Supplementary Data

Enzymatic oxidation of epigallocatechin with unripe fruits of *Citrus unshiu* and revision of structures and production mechanism of oolongtheanins

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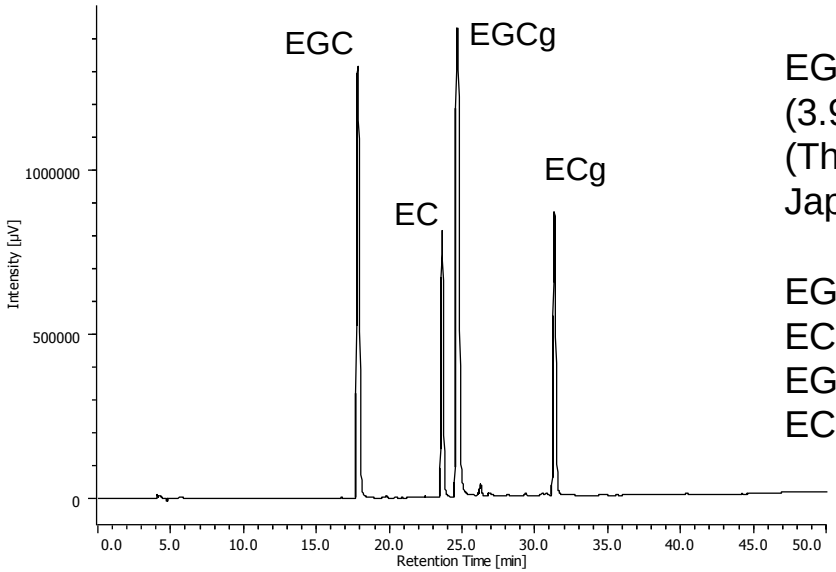
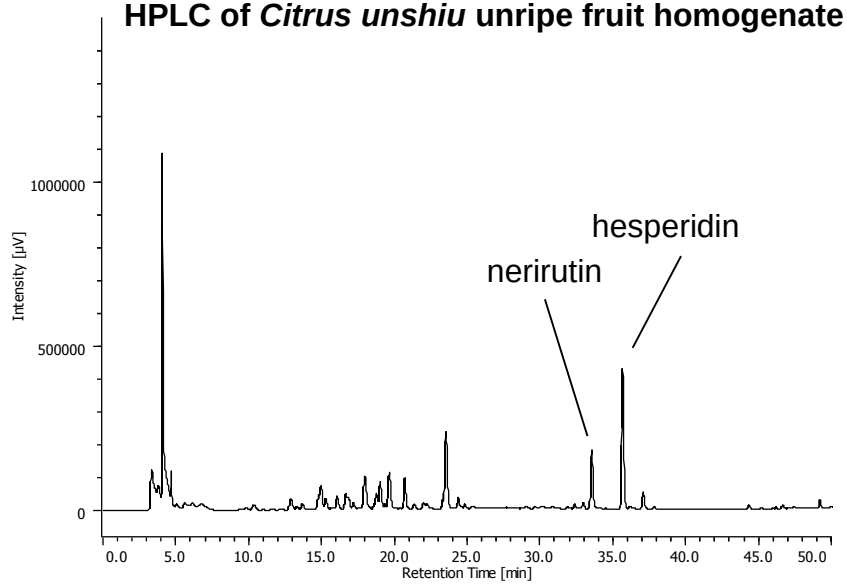
S1. HPLC of green tea catechin mixture used in this experiment.



EGC (2.5 mg, 8.2 μmol), EC (0.6 mg, 2.1 μmol), EGCg (3.9 mg, 8.5 μmol), ECg (0.9 mg, 2.0 μmol) /mL water. (The proportion was based on concentration in Japanese green tea leaves.)

EGC: (−)-epigallocatechin
EC: (−)-epicatechin
EGCg: (−)-epigallocatechin-3-*O*-gallate
ECg: (−)-epicatechin-3-*O*-gallate

HPLC of *Citrus unshiu* unripe fruit homogenate



HPLC of Japanese pear homogenate

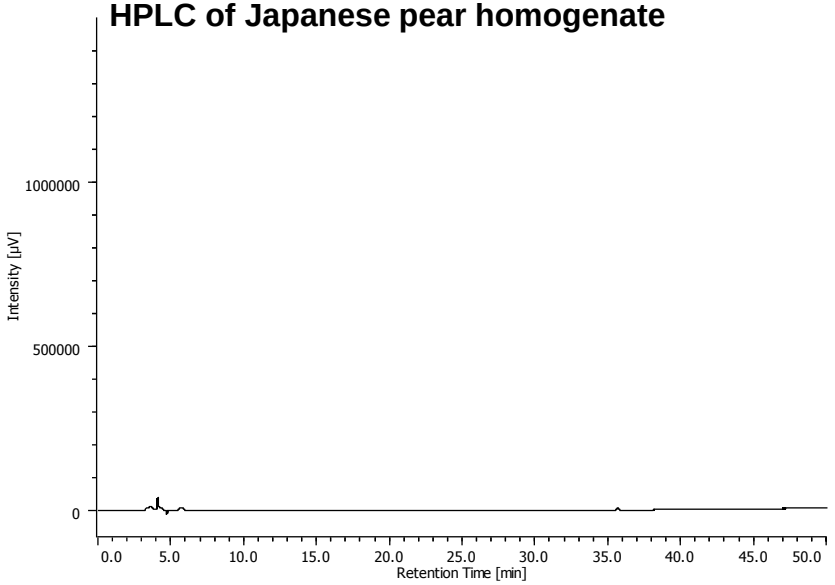
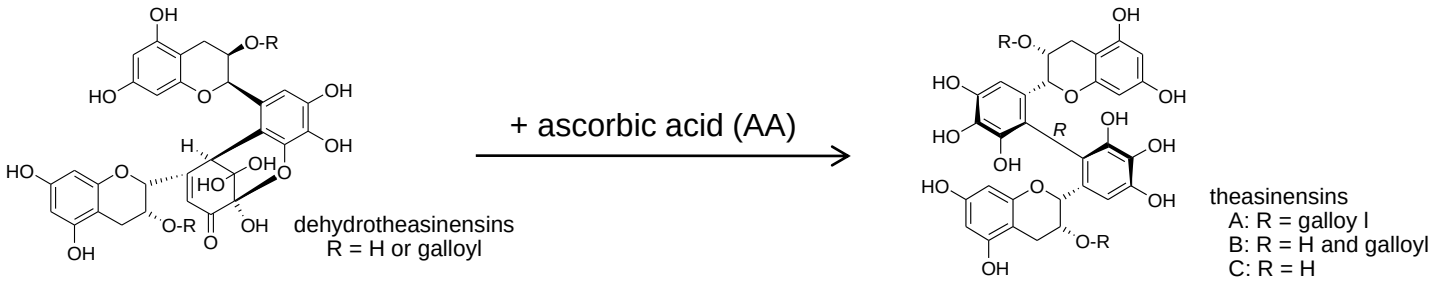
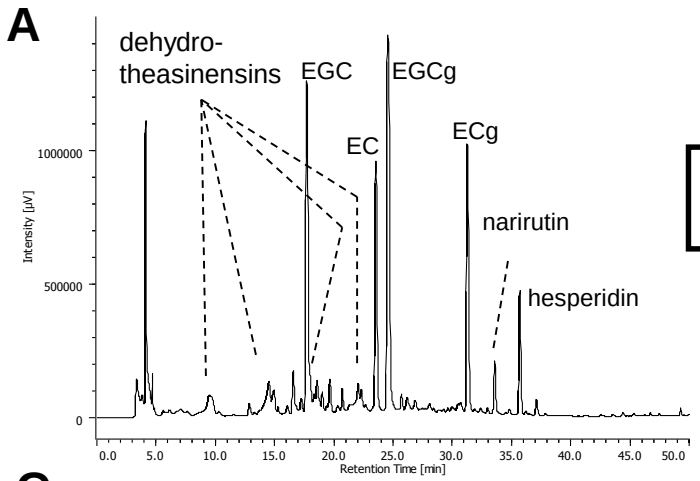


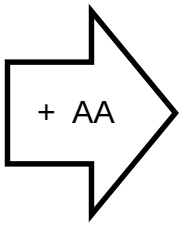
Fig. S1 HPLC of tea catechin mixture, *Citrus unshu* unripe fruit homogenate, and Japanese pear fruit homogenate.

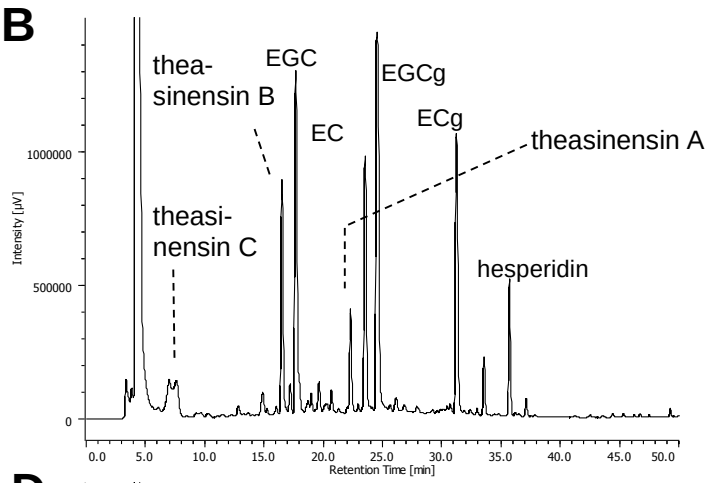
S2. HPLC of tea catechin mixture treated with homogenates of *Citrus unshiu* unripe fruits and Japanese pear.

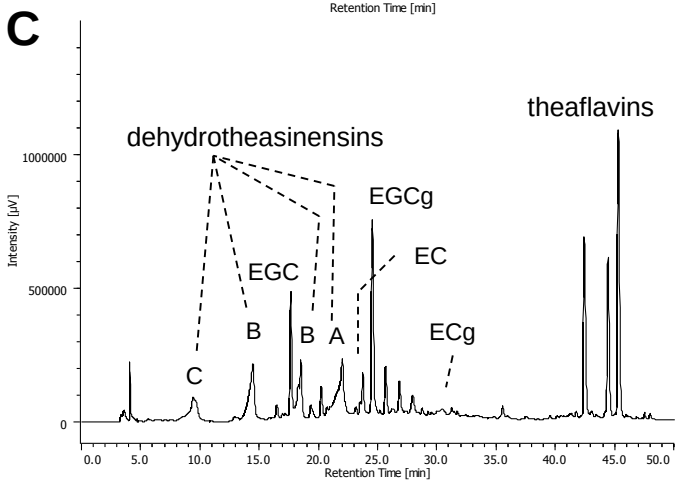
A: catechin mixture stirred with *Citrus unshiu* unripe fruit homogenate; B: after heating with ascorbic acid;
C: catechin mixture stirred with Japanese pear homogenate; D: after heating with ascorbic acid.

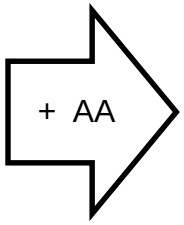


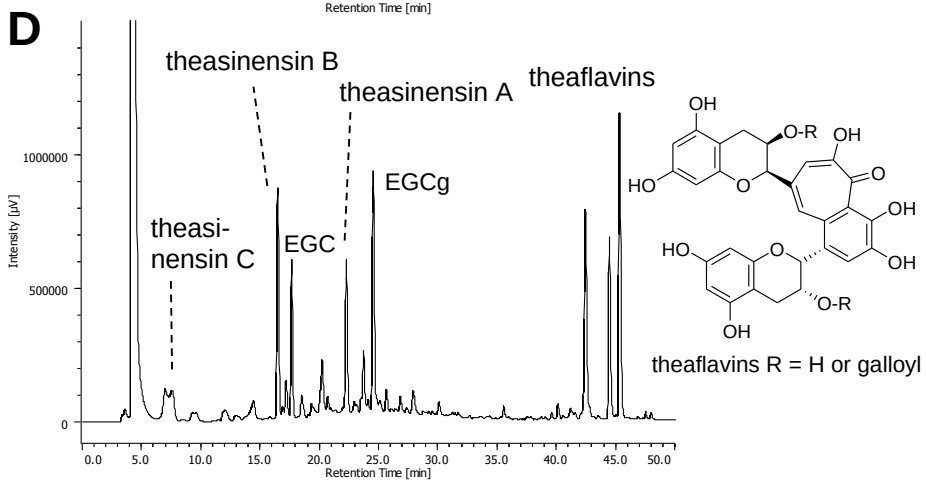












S3. Decrease of tea catechins by treatment with fruits homogenates (relative value)

	tea catechin	A	B	C	D
EGC	100%	72%	82%	18%	25%
EC	100%	100%	101%	10%	15%
EGCg	100%	75%	78%	27%	33%
ECg	100%	93%	99%	2%	4%

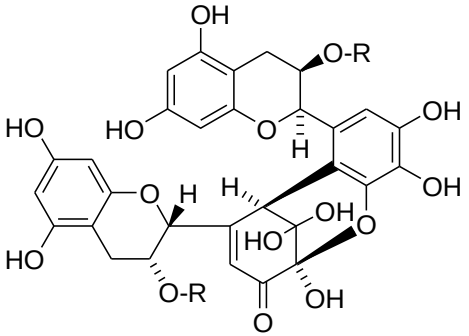
A: catechin mixture treated with homogenate of *Citrus unshu* unripe fruites for 60 min at r.t.

B: the reaction micture of A after heating with ascorbic acid.

C: catechin mixture treated with homogenate of Japanese pear fruits for 60 min at r.t.

D: the reaction micture of C after heating with ascorbic acid.

S4. Redox dismutation of dehydrotheasinensins.

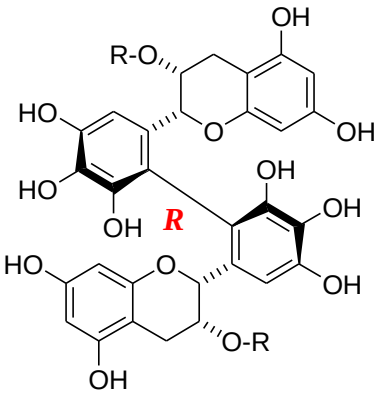


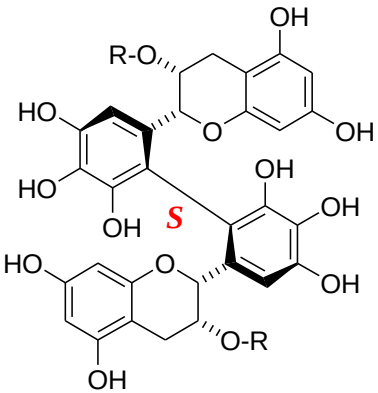
dehydrotheasinensins R = H or galloyl

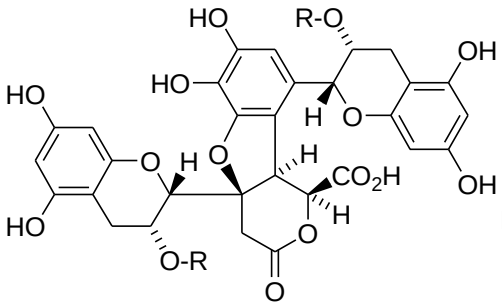
redox dismutation

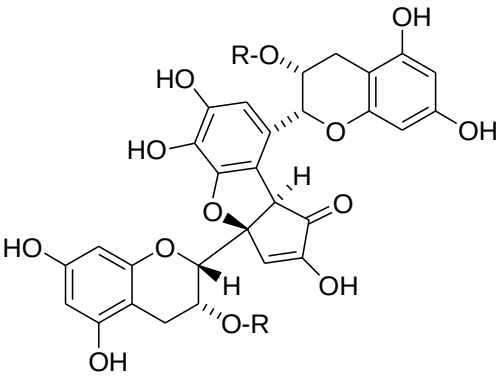
reduction products

oxidation products







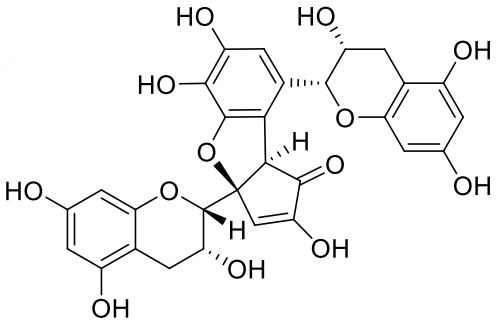


theasinensins
A (R = galloyl)
B (R = H and galloyl)
C (R = H)

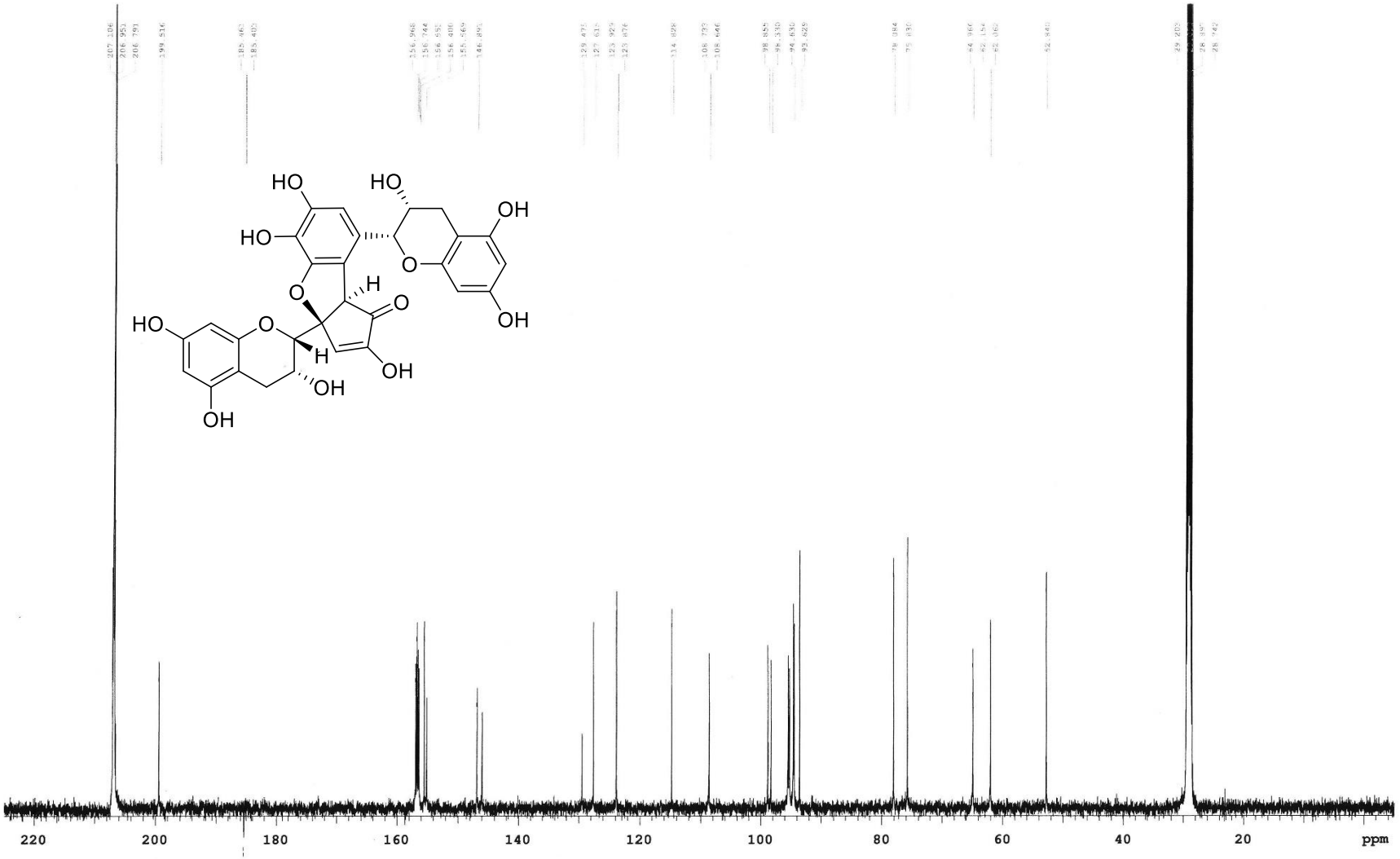
theasinensins
D (R = galloyl)
H (R = H and galloyl)
E (R = H)

oolongtheanins

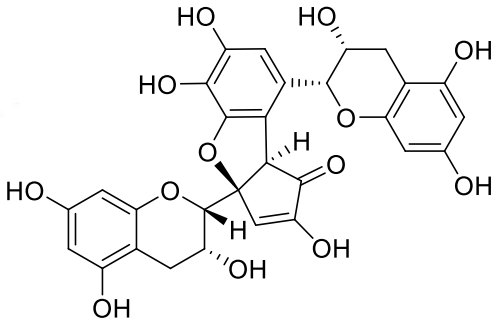
S5. ^{1}H-NMR spectrum of 11 (acetone-d_6 + D_2O, 500 MHz).



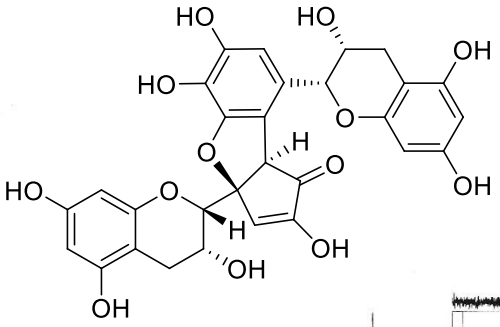
S6. ^{13}C-NMR spectrum of 11 (acetone-d_6 + D_2O, 125 MHz).



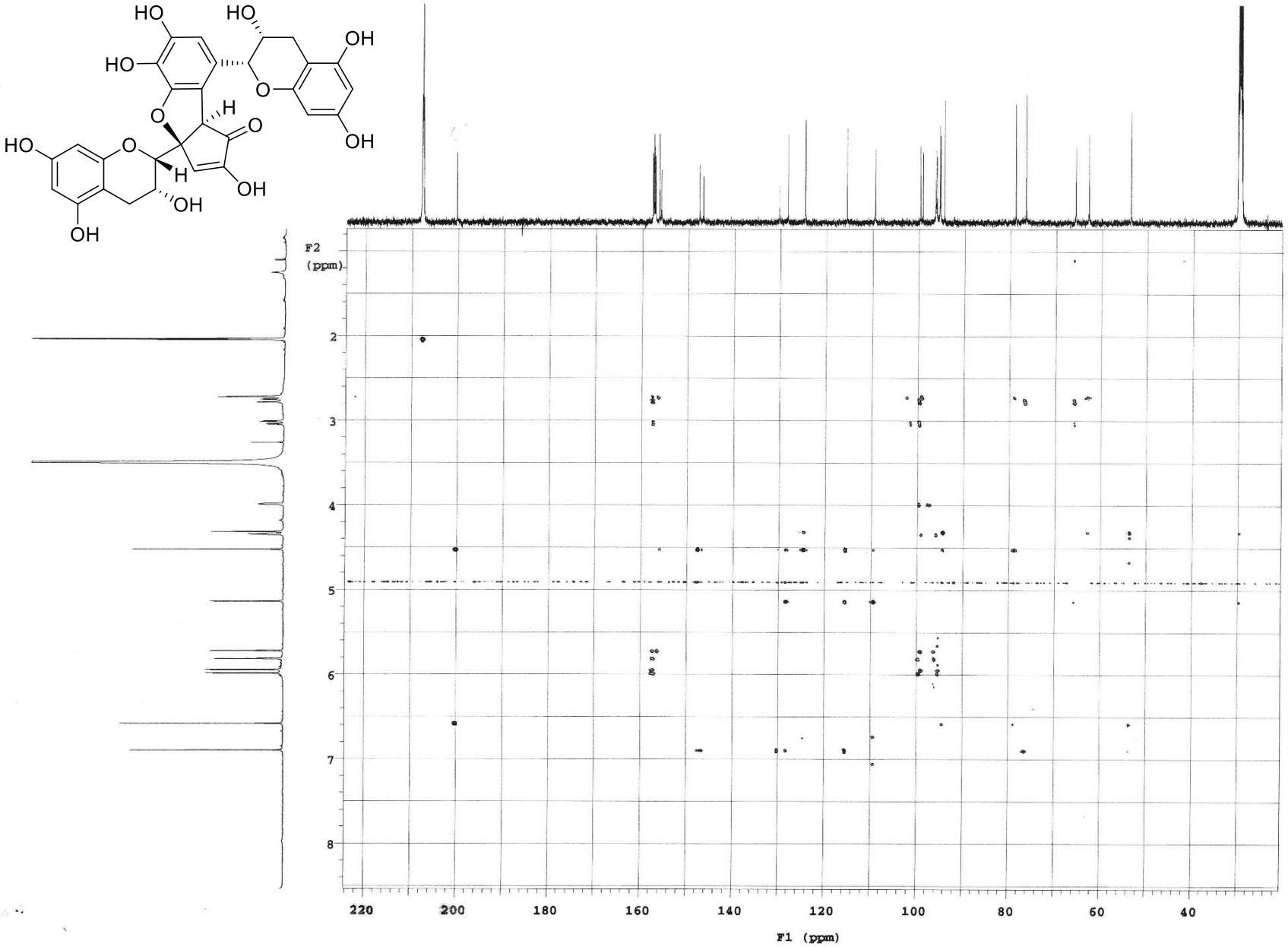
S7. ^{1}H-^{1}H COSY spectrum of 11 (acetone-d_6 + D_2O).



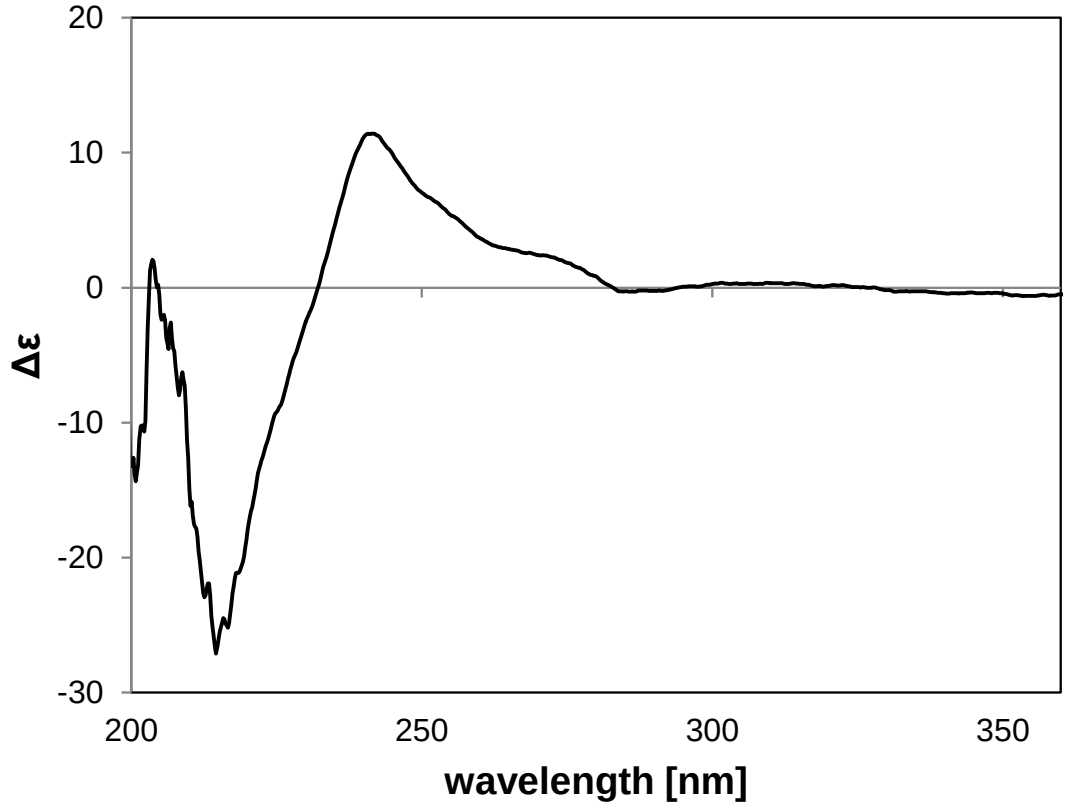
S8. HSQC spectrum of 11 (acetone-d_6 + D_2O).



S9. HMBC spectrum of 11 (acetone-d_6 + D_2O).

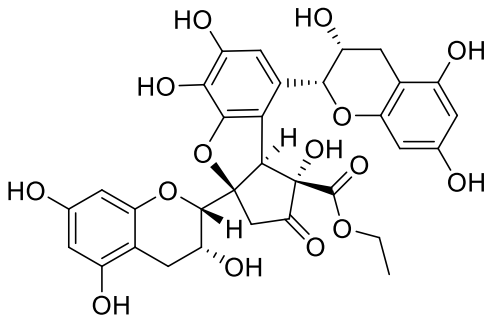


S10. Experimental ECD spectrum of 11 in MeOH.

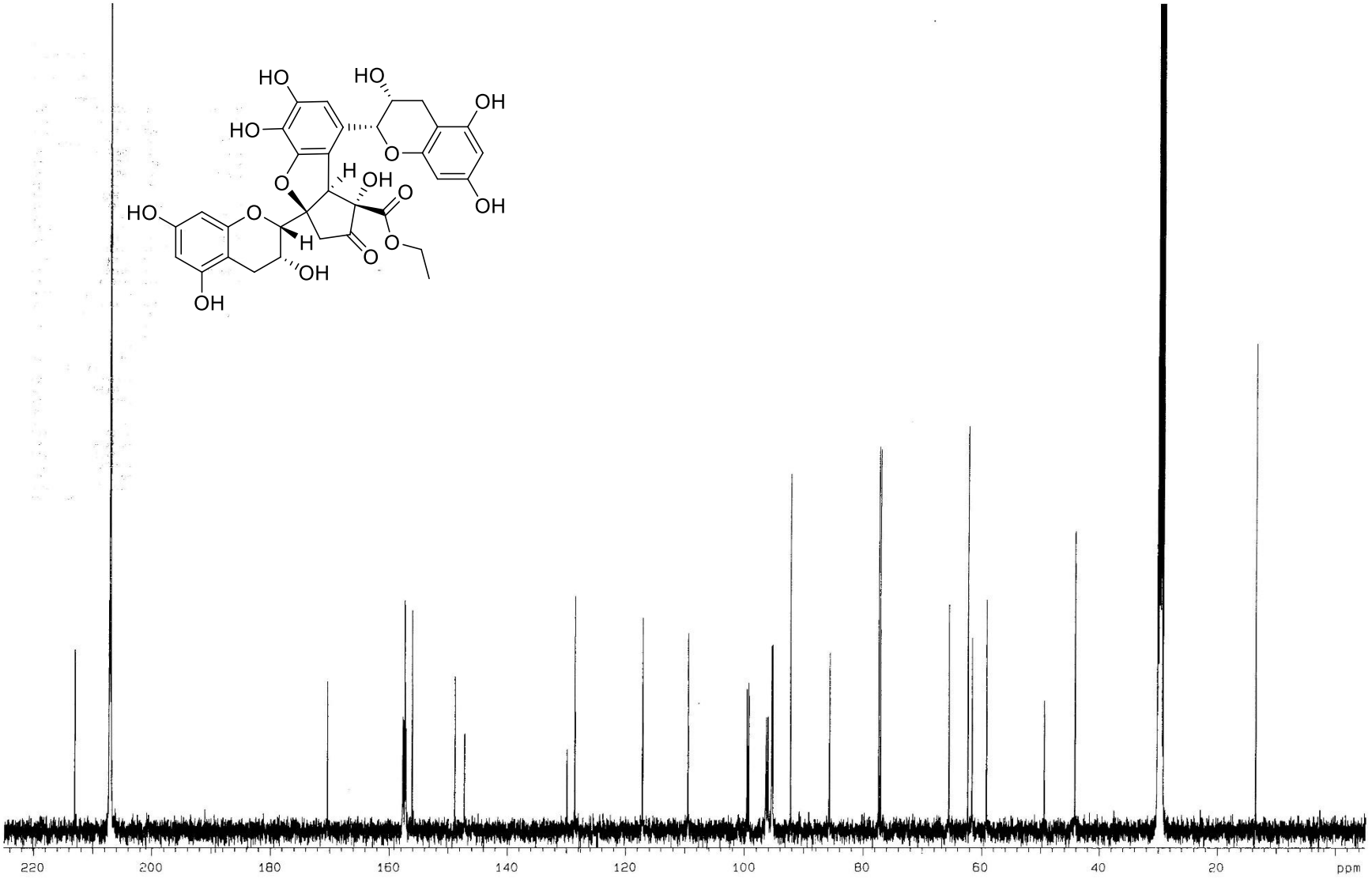


λ_{max} ($\Delta\varepsilon$): 241 (+11.4), 232 (0), 215 (–27.1) nm.

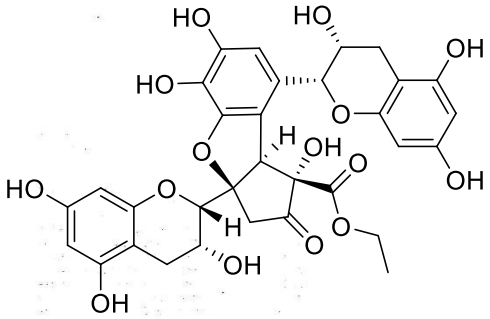
S11. ^{1}H-NMR spectrum of 12 (acetone-d_6, 500 MHz)



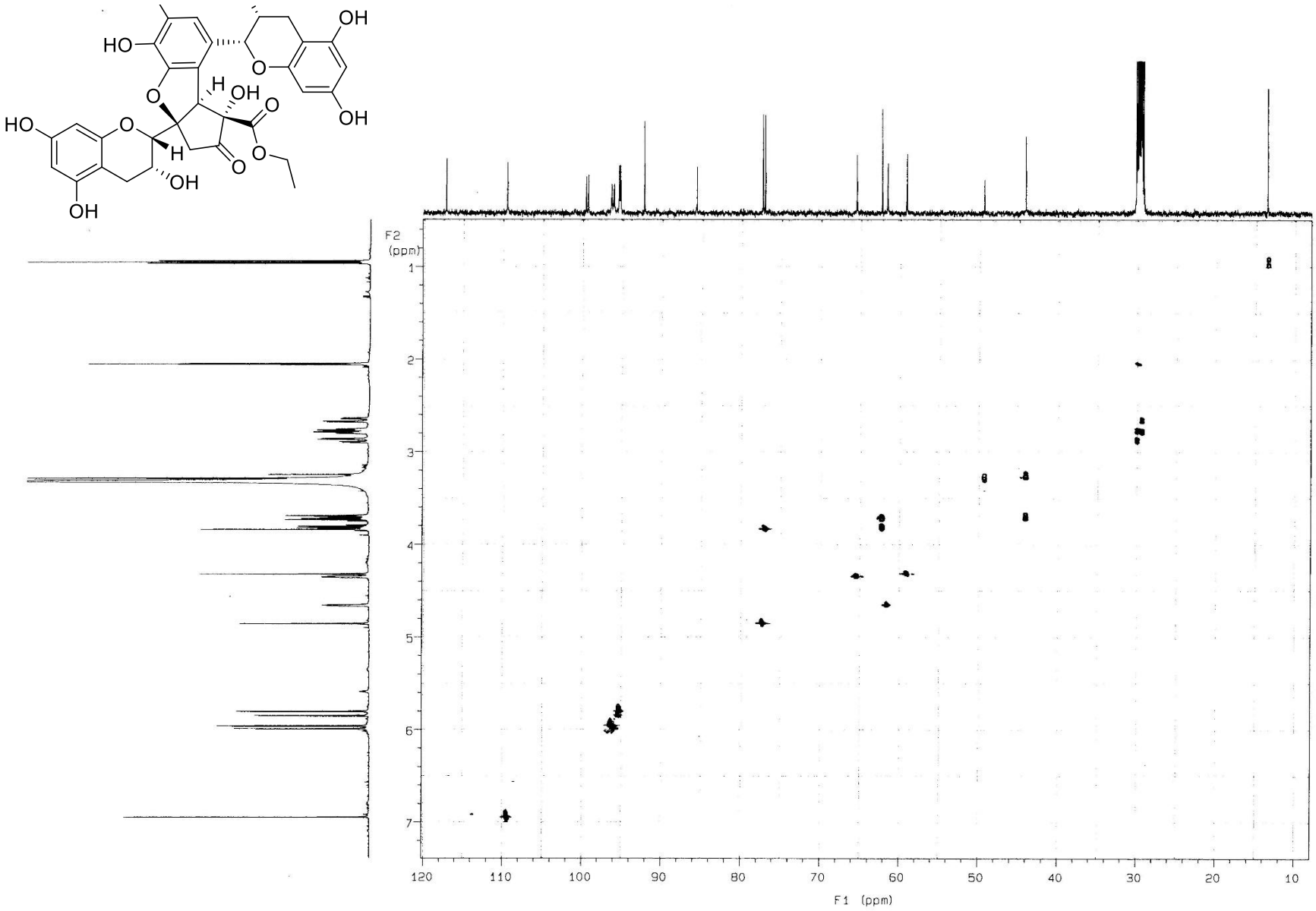
S12. ^{13}C-NMR spectrum of 12 (acetone-d_6, 125 MHz).



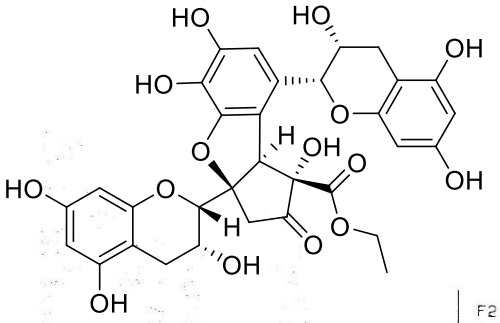
S13. ^{1}H-^{1}H COSY spectrum of 12 (acetone-d_6).

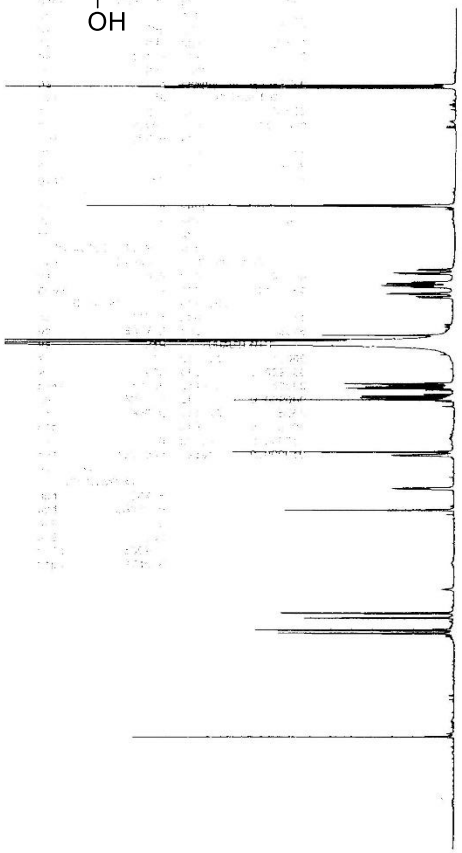


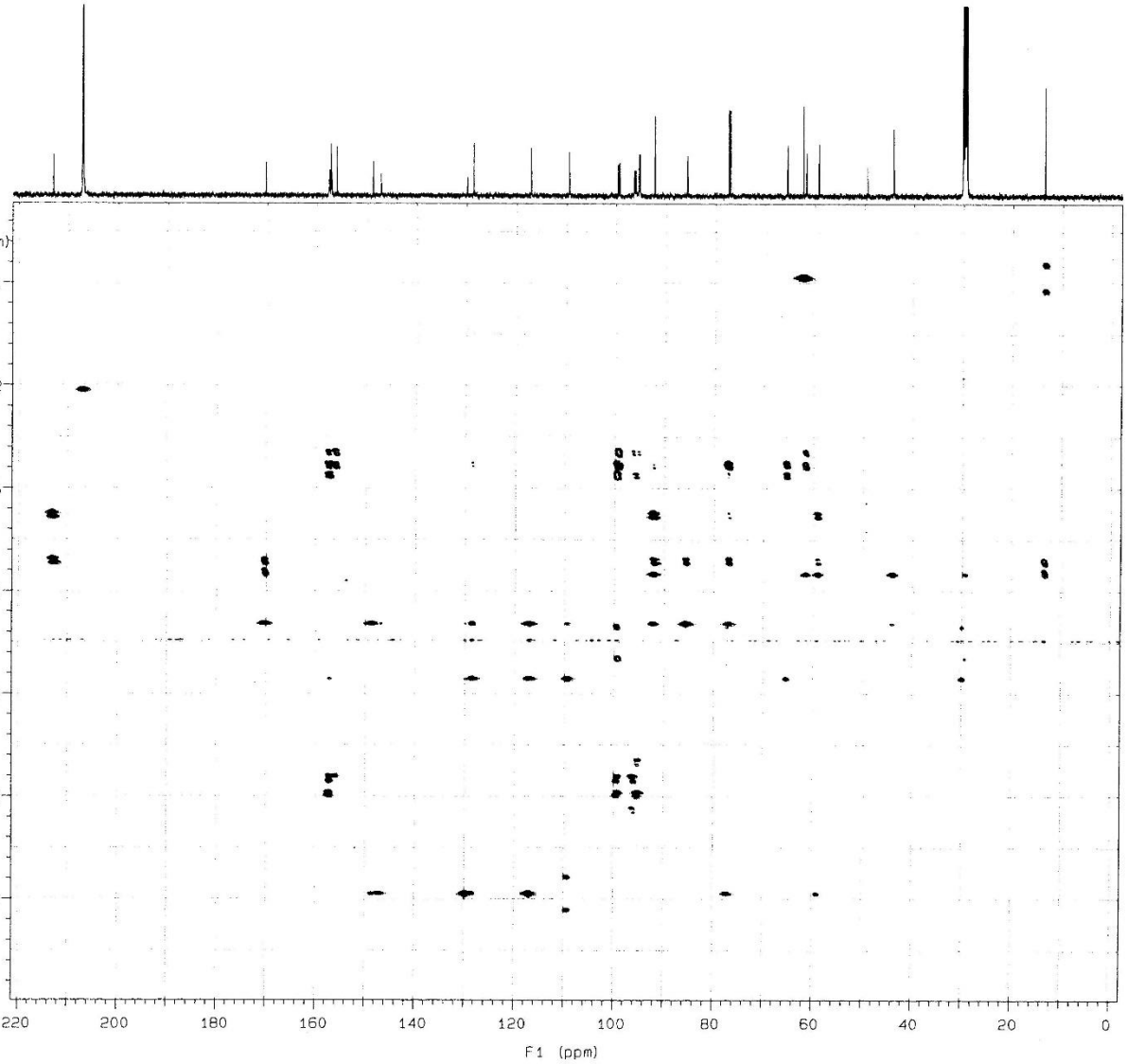
S14. HSQC spectrum of 12 (acetone-d_6).



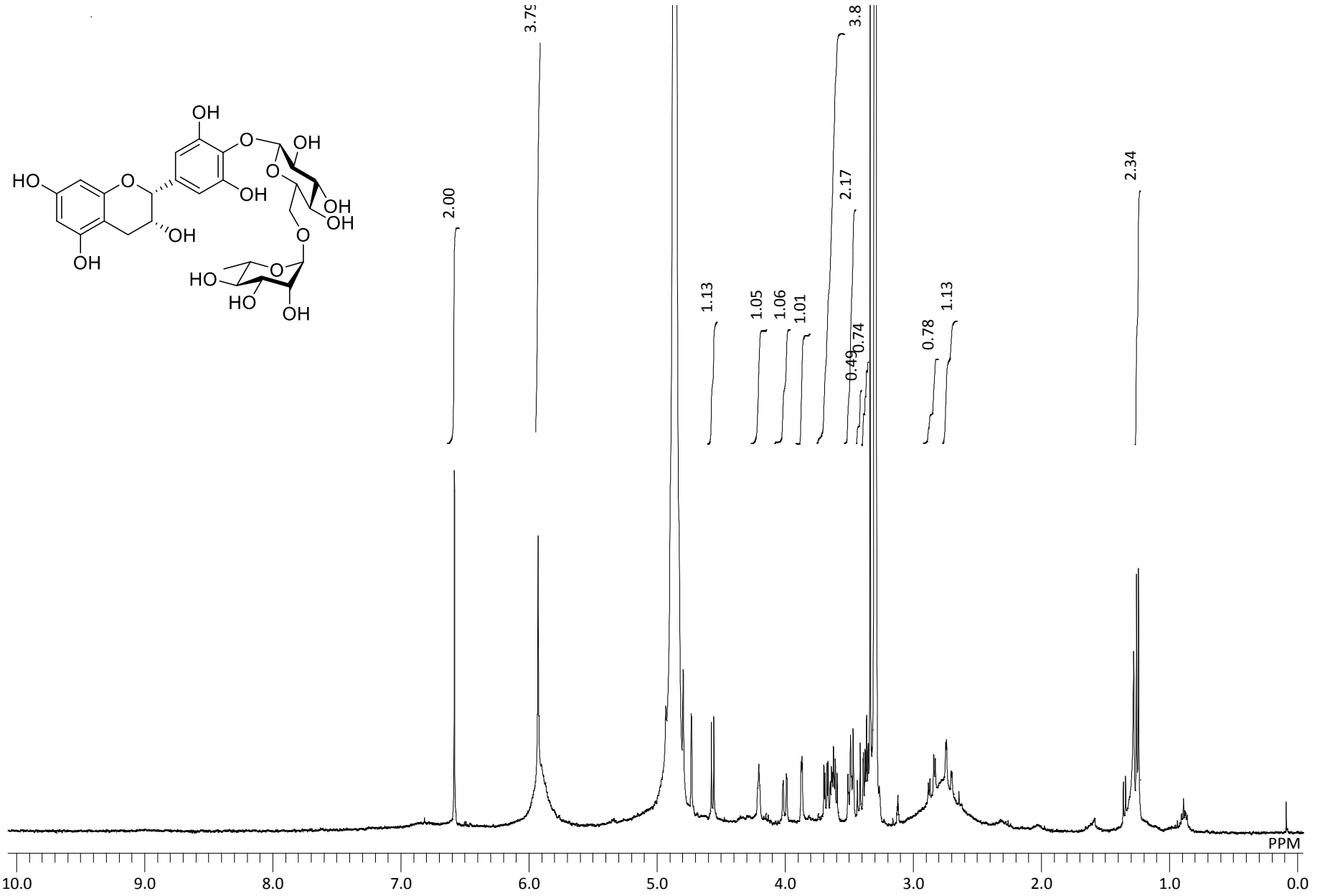
S15. HMBC spectrum of 12 (acetone-d_6).



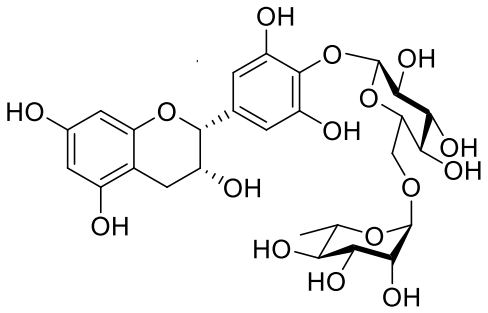




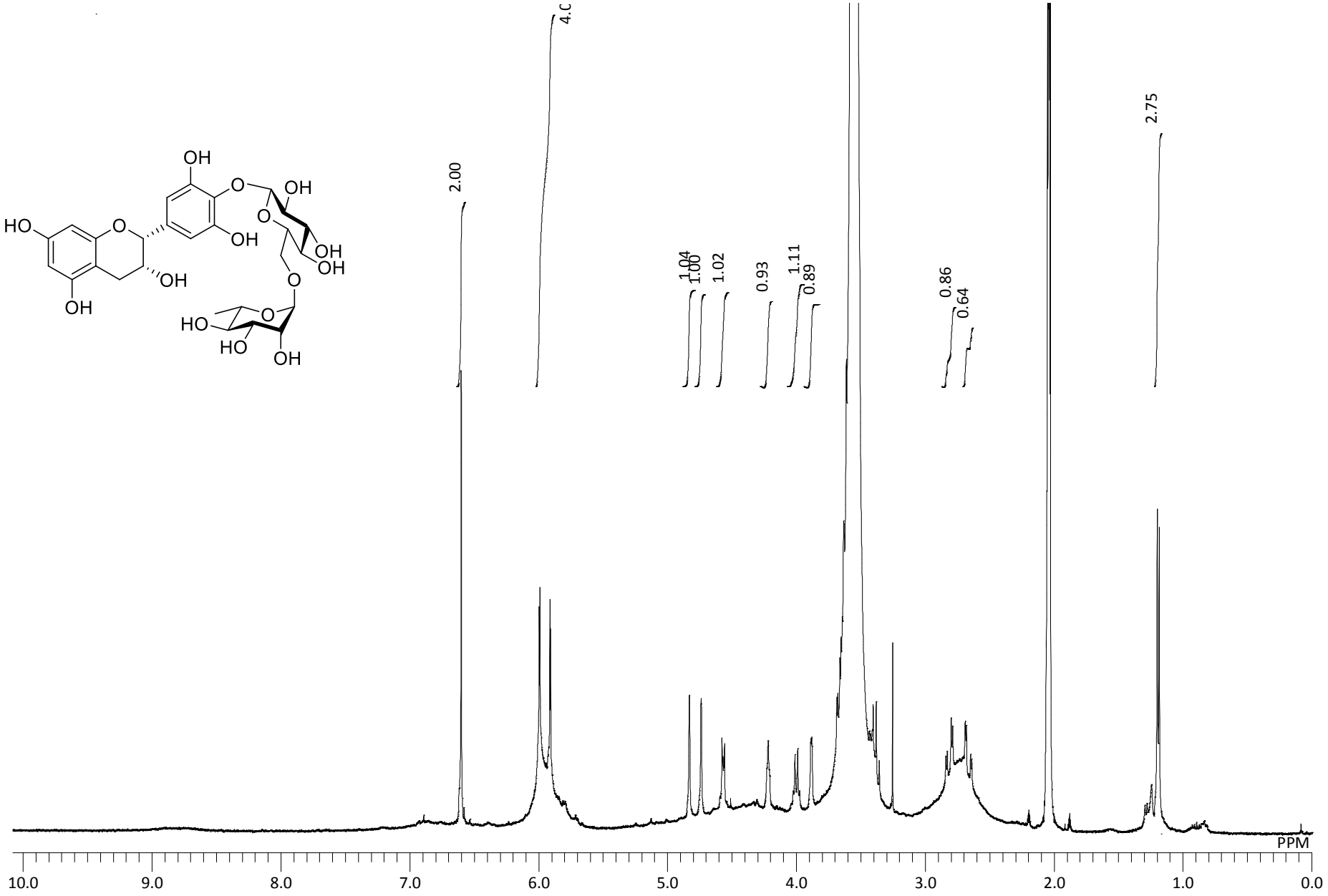
S16. ^{1}H-NMR spectrum of 13 (CD_3OD, 400 MHz).



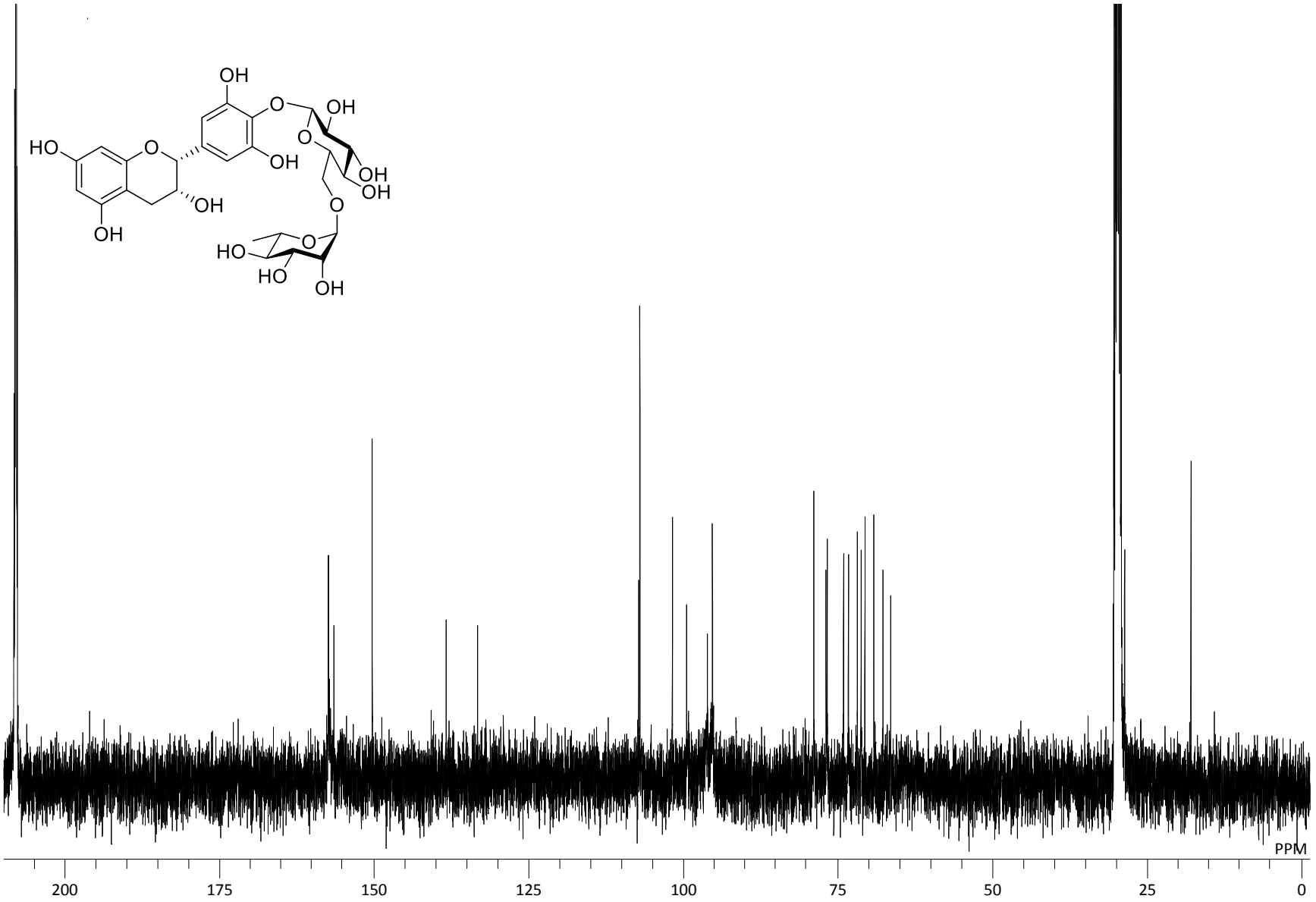
S17. ^{13}C-NMR spectrum of 13 (CD_3OD, 100 MHz).



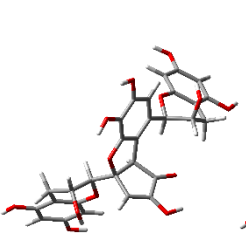
S18. ^{1}H-NMR spectrum of 13 (acetone-d_6 + D_2O, 400 MHz).



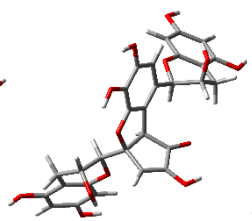
S19. ^{13}C-NMR spectrum of 13 (acetone-d_6 + D_2O, 100 MHz).



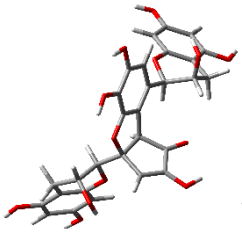
S20. Optimized conformers of (1‴*R*,5‴*R*)-11 at the B3LYP/6-31G(d,p) level in MeOH (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (Δ*G*).



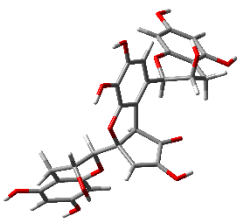
(1‴*R*,5‴*R*)-**11A**
(8.5%)



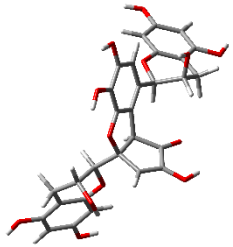
(1‴*R*,5‴*R*)-**11B**
(8.5%)



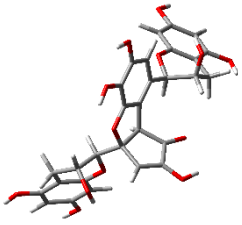
(1‴*R*,5‴*R*)-**11C**
(7.7%)



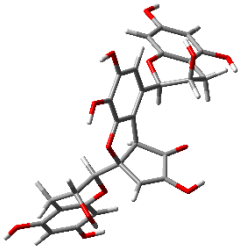
(1‴*R*,5‴*R*)-**11D**
(6.8%)



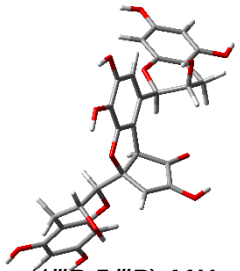
(1‴*R*,5‴*R*)-**11E**
(5.0%)



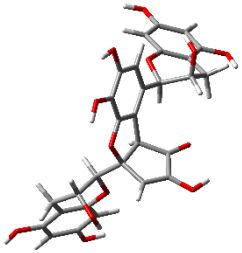
(1‴*R*,5‴*R*)-**11F**
(5.0%)



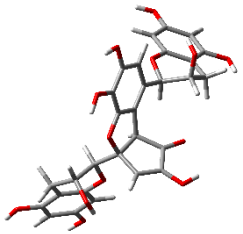
(1‴*R*,5‴*R*)-**11G**
(4.6%)



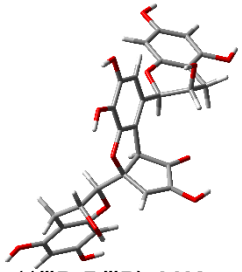
(1‴*R*,5‴*R*)-**11H**
(4.4%)



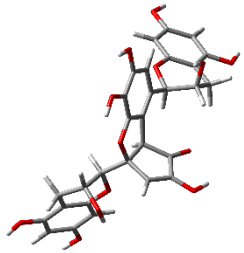
(1‴*R*,5‴*R*)-**11I**
(4.3%)



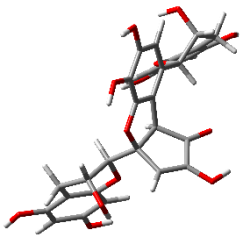
(1‴*R*,5‴*R*)-**11J**
(3.9%)



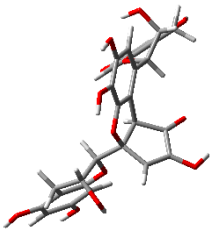
(1‴*R*,5‴*R*)-**11K**
(3.3%)



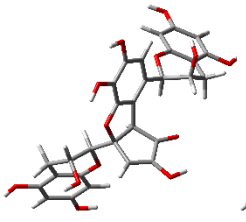
(1‴*R*,5‴*R*)-**11L**
(2.8%)



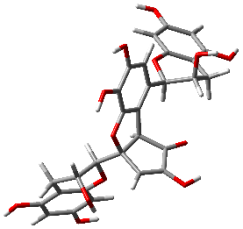
(1‴*R*,5‴*R*)-**11M**
(2.5%)



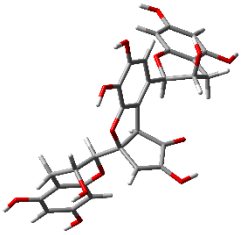
(1‴*R*,5‴*R*)-**11N**
(2.1%)



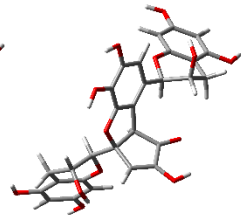
(1‴*R*,5‴*R*)-**11O**
(1.9%)



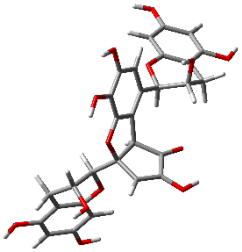
(1‴*R*,5‴*R*)-**11P**
(1.8%)



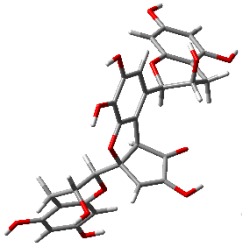
(1‴*R*,5‴*R*)-**11Q**
(1.7%)



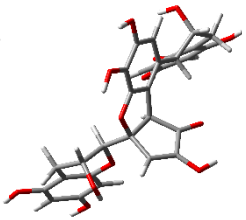
(1‴*R*,5‴*R*)-**11R**
(1.4%)



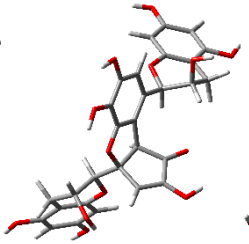
(1‴*R*,5‴*R*)-**11S**
(1.3%)



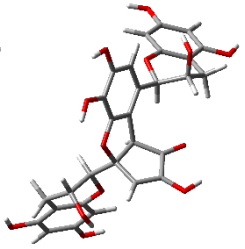
(1‴*R*,5‴*R*)-**11T**
(1.3%)



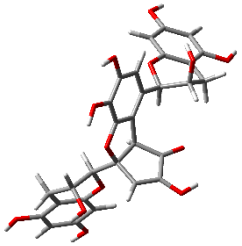
(1‴*R*,5‴*R*)-**11U**
(1.3%)



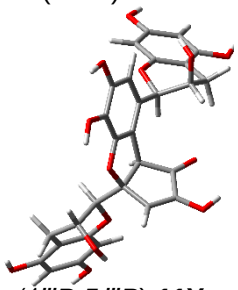
(1‴*R*,5‴*R*)-**11V**
(1.3%)



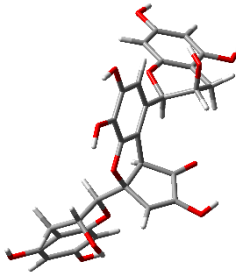
(1‴*R*,5‴*R*)-**11W**
(1.2%)



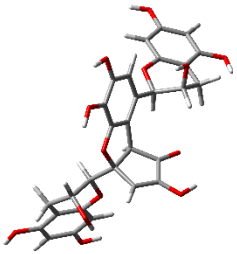
(1‴*R*,5‴*R*)-**11X**
(1.2%)



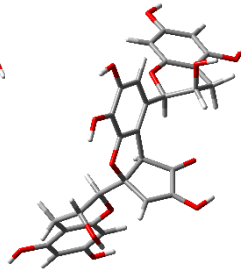
(1‴*R*,5‴*R*)-**11Y**
(1.2%)



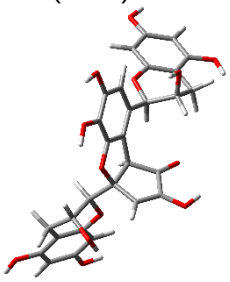
(1‴*R*,5‴*R*)-**11Z**
(1.1%)



(1‴*R*,5‴*R*)-**11AA**
(1.1%)

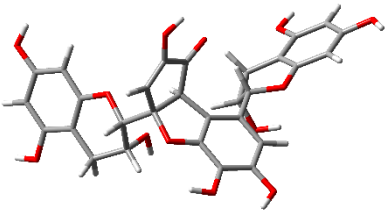


(1‴*R*,5‴*R*)-**11AB**
(1.1%)

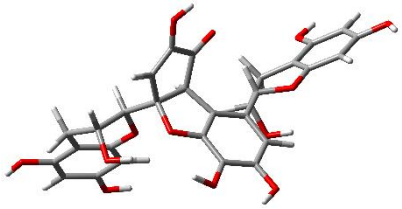


(1‴*R*,5‴*R*)-**11AC**
(1.0%)

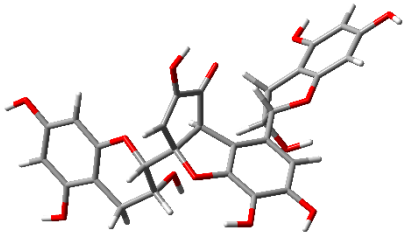
S21. Optimized conformers of (1‴*S*,5‴*S*)-11 at the B3LYP/6-31G(d,p) level in MeOH (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (Δ*G*).



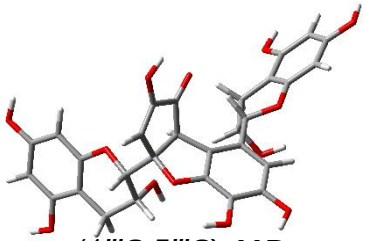
(1‴*S*,5‴*S*)-**11A**
(13.7%)



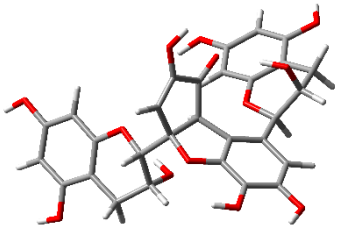
(1‴*S*,5‴*S*)-**11B**
(10.9%)



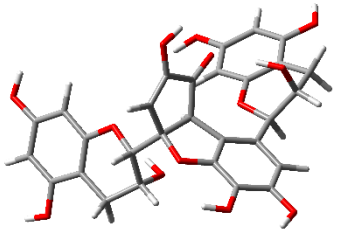
(1‴*S*,5‴*S*)-**11C**
(9.9%)



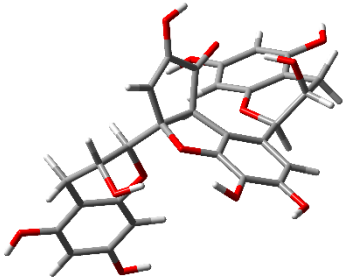
(1‴*S*,5‴*S*)-**11D**
(8.7%)



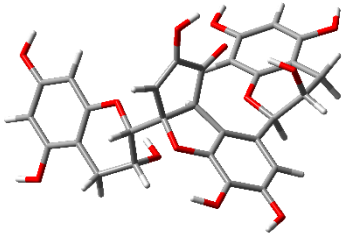
(1‴*S*,5‴*S*)-**11E**
(7.9%)



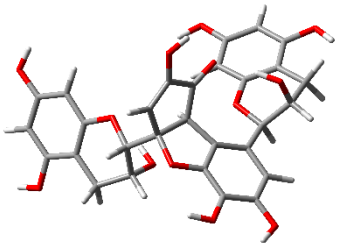
(1‴*S*,5‴*S*)-**11F**
(7.3%)



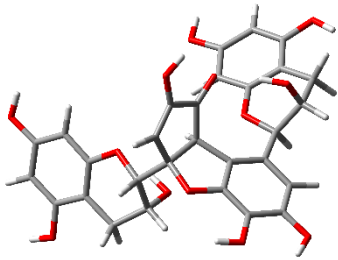
(1‴*S*,5‴*S*)-**11G**
(5.9%)



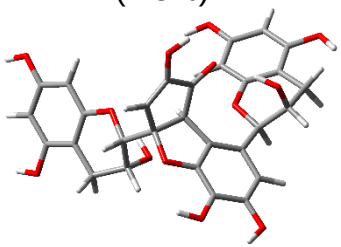
(1‴*S*,5‴*S*)-**11H**
(5.5%)



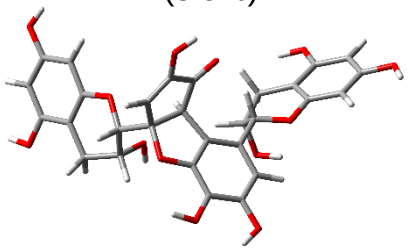
(1‴*S*,5‴*S*)-**11I**
(3.4%)



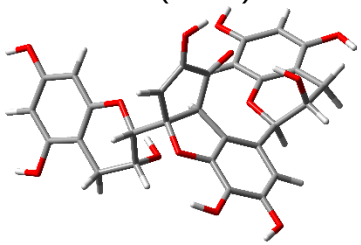
(1‴*S*,5‴*S*)-**11J**
(3.1%)



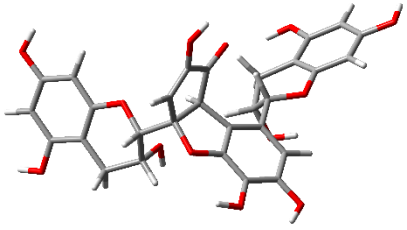
(1‴*S*,5‴*S*)-**11K**
(3.0%)



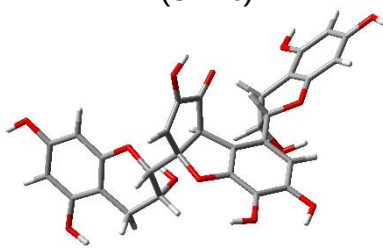
(1‴*S*,5‴*S*)-**11L**
(2.8%)



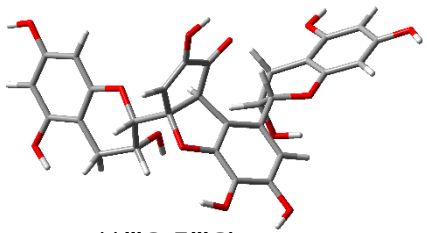
(1‴*S*,5‴*S*)-**11M**
(2.4%)



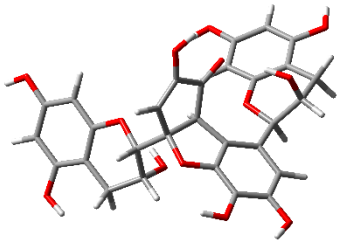
(1‴*S*,5‴*S*)-**11N**
(2.2%)



(1‴*S*,5‴*S*)-**11O**
(2.0%)



(1‴*S*,5‴*S*)-**11P**
(1.6%)



(1‴*S*,5‴*S*)-**11Q**
(1.4%)

S22. Important thermodynamic parameters and conformational analysis of of (1‴*R*,5‴*R*)-11.

conformers	*E* (a.u.)	*E'* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(1‴*R*,5‴*R*)-**11A**	-2097.470166	-2096.971438	-2096.933771	-2097.040694	0.00	8.5
(1‴*R*,5‴*R*)-**11B**	-2097.469808	-2096.971211	-2096.933481	-2097.040691	0.00	8.5
(1‴*R*,5‴*R*)-**11C**	-2097.469865	-2096.971264	-2096.933561	-2097.040598	0.06	7.7
(1‴*R*,5‴*R*)-**11D**	-2097.469508	-2096.971010	-2096.933257	-2097.040479	0.13	6.8
(1‴*R*,5‴*R*)-**11E**	-2097.470645	-2096.971609	-2096.934163	-2097.040193	0.31	5.0
(1‴*R*,5‴*R*)-**11F**	-2097.468463	-2096.970169	-2096.932317	-2097.040185	0.32	5.0
(1‴*R*,5‴*R*)-**11G**	-2097.468757	-2096.970287	-2096.932494	-2097.040110	0.37	4.6
(1‴*R*,5‴*R*)-**11H**	-2097.470344	-2096.971370	-2096.933886	-2097.040064	0.40	4.4
(1‴*R*,5‴*R*)-**11I**	-2097.468798	-2096.970311	-2096.932524	-2097.040054	0.40	4.3
(1‴*R*,5‴*R*)-**11J**	-2097.468504	-2096.970139	-2096.932320	-2097.039946	0.47	3.9
(1‴*R*,5‴*R*)-**11K**	-2097.470298	-2096.971281	-2096.933827	-2097.039798	0.56	3.3
(1‴*R*,5‴*R*)-**11L**	-2097.469999	-2096.971042	-2096.933554	-2097.039649	0.66	2.8
(1‴*R*,5‴*R*)-**11M**	-2097.469248	-2096.970275	-2096.932740	-2097.039531	0.73	2.5
(1‴*R*,5‴*R*)-**11N**	-2097.468606	-2096.969845	-2096.932223	-2097.039356	0.84	2.1
(1‴*R*,5‴*R*)-**11O**	-2097.468712	-2096.970094	-2096.932388	-2097.039271	0.89	1.9
(1‴*R*,5‴*R*)-**11P**	-2097.468516	-2096.969875	-2096.932179	-2097.039216	0.93	1.8
(1‴*R*,5‴*R*)-**11Q**	-2097.468368	-2096.969869	-2096.932113	-2097.039168	0.96	1.7
(1‴*R*,5‴*R*)-**11R**	-2097.468558	-2096.969861	-2096.932171	-2097.038957	1.09	1.4
(1‴*R*,5‴*R*)-**11S**	-2097.469198	-2096.970393	-2096.932869	-2097.038947	1.10	1.3
(1‴*R*,5‴*R*)-**11T**	-2097.468370	-2096.969773	-2096.932061	-2097.038924	1.11	1.3
(1‴*R*,5‴*R*)-**11U**	-2097.467563	-2096.968811	-2096.931162	-2097.038906	1.12	1.3
(1‴*R*,5‴*R*)-**11V**	-2097.468211	-2096.969675	-2096.931948	-2097.038900	1.13	1.3
(1‴*R*,5‴*R*)-**11W**	-2097.468547	-2096.969802	-2096.932115	-2097.038855	1.15	1.2
(1‴*R*,5‴*R*)-**11X**	-2097.468029	-2096.969548	-2096.931787	-2097.038814	1.18	1.2
(1‴*R*,5‴*R*)-**11Y**	-2097.468205	-2096.969607	-2096.931870	-2097.038808	1.18	1.2
(1‴*R*,5‴*R*)-**11Z**	-2097.468192	-2096.969559	-2096.931816	-2097.038784	1.20	1.1
(1‴*R*,5‴*R*)-**11AA**	-2097.469220	-2096.970238	-2096.932752	-2097.038745	1.22	1.1
(1‴*R*,5‴*R*)-**11AB**	-2097.468133	-2096.969565	-2096.931845	-2097.038724	1.24	1.1
(1‴*R*,5‴*R*)-**11AC**	-2097.469168	-2096.970202	-2096.932709	-2097.038699	1.25	1.0

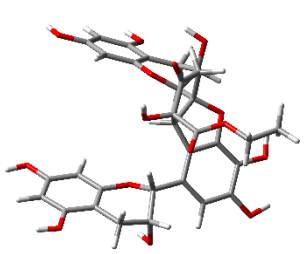
E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in MeOH using the PCM model. P_G: conformational distribution calculated from relative Gibbs free energy.

S23. Important thermodynamic parameters and conformational analysis of of (1‴*S*,5‴*S*)-11.

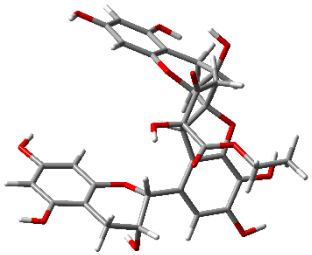
conformers	*E* (a.u.)	*E'* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(1‴*S*,5‴*S*)-**11A**	-2097.468412	-2096.969876	-2096.932081	-2097.039416	0.00	13.7
(1‴*S*,5‴*S*)-**11B**	-2097.469427	-2096.970320	-2096.932930	-2097.039200	0.14	10.9
(1‴*S*,5‴*S*)-**11C**	-2097.468092	-2096.969564	-2096.931749	-2097.039116	0.19	9.9
(1‴*S*,5‴*S*)-**11D**	-2097.468065	-2096.969527	-2096.931729	-2097.038984	0.27	8.7
(1‴*S*,5‴*S*)-**11E**	-2097.469725	-2096.970705	-2096.933444	-2097.038897	0.33	7.9
(1‴*S*,5‴*S*)-**11F**	-2097.470041	-2096.970881	-2096.933676	-2097.038829	0.37	7.3
(1‴*S*,5‴*S*)-**11G**	-2097.470987	-2096.971453	-2096.934526	-2097.038615	0.50	5.9
(1‴*S*,5‴*S*)-**11H**	-2097.469783	-2096.970621	-2096.933399	-2097.038561	0.54	5.5
(1‴*S*,5‴*S*)-**11I**	-2097.468792	-2096.969782	-2096.932490	-2097.038095	0.83	3.4
(1‴*S*,5‴*S*)-**11J**	-2097.468830	-2096.969781	-2096.932498	-2097.038017	0.88	3.1
(1‴*S*,5‴*S*)-**11K**	-2097.468474	-2096.969547	-2096.932221	-2097.037979	0.90	3.0
(1‴*S*,5‴*S*)-**11L**	-2097.467033	-2096.968529	-2096.930708	-2097.037923	0.94	2.8
(1‴*S*,5‴*S*)-**11M**	-2097.468480	-2096.969486	-2096.932184	-2097.037775	1.03	2.4
(1‴*S*,5‴*S*)-**11N**	-2097.466991	-2096.968446	-2096.930650	-2097.037704	1.07	2.2
(1‴*S*,5‴*S*)-**11O**	-2097.467410	-2096.968602	-2096.930923	-2097.037589	1.15	2.0
(1‴*S*,5‴*S*)-**11P**	-2097.466651	-2096.968051	-2096.930243	-2097.037395	1.27	1.6
(1‴*S*,5‴*S*)-**11Q**	-2097.468342	-2096.969233	-2096.931969	-2097.037294	1.33	1.4

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in MeOH using the PCM model. P_G: conformational distribution calculated from relative Gibbs free energy.

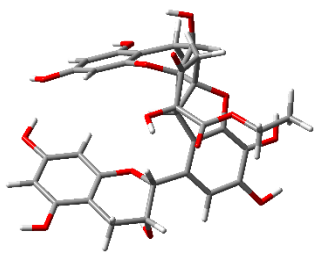
S24. Optimized conformers of (4‴*S*)-12 at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (Δ*G*).



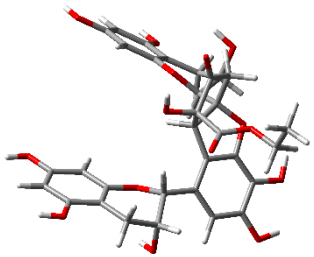
(4‴*S*)-**12A**
(19.2%)



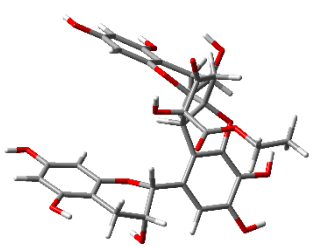
(4‴*S*)-**12B**
(12.1%)



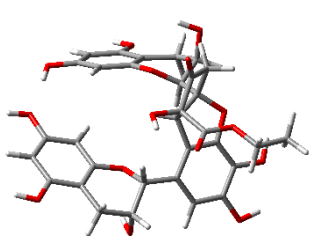
(4‴*S*)-**12C**
(9.9%)



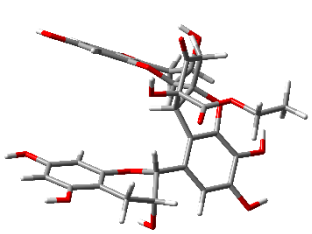
(4‴*S*)-**12D**
(9.5%)



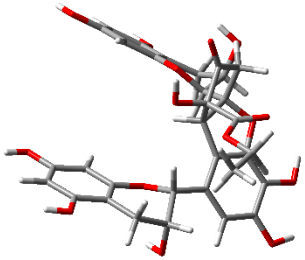
(4‴*S*)-**12E**
(6.6%)



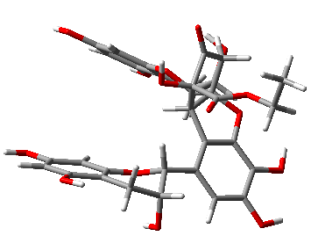
(4‴*S*)-**12F**
(4.5%)



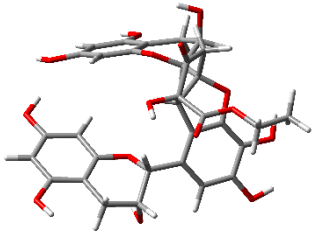
(4‴*S*)-**12G**
(4.1%)



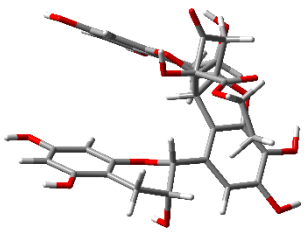
(4‴*S*)-**12H**
(3.1%)



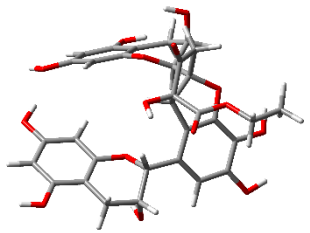
(4‴*S*)-**12I**
(3.1%)



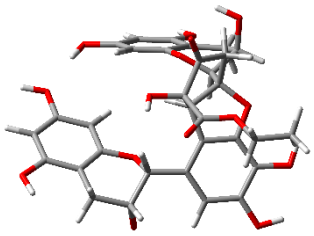
(4‴*S*)-**12J**
(2.7%)



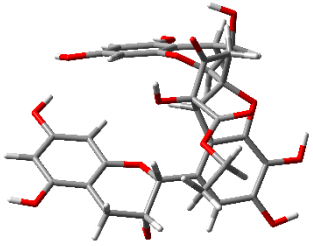
(4‴*S*)-**12K**
(2.7%)



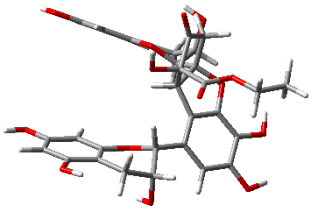
(4‴*S*)-**12L**
(2.5%)



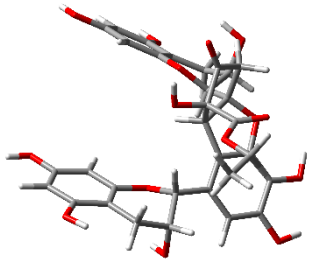
(4‴*S*)-**12M**
(1.8%)



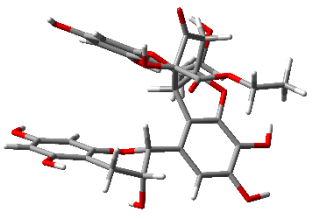
(4‴*S*)-**12N**
(1.8%)



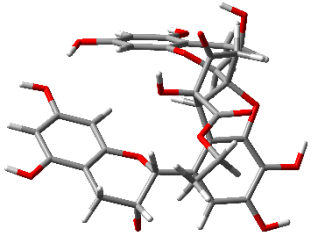
(4‴*S*)-**12O**
(1.5%)



(4‴*S*)-**12P**
(1.5%)

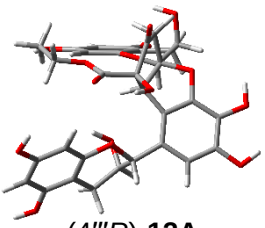


(4‴*S*)-**12Q**
(1.4%)

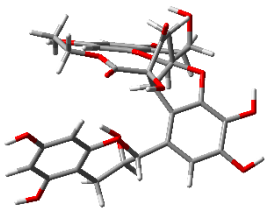


(4‴*S*)-**12R**
(1.0%)

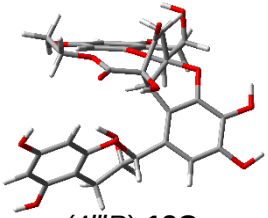
S25. Optimized conformers of (4‴*R*)-12 at the B3LYP/6-31G(d,p) level in acetone (PCM) with populations greater than 1% calculated from their relative Gibbs free energies (Δ*G*).



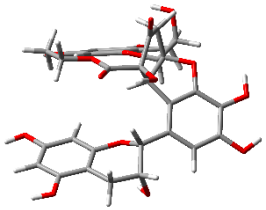
(4‴*R*)-**12A**
(13.5%)



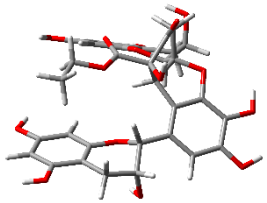
(4‴*R*)-**12B**
(6.6%)



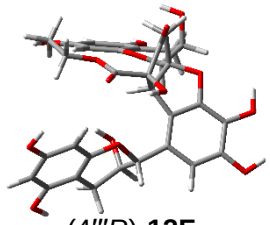
(4‴*R*)-**12C**
(6.3%)



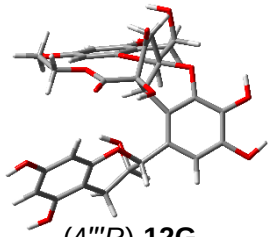
(4‴*R*)-**12D**
(6.0%)



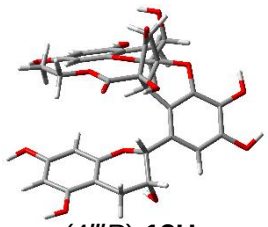
(4‴*R*)-**12E**
(5.8%)



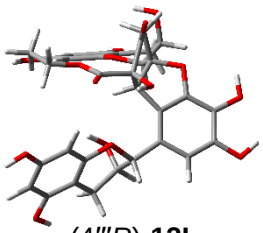
(4‴*R*)-**12F**
(4.3%)



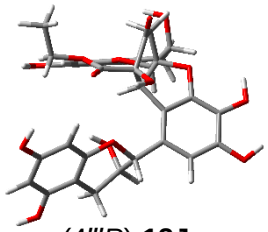
(4‴*R*)-**12G**
(3.7%)



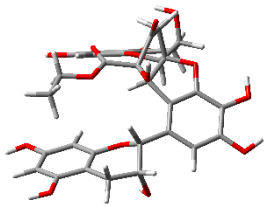
(4‴*R*)-**12H**
(3.4%)



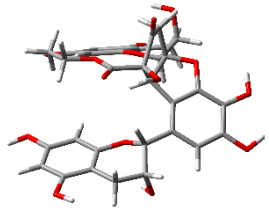
(4‴*R*)-**12I**
(3.3%)



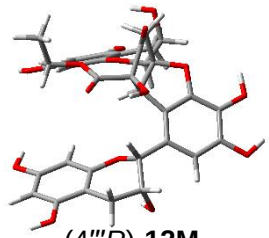
(4‴*R*)-**12J**
(2.8%)



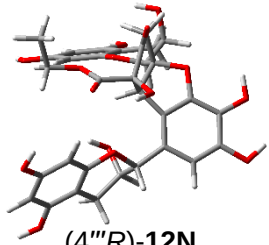
(4‴*R*)-**12K**
(2.8%)



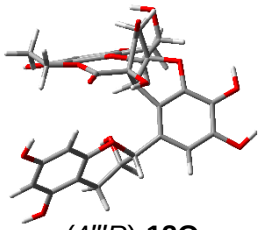
(4‴*R*)-**12L**
(2.6%)



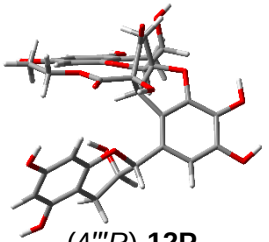
(4‴*R*)-**12M**
(2.4%)



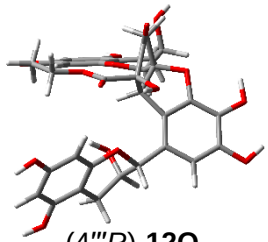
(4‴*R*)-**12N**
(2.2%)



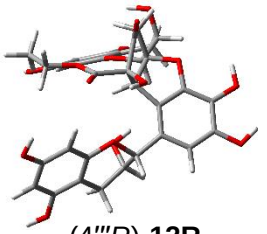
(4‴*R*)-**12O**
(2.0%)



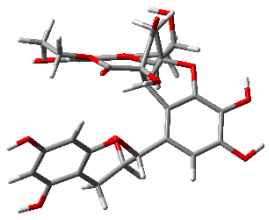
(4‴*R*)-**12P**
(1.8%)



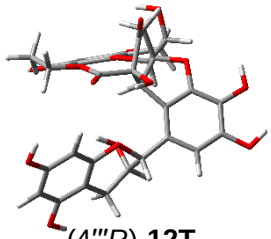
(4‴*R*)-**12Q**
(1.8%)



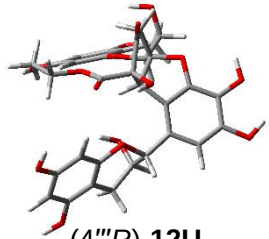
(4‴*R*)-**12R**
(1.8%)



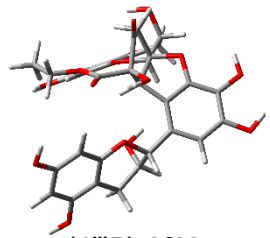
(4‴*R*)-**12S**
(1.6%)



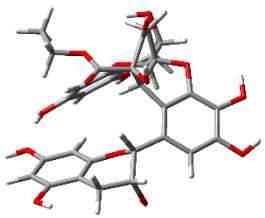
(4‴*R*)-**12T**
(1.5%)



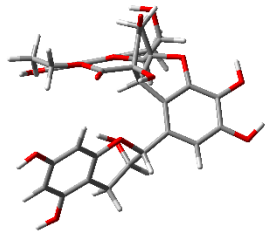
(4‴*R*)-**12U**
(1.5%)



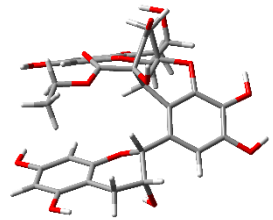
(4‴*R*)-**12V**
(1.4%)



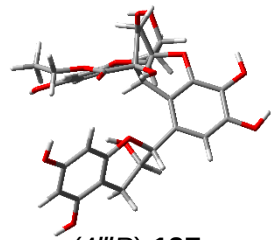
(4‴*R*)-**12W**
(1.2%)



(4‴*R*)-**12X**
(1.2%)



(4‴*R*)-**12Y**
(1.1%)



(4‴*R*)-**12Z**
(1.0%)

S26. Important thermodynamic parameters and conformational analysis of (4‴*S*)-12.

conformers	*E* (a.u.)	*E'* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(4‴*S*)-**12A**	-2365.878300	-2365.286274	-2365.242155	-2365.363965	0.00	19.2
(4‴*S*)-**12B**	-2365.878424	-2365.285928	-2365.242030	-2365.363534	0.27	12.1
(4‴*S*)-**12C**	-2365.883069	-2365.289719	-2365.246516	-2365.363340	0.39	9.9
(4‴*S*)-**12D**	-2365.877484	-2365.285310	-2365.241195	-2365.363304	0.41	9.5
(4‴*S*)-**12E**	-2365.877313	-2365.285292	-2365.241143	-2365.362965	0.63	6.6
(4‴*S*)-**12F**	-2365.881955	-2365.288705	-2365.245384	-2365.362599	0.86	4.5
(4‴*S*)-**12G**	-2365.876865	-2365.284760	-2365.240626	-2365.362512	0.91	4.1
(4‴*S*)-**12H**	-2365.877114	-2365.285063	-2365.241031	-2365.362249	1.08	3.1
(4‴*S*)-**12I**	-2365.876512	-2365.284288	-2365.240166	-2365.362240	1.08	3.1
(4‴*S*)-**12J**	-2365.881674	-2365.288410	-2365.245127	-2365.362126	1.15	2.7
(4‴*S*)-**12K**	-2365.876440	-2365.284355	-2365.240276	-2365.362106	1.17	2.7
(4‴*S*)-**12L**	-2365.881825	-2365.288452	-2365.245240	-2365.362062	1.19	2.5
(4‴*S*)-**12M**	-2365.880982	-2365.287768	-2365.244406	-2365.361740	1.40	1.8
(4‴*S*)-**12N**	-2365.880535	-2365.287436	-2365.244012	-2365.361726	1.40	1.8
(4‴*S*)-**12O**	-2365.875869	-2365.283771	-2365.239604	-2365.361548	1.52	1.5
(4‴*S*)-**12P**	-2365.876045	-2365.284132	-2365.240004	-2365.361540	1.52	1.5
(4‴*S*)-**12Q**	-2365.875971	-2365.283925	-2365.239757	-2365.361527	1.53	1.4
(4‴*S*)-**12R**	-2365.879505	-2365.286733	-2365.243149	-2365.361194	1.74	1.0

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in acetone using the PCM model. P_G*: conformational distribution calculated from relative Gibbs free energy.*

S27. Important thermodynamic parameters and conformational analysis of (4‴*R*)-12.

conformers	*E* (a.u.)	*E'* (a.u.)	*H* (a.u.)	*G* (a.u.)	Δ*G* (kcal/mol)	P_G (%)
(4‴*R*)-**12A**	-2365.880343	-2365.288184	-2365.244079	-2365.365802	0.00	13.5
(4‴*R*)-**12B**	-2365.879751	-2365.287669	-2365.243537	-2365.365124	0.43	6.6
(4‴*R*)-**12C**	-2365.880140	-2365.287998	-2365.243910	-2365.365082	0.45	6.3
(4‴*R*)-**12D**	-2365.879525	-2365.287318	-2365.243297	-2365.365039	0.48	6.0
(4‴*R*)-**12E**	-2365.878911	-2365.286953	-2365.242764	-2365.365004	0.50	5.8
(4‴*R*)-**12F**	-2365.878707	-2365.286767	-2365.242541	-2365.364721	0.68	4.3
(4‴*R*)-**12G**	-2365.879551	-2365.287500	-2365.243366	-2365.364587	0.76	3.7
(4‴*R*)-**12H**	-2365.879803	-2365.287684	-2365.243689	-2365.364497	0.82	3.4
(4‴*R*)-**12I**	-2365.878458	-2365.286532	-2365.242315	-2365.364475	0.83	3.3
(4‴*R*)-**12J**	-2365.879822	-2365.287425	-2365.243472	-2365.364304	0.94	2.8
(4‴*R*)-**12K**	-2365.878147	-2365.286200	-2365.242007	-2365.364301	0.94	2.8
(4‴*R*)-**12L**	-2365.878541	-2365.286262	-2365.242233	-2365.364240	0.98	2.6
(4‴*R*)-**12M**	-2365.879902	-2365.287255	-2365.243423	-2365.364177	1.02	2.4
(4‴*R*)-**12N**	-2365.879628	-2365.287273	-2365.243308	-2365.364081	1.08	2.2
(4‴*R*)-**12O**	-2365.879393	-2365.287389	-2365.243294	-2365.363994	1.13	2.0
(4‴*R*)-**12P**	-2365.878958	-2365.286993	-2365.242909	-2365.363916	1.18	1.8
(4‴*R*)-**12Q**	-2365.878350	-2365.286518	-2365.242357	-2365.363912	1.19	1.8
(4‴*R*)-**12R**	-2365.879474	-2365.287360	-2365.243323	-2365.363893	1.20	1.8
(4‴*R*)-**12S**	-2365.878762	-2365.286891	-2365.242702	-2365.363769	1.28	1.6
(4‴*R*)-**12T**	-2365.878492	-2365.286530	-2365.242345	-2365.363712	1.31	1.5
(4‴*R*)-**12U**	-2365.878748	-2365.286572	-2365.242470	-2365.363710	1.31	1.5
(4‴*R*)-**12V**	-2365.879820	-2365.287544	-2365.243587	-2365.363677	1.33	1.4
(4‴*R*)-**12W**	-2365.880097	-2365.287657	-2365.243801	-2365.363540	1.42	1.2
(4‴*R*)-**12X**	-2365.878159	-2365.286051	-2365.241910	-2365.363479	1.46	1.2
(4‴*R*)-**12Y**	-2365.877581	-2365.285600	-2365.241396	-2365.363441	1.48	1.1
(4‴*R*)-**12Z**	-2365.878901	-2365.286663	-2365.242609	-2365.363368	1.53	1.0

E: total energy; E': total energy with zero point energy; H: enthalpy; G: Gibbs free energy; ΔG: relative Gibbs free energy at the B3LYP/6-31G(d,p) level in acetone using the PCM model. P_G *: conformational distribution calculated from relative Gibbs free energy.*

S28. Calculated ^{1}H-NMR chemical shifts of (4‴*S*)-12.

Position	calculated[a]																			experimental[b]
	(4‴*S*)-**12A**	(4‴*S*)-**12B**	(4‴*S*)-**12C**	(4‴*S*)-**12D**	(4‴*S*)-**12E**	(4‴*S*)-**12F**	(4‴*S*)-**12G**	(4‴*S*)-**12H**	(4‴*S*)-**12I**	(4‴*S*)-**12J**	(4‴*S*)-**12K**	(4‴*S*)-**12L**	(4‴*S*)-**12M**	(4‴*S*)-**12N**	(4‴*S*)-**12O**	(4‴*S*)-**12P**	(4‴*S*)-**12Q**	(4‴*S*)-**12R**	(4‴*S*)-**12** (averaged)[c]	**12**
2	5.39	5.27	5.37	5.36	5.38	5.35	5.38	5.52	5.35	5.37	5.48	5.38	5.34	5.50	5.37	5.49	5.33	5.42	5.37	4.85
3	4.65	4.57	4.77	4.61	4.72	4.77	4.63	4.73	4.69	4.85	4.79	4.78	4.85	4.83	4.70	4.81	4.70	4.88	4.69	4.35
4	3.12	3.08	3.12	3.13	3.13	3.19	3.11	3.16	3.15	3.09	3.14	3.12	3.17	3.17	3.13	3.17	3.13	3.20	3.12	2.88
	3.07	3.03	3.03	3.07	2.90	3.05	3.07	3.08	2.90	2.83	3.08	3.03	2.92	3.09	2.90	2.91	2.91	3.05	3.02	2.77
6	6.28	6.39	6.32	6.26	6.41	6.29	6.28	6.30	6.38	6.53	6.30	6.32	6.46	6.37	6.42	6.48	6.55	6.26	6.34	5.85[a]
8	6.42	6.23	6.30	6.40	6.43	6.63	6.41	6.43	6.41	6.30	6.45	6.31	6.64	6.28	6.42	6.45	6.29	6.70	6.39	5.99[a]
6'	7.89	8.02	7.81	8.03	7.87	7.74	7.90	7.91	8.01	7.79	7.80	7.82	7.72	7.78	7.88	7.87	7.87	7.69	7.89	6.95
2''	4.22	4.11	3.81	4.17	4.21	3.92	4.19	4.29	4.17	3.81	4.28	3.82	3.93	3.90	4.19	4.28	4.16	3.97	4.10	3.84
3''	4.79	4.82	4.80	4.78	4.79	4.76	4.83	4.83	4.78	4.80	4.85	4.87	4.76	4.73	4.83	4.83	4.84	4.68	4.80	4.65
4''	3.11	2.78	2.91	3.12	3.11	3.00	2.80	3.09	3.12	2.91	3.12	2.76	3.00	2.93	2.79	3.09	2.83	2.98	2.99	2.78
	2.94	2.90	3.10	2.96	2.94	3.07	2.90	2.98	2.96	3.10	2.96	3.05	3.07	3.14	2.91	2.98	2.90	3.11	2.98	2.66
6''	6.20	6.57	6.23	6.12	6.20	6.31	6.41	6.16	6.11	6.22	6.23	6.46	6.31	6.19	6.41	6.17	6.59	6.34	6.28	5.80[b]
8''	6.30	6.18	6.77	6.30	6.30	6.56	6.33	6.30	6.30	6.77	6.31	6.80	6.55	6.77	6.32	6.30	6.16	6.66	6.40	5.96[b]
2'''	3.76	3.64	3.67	3.79	3.76	3.67	3.75	4.00	3.80	3.66	3.97	3.67	3.67	3.98	3.76	4.00	3.75	4.00	3.75	3.26
	4.17	4.05	4.19	4.29	4.19	4.44	4.12	4.47	4.30	4.20	4.45	4.14	4.45	4.45	4.13	4.47	4.14	4.66	4.23	3.70
5'''	4.77	4.75	5.07	4.71	4.75	5.19	4.74	4.85	4.69	5.06	4.95	5.06	5.18	5.01	4.71	4.85	4.70	5.08	4.85	4.32
Ethyl-CH_2	3.71	3.82	3.98	3.72	3.70	3.98	3.70	4.11	3.72	3.98	3.92	3.97	3.98	4.02	3.69	4.11	3.71	4.04	3.83	3.72
	3.95	4.12	4.10	4.47	3.95	4.12	3.96	3.76	4.46	4.09	4.74	4.10	4.12	3.68	3.96	3.75	3.95	3.69	4.09	3.82
Ethyl-CH_3	1.27	1.31	1.32	1.17	1.27	1.32	1.26	1.37	1.16	1.32	0.94	1.33	1.33	1.31	1.26	1.36	1.26	1.33	1.27	0.95

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone using the PCM model. [b] Measured in acetone-d_6 + D_2O (500 MHz). [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d,e] May be interchanged.

S29. Calculated ^{1}H-NMR chemical shifts of (4‴*R*)-12.

Position	calculated[a]																												experimental[b]
	(4‴*R*)-**12A**	(4‴*R*)-**12B**	(4‴*R*)-**12C**	(4‴*R*)-**12D**	(4‴*R*)-**12E**	(4‴*R*)-**12F**	(4‴*R*)-**12G**	(4‴*R*)-**12H**	(4‴*R*)-**12I**	(4‴*R*)-**12J**	(4‴*R*)-**12K**	(4‴*R*)-**12L**	(4‴*R*)-**12M**	(4‴*R*)-**12N**	(4‴*R*)-**12O**	(4‴*R*)-**12P**	(4‴*R*)-**12Q**	(4‴*R*)-**12R**	(4‴*R*)-**12S**	(4‴*R*)-**12T**	(4‴*R*)-**12U**	(4‴*R*)-**12V**	(4‴*R*)-**12W**	(4‴*R*)-**12X**	(4‴*R*)-**12Y**	(4‴*R*)-**12Z**	(4‴*R*)-**12** (averaged)[c]	**12**
2	5.16	5.17	5.17	4.97	5.49	5.14	5.17	4.97	5.15	5.16	5.52	4.95	4.94	5.15	5.17	5.16	5.16	5.22	5.19	5.15	5.16	5.23	4.99	5.16	5.49	5.16	5.17	4.85
3	3.99	3.96	3.98	4.81	4.86	4.07	3.96	4.82	4.03	3.97	4.86	4.89	4.78	3.95	4.32	4.03	4.00	4.26	4.31	4.06	3.97	4.27	4.82	3.95	4.94	3.96	4.27	4.35
4	3.26	3.23	3.24	2.96	3.13	3.22	3.22	2.96	3.18	3.27	3.13	2.93	2.95	3.26	3.09	3.27	3.25	3.08	3.09	3.23	3.25	3.08	3.06	3.23	3.08	3.24	3.16	2.88
	2.96	2.96	2.96	2.98	3.09	2.78	2.96	2.99	2.77	2.95	3.11	2.83	2.94	2.97	2.84	2.97	2.97	2.97	2.82	2.77	2.95	2.96	2.73	2.96	2.87	2.96	2.94	2.77
6	6.15	5.94	6.15	6.14	6.38	6.39	5.94	6.14	6.24	6.15	6.18	6.36	6.29	6.14	6.09	6.16	5.95	6.13	5.88	6.39	6.15	6.12	6.53	5.94	6.56	6.15	6.17	5.85[a]
8	6.44	6.63	6.46	6.66	6.29	6.51	6.64	6.65	6.68	6.49	6.48	6.67	6.33	6.51	6.42	6.44	6.62	6.46	6.59	6.52	6.45	6.46	6.64	6.62	6.31	6.46	6.51	5.99[a]
6'	6.99	6.99	6.98	7.47	7.66	6.98	6.99	7.46	6.97	7.01	7.66	7.46	7.72	7.00	6.99	6.98	6.98	7.05	7.00	6.97	6.99	7.04	7.79	6.99	7.60	6.99	7.17	6.95
2''	4.37	4.36	4.36	4.37	4.34	4.37	4.36	4.37	4.36	4.34	4.35	4.37	4.30	4.34	4.30	4.41	4.41	4.17	4.31	4.35	4.35	4.15	4.11	4.35	4.33	4.35	4.35	3.84
3''	4.68	4.68	4.66	4.75	4.73	4.69	4.66	4.76	4.68	4.68	4.73	4.75	4.76	4.68	4.67	4.98	4.98	4.70	4.67	4.67	4.75	4.71	4.70	4.76	4.73	4.74	4.71	4.65
4''	2.96	2.99	2.96	3.06	3.02	2.96	2.97	3.07	2.98	2.95	3.01	3.07	3.03	2.95	2.95	2.92	2.93	2.97	2.97	2.95	2.78	2.98	3.06	2.80	3.02	2.78	2.98	2.78
	2.93	2.93	2.93	2.98	2.98	2.93	2.93	2.98	2.93	2.94	2.99	2.98	2.96	2.94	2.91	2.89	2.89	2.95	2.92	2.93	2.95	2.95	3.09	2.95	2.98	2.95	2.95	2.66
6''	6.31	6.29	6.11	6.23	6.45	6.31	6.10	6.39	6.30	6.30	6.28	6.23	6.28	6.11	6.08	6.11	6.10	6.10	6.07	6.12	6.52	6.29	6.38	6.51	6.45	6.35	6.26	5.80[b]
8''	6.27	6.27	6.43	6.76	6.43	6.26	6.43	6.60	6.26	6.24	6.60	6.76	6.65	6.39	6.44	6.37	6.37	6.48	6.44	6.42	6.31	6.33	6.54	6.31	6.44	6.45	6.42	5.96[b]
2'''	3.59	3.60	3.58	3.62	3.52	3.59	3.59	3.63	3.60	3.58	3.52	3.62	3.49	3.57	3.57	3.57	3.58	3.61	3.58	3.58	3.56	3.62	3.51	3.56	3.53	3.55	3.58	3.26
	3.66	3.66	3.67	3.75	4.12	3.65	3.67	3.73	3.66	3.68	4.15	3.75	3.87	3.67	3.66	3.71	3.72	3.68	3.67	3.66	3.65	3.67	3.98	3.65	4.13	3.66	3.74	3.70
5'''	5.35	5.33	5.32	5.49	5.16	5.29	5.31	5.49	5.28	5.25	5.19	5.47	5.26	5.24	5.64	5.46	5.45	5.41	5.64	5.27	5.32	5.39	5.32	5.32	5.17	5.31	5.34	4.32
Ethyl-CH_2	4.38	4.37	4.42	4.22	4.09	4.39	4.41	4.19	4.39	4.19	4.10	4.24	4.40	5.03	4.38	4.33	4.34	4.44	4.39	4.42	4.42	4.45	4.07	4.38	4.09	4.42	4.34	3.72
	4.41	4.52	4.41	4.14	3.87	4.43	4.49	4.14	4.53	5.03	3.88	4.13	4.84	4.22	4.39	4.38	4.45	4.41	4.47	4.43	4.40	4.40	4.31	4.52	3.86	4.42	4.35	3.82
Ethyl-CH_3	1.50	1.50	1.52	1.74	1.14	1.50	1.52	1.72	1.50	1.34	1.13	1.74	1.29	1.35	1.50	1.51	1.50	1.51	1.50	1.52	1.51	1.49	1.43	1.51	1.13	1.53	1.48	0.95

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone using the PCM model. [b] Measured in acetone-d_6 + D_2O (500 MHz). [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d,e] May be interchanged.

S30. Calculated ^{13}C-NMR chemical shifts of (4‴*S*)-12.

Position	calculated[a]																			experimental[b]
	(4‴*S*)-**12A**	(4‴*S*)-**12B**	(4‴*S*)-**12C**	(4‴*S*)-**12D**	(4‴*S*)-**12E**	(4‴*S*)-**12F**	(4‴*S*)-**12G**	(4‴*S*)-**12H**	(4‴*S*)-**12I**	(4‴*S*)-**12J**	(4‴*S*)-**12K**	(4‴*S*)-**12L**	(4‴*S*)-**12M**	(4‴*S*)-**12N**	(4‴*S*)-**12O**	(4‴*S*)-**12P**	(4‴*S*)-**12Q**	(4‴*S*)-**12R**	(4‴*S*)-**12** (averaged)[c]	**12**
2	74.8	75.0	75.7	74.8	74.6	76.8	74.7	74.8	74.6	75.5	75.1	75.7	76.4	75.5	74.5	74.7	74.6	76.0	75.1	77.4
3	63.4	64.0	63.3	63.6	63.2	63.8	63.4	63.3	63.3	63.1	62.8	63.3	63.7	63.6	63.2	62.9	63.1	63.8	63.5	65.6
4	29.2	29.2	29.1	29.2	27.7	30.2	29.2	29.5	27.6	27.2	29.0	29.0	28.2	29.4	27.7	27.9	27.7	29.8	28.9	30.0
4a	100.5	100.2	99.7	100.1	98.7	101.3	100.4	100.2	98.2	97.5	99.5	99.6	99.2	99.6	98.8	98.0	98.7	101.6	99.9	99.6
5	158.4	159.0	158.5	158.4	159.5	158.5	158.4	158.4	159.4	159.1	158.2	158.6	159.1	158.7	159.5	159.1	159.9	158.4	158.7	157.4[d]
6	92.9	93.2	93.9	93.0	93.4	92.8	93.0	92.9	93.5	94.8	92.9	93.9	93.4	93.9	93.4	93.3	93.6	93.2	93.3	95.5[e]
7	158.5	158.4	158.9	158.5	159.2	156.4	158.5	158.4	159.1	159.7	158.5	159.0	157.1	158.9	159.1	159.1	159.0	156.5	158.5	157.2[d]
8	93.6	93.1	94.8	93.7	94.0	95.8	93.6	93.6	94.0	95.1	93.8	94.8	95.9	94.5	94.0	94.1	93.4	95.7	94.0	96.1[e]
8a	160.4	160.0	159.5	160.4	160.1	160.6	160.3	160.2	160.0	159.1	160.2	159.6	160.3	159.5	160.0	159.8	159.6	160.5	160.1	157.7[d]
1'	129.9	130.0	129.3	130.2	129.5	130.3	130.0	129.2	129.8	128.9	129.5	129.3	130.0	130.2	129.6	128.8	129.6	129.7	129.8	128.7
2'	119.2	119.8	118.7	119.8	119.2	120.1	119.2	117.9	119.9	118.8	118.2	118.6	120.0	118.6	119.1	118.0	119.3	118.4	119.2	117.2
3'	149.2	149.7	149.0	149.4	149.1	149.1	149.1	148.7	149.4	148.8	149.7	148.8	149.0	148.5	149.1	148.9	149.3	148.2	149.2	148.9
4'	129.6	130.7	132.7	130.3	129.7	130.2	129.6	129.1	130.3	132.7	129.9	132.7	130.1	129.8	129.7	129.1	129.8	129.8	130.4	130.0
5'	148.2	148.0	148.8	147.8	148.2	148.5	148.2	148.1	147.9	148.8	148.0	148.8	148.6	148.1	148.2	148.1	148.1	148.1	148.2	147.3
6'	108.8	109.4	109.1	109.8	108.7	109.9	108.9	108.5	109.7	109.0	108.4	109.2	109.7	109.9	108.7	108.5	108.9	109.6	109.1	109.5
2''	74.8	74.4	75.3	75.4	74.8	75.2	74.5	75.8	75.4	75.3	75.6	75.1	75.2	76.2	74.5	75.7	74.5	75.7	75.0	77.1
3''	61.9	61.8	63.7	61.8	61.9	63.7	61.8	62.0	61.8	63.7	62.1	63.6	63.7	63.7	61.8	62.0	61.8	63.7	62.4	61.7
4''	27.0	25.4	29.1	27.0	27.0	28.9	25.4	27.0	27.0	29.1	27.6	27.3	28.9	29.2	25.4	27.1	25.6	28.9	27.2	29.6
4a''	97.9	96.1	101.2	97.7	97.9	100.0	96.2	97.8	97.7	101.2	98.0	99.0	100.0	102.3	96.2	97.8	96.4	100.3	98.3	99.4
5''	158.6	159.7	159.0	158.6	158.6	159.1	159.0	158.6	158.6	158.9	158.7	159.6	159.1	158.8	159.0	158.7	159.7	159.1	158.9	157.6[d]
6''	93.0	94.7	94.3	92.9	93.0	96.2	93.8	92.9	93.0	94.3	93.1	95.5	96.2	94.5	93.8	92.9	94.5	95.9	93.8	95.3[f]
7''	159.1	159.9	156.3	159.4	159.1	159.1	159.7	159.1	159.4	156.3	158.9	157.0	159.1	156.2	159.7	159.1	159.8	159.0	158.8	157.4[d]
8''	94.1	93.5	96.3	94.1	94.1	96.6	94.2	94.2	94.1	96.3	94.2	96.5	96.6	96.1	94.2	94.2	93.5	96.6	94.7	96.4[f]
8a''	158.0	156.5	160.6	157.9	158.0	158.9	157.4	158.0	157.9	160.5	158.2	160.4	158.9	160.5	157.4	158.0	156.5	159.3	158.3	156.1[d]
1'''	94.2	93.3	94.0	94.0	94.2	94.3	94.0	93.0	94.0	94.0	93.6	93.8	94.3	93.5	94.0	93.1	94.0	94.0	93.9	92.3
2'''	43.9	43.6	42.5	44.3	43.9	42.8	43.8	43.8	44.3	42.5	43.2	42.5	42.8	42.5	43.8	43.8	43.8	42.7	43.5	44.3
3'''	222.4	220.6	220.7	221.9	222.3	220.7	222.3	220.4	221.8	220.7	220.4	220.7	220.6	221.8	222.2	220.4	222.1	221.6	221.5	213.1
4'''	85.8	86.5	86.3	85.5	85.8	86.8	85.8	86.3	85.5	86.3	86.9	86.3	86.8	86.3	85.8	86.3	85.8	86.5	86.1	85.8
5'''	58.8	57.7	57.9	58.7	58.8	57.0	58.7	60.2	58.7	57.8	59.8	58.0	56.9	58.7	58.7	60.1	58.8	58.7	58.4	59.3
6'''	173.7	175.3	175.5	173.8	173.8	175.5	173.7	174.9	173.9	175.5	174.8	175.5	175.5	175.3	173.7	174.9	173.7	175.3	174.5	170.4
Ethyl-CH_2	62.4	64.3	64.5	62.0	62.5	64.6	62.5	62.7	62.1	64.5	62.1	64.5	64.6	62.4	62.5	62.7	62.5	62.4	63.2	62.4
Ethyl-CH_3	9.4	9.3	9.5	10.6	9.4	9.4	9.4	9.7	10.6	9.5	10.9	9.5	9.4	9.5	9.4	9.7	9.4	9.5	9.6	13.6

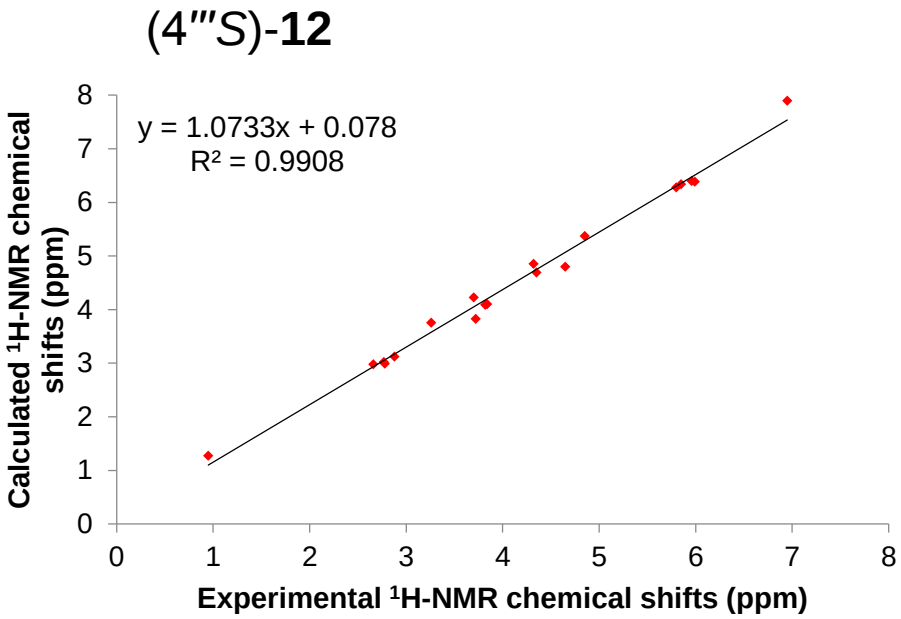
[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone using the PCM model. [b] Measured in acetone-d_6 + D_2O (500 MHz). [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d–f] May be interchanged.

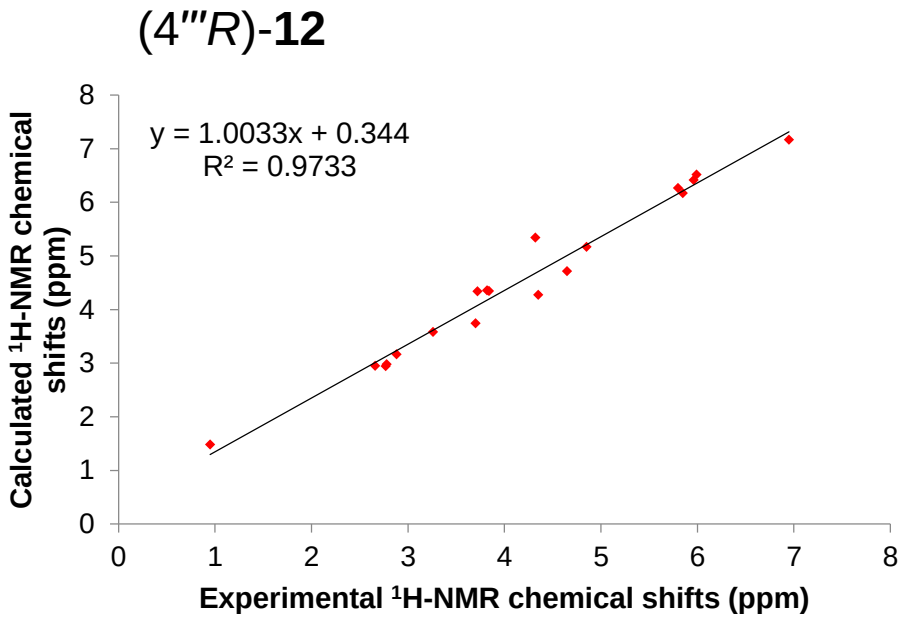
S31. Calculated ^{13}C-NMR chemical shifts of (4‴*R*)-12.

Position	calculated[a]																												experimental[b]
	(4‴*R*)-**12A**	(4‴*R*)-**12B**	(4‴*R*)-**12C**	(4‴*R*)-**12D**	(4‴*R*)-**12E**	(4‴*R*)-**12F**	(4‴*R*)-**12G**	(4‴*R*)-**12H**	(4‴*R*)-**12I**	(4‴*R*)-**12J**	(4‴*R*)-**12K**	(4‴*R*)-**12L**	(4‴*R*)-**12M**	(4‴*R*)-**12N**	(4‴*R*)-**12O**	(4‴*R*)-**12P**	(4‴*R*)-**12Q**	(4‴*R*)-**12R**	(4‴*R*)-**12S**	(4‴*R*)-**12T**	(4‴*R*)-**12U**	(4‴*R*)-**12V**	(4‴*R*)-**12W**	(4‴*R*)-**12X**	(4‴*R*)-**12Y**	(4‴*R*)-**12Z**	(4‴*R*)-**12** (averaged)[c]	**12**
2	82.1	81.8	82.0	76.2	75.8	82.4	81.7	76.2	82.0	82.2	75.8	75.9	75.8	82.1	80.6	82.4	82.2	81.0	80.4	82.2	82.0	81.0	76.1	81.7	75.6	81.9	80.1	77.4
3	68.6	68.6	68.6	62.0	62.3	67.8	68.6	62.0	67.8	68.5	62.3	61.7	62.2	68.5	68.4	68.6	68.5	68.4	68.3	67.9	68.6	68.5	63.4	68.6	62.0	68.7	66.5	65.6
4	27.4	27.3	27.2	28.9	29.0	25.7	27.2	28.9	25.8	27.5	29.1	27.0	28.1	27.4	28.0	27.6	27.6	24.7	28.0	25.6	27.3	24.7	26.9	27.3	26.9	27.2	27.4	30.0
4a	97.8	97.8	97.7	100.9	101.2	96.5	97.7	100.9	96.5	98.2	101.2	99.2	100.4	98.0	98.6	98.3	98.2	99.7	98.6	96.5	97.7	99.5	99.8	97.7	99.0	97.6	98.7	99.6
5	159.3	158.6	159.3	158.2	159.1	160.1	158.6	158.2	159.5	159.3	158.4	159.0	158.7	159.3	158.4	159.4	158.7	158.3	157.6	160.0	159.3	158.3	159.1	158.6	159.8	159.3	159.0	157.6[d]
6	94.0	93.6	94.0	93.2	93.6	95.6	93.6	93.2	95.1	93.9	93.0	94.0	94.0	94.0	92.9	94.0	93.6	93.2	92.5	95.5	94.0	93.2	93.4	93.6	94.4	94.0	93.9	95.5[e]
7	158.8	158.6	158.8	158.5	158.4	159.5	158.6	158.4	159.5	158.7	158.4	159.2	158.5	158.7	158.4	158.7	158.6	158.2	158.2	159.5	158.8	158.3	157.4	158.6	159.1	158.8	158.7	157.4[d]
8	95.4	95.9	95.4	94.2	93.1	95.4	96.0	94.2	95.7	95.4	94.1	94.5	93.0	95.4	95.2	95.5	96.1	95.3	95.8	95.5	95.4	95.3	95.2	95.9	93.4	95.4	95.0	96.1[e]
8a	158.8	159.3	158.7	160.3	159.8	158.3	159.3	160.3	158.7	158.7	160.3	159.8	159.6	158.7	158.9	158.9	159.5	158.4	159.6	158.2	158.7	158.4	159.5	159.3	159.4	158.7	159.2	157.7[d]
1'	132.2	132.3	132.3	129.0	129.2	131.6	132.3	128.9	131.6	132.2	129.2	128.6	129.8	132.2	132.5	131.9	132.0	132.0	132.6	131.7	132.3	132.1	129.7	132.3	128.7	132.3	131.2	128.7
2'	117.6	117.7	117.7	120.1	117.9	117.5	117.8	120.1	117.6	117.6	117.9	120.2	120.2	117.7	119.3	117.5	117.6	116.5	119.2	117.5	117.6	116.6	119.7	117.7	117.9	117.6	118.2	117.2
3'	148.7	148.6	148.6	148.1	147.6	148.8	148.6	148.1	148.7	148.8	147.5	148.2	148.4	148.8	148.5	148.9	148.9	149.0	148.5	148.7	148.7	149.0	148.5	148.6	147.8	148.6	148.5	148.9
4'	128.2	128.0	128.1	129.3	129.4	128.3	128.0	129.4	128.1	128.1	129.4	129.4	129.5	128.1	127.8	128.3	128.3	128.2	127.7	128.3	128.1	128.1	130.4	127.9	129.5	128.0	128.5	130.0
5'	146.7	146.7	146.7	147.9	148.3	146.8	146.7	147.9	146.8	146.6	148.3	147.9	147.3	146.6	146.3	146.8	146.8	147.6	146.2	146.8	146.7	147.5	147.6	146.7	148.3	146.7	147.1	147.3
6'	106.5	106.2	106.3	107.7	108.7	106.6	106.1	107.7	106.4	106.4	108.6	107.7	108.7	106.1	105.7	106.9	106.7	106.6	105.8	106.5	106.4	106.6	109.2	106.2	108.5	106.3	106.9	109.5
2"	73.5	73.5	73.5	74.3	74.1	73.5	73.5	74.4	73.5	73.6	74.1	74.3	74.3	73.6	73.6	72.5	72.4	73.5	73.6	73.5	73.4	73.5	74.9	73.3	74.1	73.3	73.7	77.1
3"	62.1	62.1	62.2	61.9	62.2	62.2	62.1	61.8	62.1	62.1	62.2	61.8	62.0	62.2	62.3	61.4	61.4	62.1	62.2	62.2	61.7	62.1	63.1	61.7	62.2	61.7	62.1	61.7
4"	26.5	26.6	26.7	27.0	26.6	26.5	26.7	27.0	26.6	26.6	26.6	27.0	27.2	26.7	26.9	27.3	27.3	26.9	26.9	26.7	25.7	26.9	28.6	25.7	26.6	25.8	26.7	29.6
4a"	98.2	98.4	98.3	98.0	97.5	98.1	98.4	98.1	98.4	98.2	97.3	98.0	98.0	98.3	98.5	98.7	98.8	98.1	98.6	98.1	96.9	98.4	101.9	97.2	97.4	97.0	98.2	99.4
5"	158.9	158.9	158.3	158.5	158.9	158.9	158.3	159.1	158.9	158.9	158.2	158.5	158.4	158.3	158.3	157.7	157.7	158.4	158.3	158.3	159.4	159.0	159.2	159.4	158.9	158.9	158.7	157.2[d]
6"	93.4	93.6	93.1	93.2	93.5	93.4	93.1	93.6	93.5	93.4	93.1	93.2	93.3	93.0	93.1	91.9	91.9	93.3	93.1	93.0	94.4	93.7	95.8	94.6	93.5	94.0	93.4	95.3[f]
7"	158.9	158.9	158.8	158.9	159.2	159.0	158.8	159.0	158.9	158.9	159.1	158.9	159.0	158.8	158.7	158.5	158.5	158.8	158.7	158.8	159.6	158.9	158.9	159.6	159.2	159.5	158.9	157.4[d]
8"	93.6	93.5	94.1	94.6	93.8	93.6	94.0	93.8	93.5	93.4	94.6	94.6	94.2	93.9	94.2	93.8	93.8	94.3	94.1	94.1	93.7	93.6	96.8	93.7	93.8	94.1	93.9	96.4[f]
8a"	157.6	157.7	158.4	158.5	157.4	157.6	158.4	157.9	157.6	157.6	158.1	158.5	158.5	158.3	158.6	158.4	158.4	158.1	158.7	158.3	157.4	157.6	158.5	157.4	157.4	158.0	158.0	156.1[d]
1""	96.4	96.3	96.3	96.8	95.5	96.2	96.3	96.8	96.2	96.1	95.5	96.9	96.5	95.9	96.5	97.0	97.0	96.1	96.6	96.1	96.2	96.2	96.5	96.2	95.4	96.2	96.3	92.3
2""	42.6	42.6	42.6	43.5	43.8	42.5	42.6	43.5	42.5	42.6	43.9	43.5	44.0	42.6	42.7	43.1	43.1	42.7	42.7	42.5	42.5	42.8	44.9	42.5	43.8	42.5	43.0	44.3
3""	221.9	221.9	221.7	221.3	221.8	221.7	221.8	221.4	221.8	221.6	221.9	221.3	220.5	221.5	221.8	222.7	222.7	221.2	221.8	221.6	221.5	221.1	221.8	221.6	221.7	221.5	221.7	213.1
4""	80.8	80.8	80.8	79.1	81.1	80.8	80.9	79.1	80.8	81.2	81.1	79.2	80.8	81.1	81.0	81.1	81.1	81.0	81.0	80.8	80.9	81.1	80.4	80.9	81.2	80.9	80.7	85.8
5""	56.6	56.4	56.6	55.4	57.4	56.6	56.5	55.5	56.5	57.0	57.3	55.3	55.2	57.0	56.3	56.5	56.5	56.1	56.2	56.6	56.6	56.1	54.4	56.5	57.4	56.6	56.4	59.3
6""	177.2	177.2	177.3	177.5	177.4	177.2	177.2	177.6	177.2	176.9	177.3	177.5	176.9	176.9	177.2	177.2	177.1	177.0	177.1	177.3	177.2	177.0	175.5	177.1	177.3	177.2	177.2	170.4
Ethyl-CH_2	64.8	64.9	64.9	64.8	62.6	64.9	65.0	64.7	65.0	64.1	62.5	64.9	64.2	64.1	64.8	64.7	64.7	65.0	64.9	65.0	64.9	65.0	62.9	65.0	62.6	65.0	64.5	62.4
Ethyl-CH_3	10.2	10.1	10.2	10.5	9.4	10.2	10.2	10.4	10.2	10.2	9.4	10.5	10.2	10.2	10.1	10.2	10.2	10.1	10.1	10.2	10.2	10.0	9.8	10.2	9.4	10.2	10.1	13.6

[a] Calculated using the GIAO method at the mPW1PW91/6-311+G(2d,p) level in acetone using the PCM model. [b] Measured in acetone-d_6 + D_2O (500 MHz). [c] Averaged according to the Boltzmann distribution theory at 298 K based on relative Gibbs free energies. [d-f] May be interchanged.

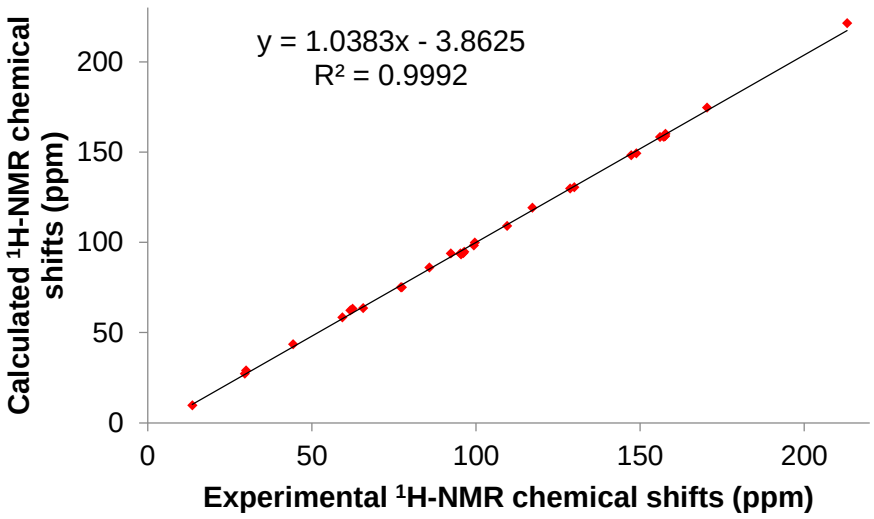
S32. Correlation plots of experimental ^{1}H-NMR chemical shifts versus corresponding calculated ^{1}H-NMR chemical shifts of 12.



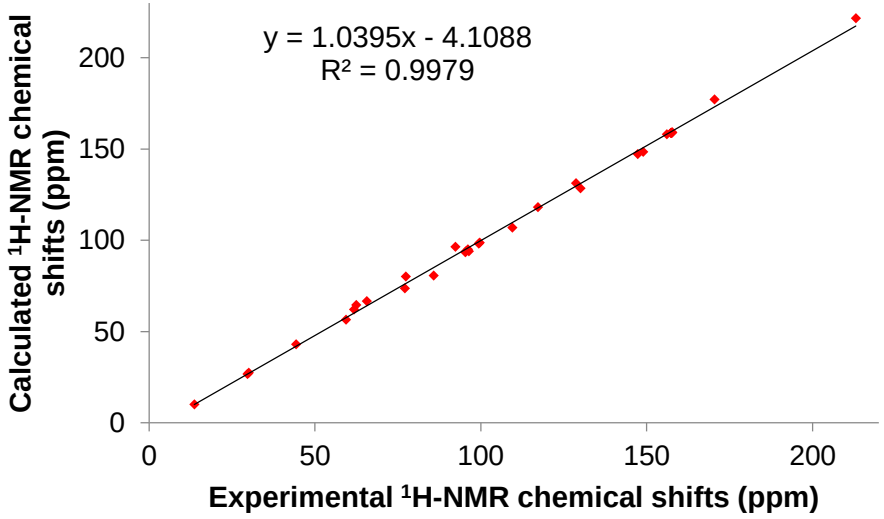


S33. Correlation plots of experimental ^{13}C-NMR chemical shifts versus corresponding calculated ^{13}C-NMR chemical shifts of 12.

(4‴*S*)-**12**



(4‴*R*)-**12**



S34. Statistical parameters of calculated ^{1}H-NMR chemical shifts of 12 (ppm).

	R^2	CMaxErr	CMAE
(4'''*S*)-**12**	0.9908	0.33	0.11
(4'''*R*)-**12**	0.9733	0.66	0.19

R^2: correlation coefficient; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

S35. Statistical parameters of calculated ^{13}C-NMR chemical shifts of 12 (ppm).

	R^2	CMaxErr	CMAE
(4'''*S*)-**12**	0.9992	3.9	1.1
(4'''*R*)-**12**	0.9979	4.3	1.7

R^2: correlation coefficient; CMaxErr: corrected maximum absolute error with respect to the linear fit; CMAE: corrected mean absolute error with respect to the linear fit

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11A at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.866857	3.758906	0.100095
2	6	0	5.826645	3.407937	-0.856917
3	6	0	5.865815	2.097090	-1.330395
4	6	0	4.970133	1.111854	-0.874053
5	6	0	4.017978	1.513318	0.069486
6	6	0	3.951343	2.817455	0.569289
7	6	0	5.045038	-0.318182	-1.364918
8	6	0	4.232086	-1.255217	-0.460847
9	6	0	2.886581	-0.575345	-0.168426
10	8	0	3.106720	0.620285	0.595064
11	8	0	4.932252	-1.582908	0.738774
12	6	0	1.855352	-1.404749	0.615881
13	6	0	2.234233	-1.788244	2.024334
14	6	0	1.296657	-1.400386	2.908211
15	6	0	0.179590	-0.708287	2.235959
16	6	0	0.459214	-0.701905	0.735409
17	6	0	-0.450416	-1.608503	-0.066779
18	6	0	0.320973	-2.675375	-0.525276
19	8	0	1.647522	-2.617683	-0.186577
20	6	0	-1.810583	-1.538589	-0.385692
21	6	0	-2.355038	-2.566796	-1.172084
22	6	0	-1.569711	-3.630977	-1.618084
23	6	0	-0.204330	-3.702575	-1.294752
24	8	0	-2.136073	-4.609891	-2.382327
25	8	0	0.511199	-4.766951	-1.775665
26	8	0	-0.782882	-0.247115	2.832161
27	8	0	1.274142	-1.562608	4.241214
28	8	0	6.779474	1.691930	-2.261035
29	8	0	4.871745	5.053749	0.532067
30	6	0	-2.668001	-0.396613	0.103295
31	8	0	-3.408335	0.114012	-1.032447
32	6	0	-4.289739	1.137711	-0.772889
33	6	0	-4.766778	1.391943	0.519434
34	6	0	-4.336627	0.545412	1.697819
35	6	0	-3.670912	-0.751529	1.222557
36	6	0	-4.703429	1.880359	-1.885356
37	6	0	-5.617184	2.916100	-1.698078
38	6	0	-6.108575	3.214891	-0.421587
39	6	0	-5.679967	2.452755	0.664655
40	8	0	-6.127816	2.691066	1.933742
41	8	0	-6.068096	3.690047	-2.729449
42	8	0	-4.625639	-1.714838	0.785143
43	1	0	0.477721	0.332550	0.375966
44	1	0	6.525245	4.157046	-1.215808
45	1	0	3.191807	3.073071	1.300716
46	1	0	4.673705	-0.393041	-2.395443
47	1	0	6.083310	-0.663347	-1.385330
48	1	0	4.051278	-2.205062	-0.968108
49	1	0	2.424158	-0.309561	-1.129455
50	1	0	5.043832	-0.765375	1.246401
51	1	0	3.155980	-2.308450	2.242625
52	1	0	-3.402042	-2.551557	-1.444463
53	1	0	-1.449201	-5.260883	-2.595603
54	1	0	1.429974	-4.698940	-1.478086
55	1	0	0.449162	-1.151016	4.558445
56	1	0	7.357115	2.433217	-2.491378
57	1	0	4.175450	5.174980	1.192886
58	1	0	-2.023721	0.404523	0.484383
59	1	0	-5.197866	0.294377	2.325029
60	1	0	-3.635132	1.096075	2.338003
61	1	0	-3.128665	-1.217953	2.047187
62	1	0	-4.302823	1.642574	-2.865423
63	1	0	-6.813112	4.030654	-0.294179
64	1	0	-6.770641	3.414048	1.917791
65	1	0	-5.662672	3.390629	-3.555364
66	1	0	-5.109801	-1.326085	0.042138

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11B at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.868873	3.760616	0.095981
2	6	0	5.829709	3.409020	-0.859745
3	6	0	5.868733	2.098097	-1.333047
4	6	0	4.971877	1.113415	-0.877807
5	6	0	4.018790	1.515488	0.064532
6	6	0	3.952268	2.819723	0.564124
7	6	0	5.046412	-0.316716	-1.368443
8	6	0	4.233228	-1.253285	-0.464116
9	6	0	2.887404	-0.573624	-0.172777
10	8	0	3.106490	0.623143	0.589245
11	8	0	4.933077	-1.580170	0.735933
12	6	0	1.856491	-1.402176	0.612896
13	6	0	2.235461	-1.781958	2.022358
14	6	0	1.298590	-1.390570	2.905400
15	6	0	0.181895	-0.699578	2.231490
16	6	0	0.459953	-0.699679	0.730657
17	6	0	-0.449886	-1.610996	-0.066089
18	6	0	0.322203	-2.678595	-0.521678
19	8	0	1.649479	-2.617142	-0.186456
20	6	0	-1.810767	-1.544394	-0.382797
21	6	0	-2.355310	-2.577071	-1.163176
22	6	0	-1.569285	-3.642075	-1.606064
23	6	0	-0.203094	-3.710050	-1.285452
24	8	0	-2.135796	-4.625284	-2.364639
25	8	0	0.513099	-4.775450	-1.763150
26	8	0	-0.779311	-0.234696	2.826883
27	8	0	1.276596	-1.548384	4.238967
28	8	0	6.783404	1.692339	-2.262429
29	8	0	4.873942	5.055491	0.527903
30	6	0	-2.668465	-0.400528	0.101372
31	8	0	-3.416419	0.098351	-1.034286
32	6	0	-4.294254	1.126894	-0.780063
33	6	0	-4.763277	1.391789	0.515225
34	6	0	-4.328656	0.552472	1.697253
35	6	0	-3.665210	-0.748007	1.228245
36	6	0	-4.712649	1.859647	-1.894363
37	6	0	-5.623071	2.899054	-1.710684
38	6	0	-6.104902	3.210525	-0.433354
39	6	0	-5.671301	2.454524	0.658285
40	8	0	-6.111438	2.705233	1.927536
41	8	0	-6.008905	3.595975	-2.820462
42	8	0	-4.621589	-1.714704	0.801907
43	1	0	0.477004	0.333052	0.366224
44	1	0	6.529176	4.157698	-1.217841
45	1	0	3.191995	3.075817	1.294616
46	1	0	4.675071	-0.391722	-2.398948
47	1	0	6.084590	-0.662149	-1.388746
48	1	0	4.052729	-2.203483	-0.970836
49	1	0	2.424996	-0.309447	-1.134247
50	1	0	5.045824	-0.762087	1.242401
51	1	0	3.156903	-2.302183	2.241872
52	1	0	-3.402683	-2.564329	-1.434352
53	1	0	-1.448058	-5.275397	-2.577797
54	1	0	1.433096	-4.703013	-1.470440
55	1	0	0.452072	-1.135113	4.555189
56	1	0	7.361626	2.433346	-2.492211
57	1	0	4.176502	5.177260	1.187415
58	1	0	-2.023946	0.405194	0.472370
59	1	0	-5.187313	0.306181	2.329895
60	1	0	-3.623965	1.106852	2.330691
61	1	0	-3.119240	-1.208268	2.053852
62	1	0	-4.329197	1.623837	-2.879793
63	1	0	-6.806614	4.028532	-0.291378
64	1	0	-6.754447	3.427945	1.910620
65	1	0	-6.635596	4.287200	-2.564984
66	1	0	-5.102117	-1.335110	0.051819

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11C at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.834587	3.765533	0.111593
2	6	0	5.797735	3.421790	-0.844897
3	6	0	5.848504	2.108332	-1.317433
4	6	0	4.961892	1.118296	-0.860391
5	6	0	4.005488	1.514352	0.084171
6	6	0	3.927838	2.815997	0.581929
7	6	0	5.046970	-0.311323	-1.351209
8	6	0	4.235463	-1.254325	-0.451754
9	6	0	2.887003	-0.580160	-0.160470
10	8	0	3.102991	0.611792	0.609562
11	8	0	4.933630	-1.582156	0.749014
12	6	0	1.855251	-1.415662	0.616568
13	6	0	2.231931	-1.809789	2.022628
14	6	0	1.292449	-1.429552	2.907805
15	6	0	0.175993	-0.733088	2.238915
16	6	0	0.458983	-0.713773	0.739092
17	6	0	-0.448872	-1.612899	-0.073284
18	6	0	0.323091	-2.676449	-0.538492
19	8	0	1.648675	-2.622723	-0.195304
20	6	0	-1.807997	-1.539020	-0.395627
21	6	0	-2.351009	-2.559983	-1.192391
22	6	0	-1.565194	-3.620946	-1.645141
23	6	0	-0.200837	-3.696512	-1.318349
24	8	0	-2.130033	-4.592734	-2.419586
25	8	0	0.515245	-4.757353	-1.806286
26	8	0	-0.788319	-0.278095	2.836817
27	8	0	1.267540	-1.602516	4.239382
28	8	0	6.766043	1.711210	-2.247533
29	8	0	4.731173	5.029928	0.615503
30	6	0	-2.665560	-0.400211	0.100454
31	8	0	-3.401699	0.121174	-1.033176
32	6	0	-4.280983	1.145174	-0.767491
33	6	0	-4.761598	1.389126	0.525469
34	6	0	-4.337718	0.530896	1.697647
35	6	0	-3.672657	-0.763089	1.213387
36	6	0	-4.688672	1.899081	-1.874572
37	6	0	-5.599695	2.936049	-1.680905
38	6	0	-6.094395	3.224845	-0.403398
39	6	0	-5.671791	2.451583	0.677339
40	8	0	-6.122907	2.679894	1.947109
41	8	0	-6.044649	3.720804	-2.706712
42	8	0	-4.627447	-1.721133	0.764697
43	1	0	0.478789	0.323838	0.389002
44	1	0	6.497716	4.166175	-1.215789
45	1	0	3.173738	3.080445	1.313261
46	1	0	4.680113	-0.387441	-2.383279
47	1	0	6.087210	-0.650801	-1.367852
48	1	0	4.060281	-2.203478	-0.962338
49	1	0	2.426480	-0.310914	-1.121462
50	1	0	5.028743	-0.767557	1.264729
51	1	0	3.153558	-2.331146	2.238720
52	1	0	-3.397156	-2.541424	-1.467827
53	1	0	-1.442989	-5.242310	-2.636563
54	1	0	1.433431	-4.692052	-1.506295
55	1	0	0.442044	-1.193425	4.558499
56	1	0	7.338734	2.455987	-2.478748
57	1	0	5.404157	5.595503	0.211615
58	1	0	-2.021417	0.396707	0.490491
59	1	0	-5.201851	0.275915	2.319274
60	1	0	-3.637591	1.074301	2.345482
61	1	0	-3.133899	-1.237410	2.035786
62	1	0	-4.285473	1.668996	-2.855409
63	1	0	-6.796535	4.041879	-0.270972
64	1	0	-6.762584	3.405755	1.935921
65	1	0	-5.637000	3.427914	-3.533870
66	1	0	-5.107643	-1.325837	0.022578

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11D at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.831579	3.769034	0.109305
2	6	0	5.795521	3.425959	-0.846621
3	6	0	5.847396	2.112564	-1.319225
4	6	0	4.961156	1.121928	-0.862755
5	6	0	4.003952	1.517323	0.081267
6	6	0	3.925177	2.818897	0.579055
7	6	0	5.047326	-0.307623	-1.353588
8	6	0	4.236509	-1.251246	-0.454138
9	6	0	2.887329	-0.578395	-0.163258
10	8	0	3.101798	0.614233	0.606183
11	8	0	4.934811	-1.578313	0.746776
12	6	0	1.856483	-1.414292	0.614574
13	6	0	2.233554	-1.805774	2.021290
14	6	0	1.294147	-1.424186	2.905939
15	6	0	0.177368	-0.729309	2.235982
16	6	0	0.459420	-0.713719	0.735957
17	6	0	-0.447813	-1.616485	-0.073137
18	6	0	0.325387	-2.679984	-0.536383
19	8	0	1.651385	-2.622858	-0.195265
20	6	0	-1.807372	-1.545573	-0.394379
21	6	0	-2.349674	-2.569834	-1.187334
22	6	0	-1.562654	-3.630854	-1.637923
23	6	0	-0.197768	-3.703170	-1.312659
24	8	0	-2.126849	-4.605811	-2.408825
25	8	0	0.519514	-4.764221	-1.798420
26	8	0	-0.786531	-0.272810	2.833430
27	8	0	1.269597	-1.594459	4.237893
28	8	0	6.765771	1.716106	-2.248783
29	8	0	4.727119	5.033328	0.613292
30	6	0	-2.665747	-0.405761	0.098088
31	8	0	-3.407337	0.106935	-1.035669
32	6	0	-4.282674	1.135865	-0.774231
33	6	0	-4.757675	1.387225	0.521558
34	6	0	-4.332116	0.532840	1.696058
35	6	0	-3.668868	-0.763744	1.215997
36	6	0	-4.692097	1.883442	-1.881994
37	6	0	-5.599189	2.924395	-1.690783
38	6	0	-6.086871	3.222466	-0.412490
39	6	0	-5.662187	2.451866	0.672441
40	8	0	-6.108103	2.689209	1.942245
41	8	0	-5.975962	3.636344	-2.794148
42	8	0	-4.624850	-1.723832	0.774207
43	1	0	0.477542	0.322886	0.382820
44	1	0	6.495257	4.170808	-1.217037
45	1	0	3.170458	3.082816	1.309940
46	1	0	4.680550	-0.384021	-2.385663
47	1	0	6.087823	-0.646314	-1.370190
48	1	0	4.062297	-2.200636	-0.964624
49	1	0	2.426541	-0.310243	-1.124420
50	1	0	5.029969	-0.763407	1.261991
51	1	0	3.155446	-2.326350	2.238127
52	1	0	-3.395966	-2.553488	-1.462419
53	1	0	-1.438682	-5.254150	-2.625940
54	1	0	1.438612	-4.694905	-1.502153
55	1	0	0.444017	-1.184967	4.556284
56	1	0	7.337813	2.461402	-2.479937
57	1	0	5.399737	5.599425	0.209532
58	1	0	-2.021766	0.394699	0.481174
59	1	0	-5.195056	0.281263	2.320757
60	1	0	-3.629849	1.078068	2.340048
61	1	0	-3.128039	-1.234128	2.039274
62	1	0	-4.304039	1.657992	-2.868046
63	1	0	-6.786013	4.041658	-0.264718
64	1	0	-6.747467	3.415258	1.930818
65	1	0	-6.599948	4.328086	-2.533488
66	1	0	-5.099729	-1.335701	0.024896

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11E at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.089273	-3.693678	-0.028218
2	6	0	-6.049152	-3.276272	-0.958079
3	6	0	-6.046611	-1.949505	-1.386916
4	6	0	-5.107310	-1.013978	-0.914136
5	6	0	-4.158088	-1.480786	0.001804
6	6	0	-4.133248	-2.802299	0.457704
7	6	0	-5.134005	0.432568	-1.359157
8	6	0	-4.278907	1.309958	-0.434720
9	6	0	-2.955245	0.574289	-0.179830
10	8	0	-3.207511	-0.639626	0.543253
11	8	0	-4.955300	1.623357	0.782038
12	6	0	-1.889916	1.339797	0.624298
13	6	0	-2.250637	1.693695	2.045089
14	6	0	-1.341711	1.217864	2.915688
15	6	0	-0.262178	0.491550	2.219379
16	6	0	-0.521476	0.579081	0.717950
17	6	0	0.426176	1.490563	-0.036037
18	6	0	-0.309709	2.593277	-0.469299
19	8	0	-1.638126	2.567177	-0.141673
20	6	0	1.782508	1.387158	-0.361949
21	6	0	2.357765	2.417730	-1.127233
22	6	0	1.606154	3.519346	-1.543935
23	6	0	0.247050	3.627107	-1.208492
24	8	0	2.199489	4.492712	-2.291270
25	8	0	-0.436671	4.724297	-1.658677
26	8	0	0.658707	-0.063963	2.800438
27	8	0	-1.320138	1.321081	4.254436
28	8	0	-6.959301	-1.479656	-2.287573
29	8	0	-5.134961	-5.000953	0.361727
30	6	0	2.631696	0.229157	0.111324
31	8	0	3.421919	-0.204519	-1.013271
32	6	0	4.437803	-1.092688	-0.775203
33	6	0	4.907832	-1.365276	0.514226
34	6	0	4.327542	-0.666479	1.720654
35	6	0	3.541086	0.577300	1.313811
36	6	0	4.988520	-1.695617	-1.913599
37	6	0	6.034628	-2.602724	-1.755963
38	6	0	6.525636	-2.914174	-0.482829
39	6	0	5.958870	-2.291740	0.629658
40	8	0	6.400656	-2.547793	1.898977
41	8	0	6.621406	-3.234381	-2.817184
42	8	0	4.481016	1.598428	0.992016
43	1	0	-0.571257	-0.433059	0.302075
44	1	0	-6.780454	-3.986590	-1.330738
45	1	0	-3.374672	-3.109963	1.169807
46	1	0	-4.769666	0.526438	-2.390598
47	1	0	-6.158888	0.816041	-1.358019
48	1	0	-4.069382	2.268828	-0.913307
49	1	0	-2.510134	0.328348	-1.154166
50	1	0	-5.095340	0.794314	1.263237
51	1	0	-3.144485	2.253273	2.281089
52	1	0	3.392078	2.351290	-1.442522
53	1	0	1.532005	5.166816	-2.494827
54	1	0	-1.359869	4.670664	-1.371854
55	1	0	-0.523523	0.848293	4.558494
56	1	0	-7.572664	-2.188962	-2.525779
57	1	0	-4.432839	-5.168492	1.006135
58	1	0	1.983446	-0.598155	0.427679
59	1	0	5.122691	-0.370332	2.411641
60	1	0	3.662869	-1.335966	2.281574
61	1	0	2.893908	0.888344	2.141844
62	1	0	4.588673	-1.452043	-2.892646
63	1	0	7.335505	-3.629113	-0.376994
64	1	0	7.145331	-3.164148	1.860397
65	1	0	6.201716	-2.936905	-3.636616
66	1	0	3.980666	2.400470	0.782260

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11F at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.844619	3.760873	0.076752
2	6	0	5.817035	3.403704	-0.865332
3	6	0	5.869079	2.084815	-1.322371
4	6	0	4.973799	1.102803	-0.864916
5	6	0	4.008660	1.512051	0.064974
6	6	0	3.929913	2.819301	0.547695
7	6	0	5.058637	-0.332003	-1.340234
8	6	0	4.236396	-1.263250	-0.438442
9	6	0	2.887082	-0.582935	-0.166086
10	8	0	3.097976	0.618188	0.590830
11	8	0	4.923472	-1.581306	0.771337
12	6	0	1.848060	-1.406839	0.613775
13	6	0	2.215204	-1.784448	2.026962
14	6	0	1.275746	-1.383126	2.902847
15	6	0	0.167452	-0.688542	2.219226
16	6	0	0.453125	-0.699359	0.719978
17	6	0	-0.455097	-1.613644	-0.075245
18	6	0	0.317152	-2.683749	-0.524421
19	8	0	1.643111	-2.622856	-0.184531
20	6	0	-1.814986	-1.547148	-0.396116
21	6	0	-2.358789	-2.581799	-1.174079
22	6	0	-1.572251	-3.648811	-1.611534
23	6	0	-0.207177	-3.717323	-1.286158
24	8	0	-2.137484	-4.633492	-2.368726
25	8	0	0.508938	-4.785199	-1.757816
26	8	0	-0.794210	-0.214058	2.806535
27	8	0	1.245437	-1.535047	4.236901
28	8	0	6.796174	1.674313	-2.237025
29	8	0	4.739703	5.031055	0.565584
30	6	0	-2.671492	-0.401834	0.086020
31	8	0	-3.441676	0.080897	-1.040421
32	6	0	-4.303157	1.123553	-0.782720
33	6	0	-4.748065	1.407605	0.519622
34	6	0	-4.304476	0.564622	1.698809
35	6	0	-3.652968	-0.743737	1.226792
36	6	0	-4.730241	1.848690	-1.896005
37	6	0	-5.625674	2.902709	-1.708142
38	6	0	-6.078765	3.235505	-0.428632
39	6	0	-5.635985	2.488594	0.665251
40	8	0	-6.121379	2.860587	1.887428
41	8	0	-6.020867	3.590390	-2.820164
42	8	0	-4.618379	-1.705420	0.817039
43	1	0	0.474563	0.330773	0.348491
44	1	0	6.522885	4.141990	-1.237337
45	1	0	3.168975	3.094015	1.268077
46	1	0	4.700776	-0.417574	-2.374707
47	1	0	6.097857	-0.674902	-1.344162
48	1	0	4.062834	-2.217058	-0.940899
49	1	0	2.434427	-0.325314	-1.133961
50	1	0	5.022590	-0.761176	1.277424
51	1	0	3.131929	-2.309498	2.254535
52	1	0	-3.404839	-2.568866	-1.450678
53	1	0	-1.449812	-5.284763	-2.578610
54	1	0	1.428424	-4.712676	-1.463481
55	1	0	0.422202	-1.114904	4.547217
56	1	0	7.376959	2.413388	-2.466273
57	1	0	5.419341	5.589918	0.163487
58	1	0	-2.026331	0.410939	0.439883
59	1	0	-5.155507	0.297286	2.338493
60	1	0	-3.585252	1.106736	2.327752
61	1	0	-3.100812	-1.199299	2.050347
62	1	0	-4.365440	1.597502	-2.884680
63	1	0	-6.764544	4.061212	-0.267116
64	1	0	-5.727699	2.314240	2.581175
65	1	0	-6.633082	4.293376	-2.561387
66	1	0	-5.074001	-1.347448	0.041004

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11G at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.883448	3.751198	0.061109
2	6	0	5.854775	3.383816	-0.877941
3	6	0	5.894221	2.066829	-1.334131
4	6	0	4.986744	1.091884	-0.878978
5	6	0	4.023965	1.509394	0.046596
6	6	0	3.957041	2.819964	0.529266
7	6	0	5.060063	-0.344063	-1.352372
8	6	0	4.233587	-1.266707	-0.445950
9	6	0	2.887319	-0.578942	-0.176426
10	8	0	3.101703	0.627487	0.571353
11	8	0	4.920124	-1.583182	0.764516
12	6	0	1.846926	-1.393955	0.611046
13	6	0	2.214271	-1.758083	2.027793
14	6	0	1.277396	-1.344032	2.900503
15	6	0	0.170679	-0.653128	2.210834
16	6	0	0.452767	-0.683801	0.711234
17	6	0	-0.458167	-1.608445	-0.069075
18	6	0	0.313025	-2.683247	-0.508729
19	8	0	1.640361	-2.617174	-0.175360
20	6	0	-1.819542	-1.547102	-0.384777
21	6	0	-2.365742	-2.591610	-1.147750
22	6	0	-1.580237	-3.663354	-1.575389
23	6	0	-0.213718	-3.726717	-1.255140
24	8	0	-2.147972	-4.657953	-2.317556
25	8	0	0.501218	-4.799735	-1.716766
26	8	0	-0.787675	-0.167261	2.794359
27	8	0	1.248593	-1.480884	4.236260
28	8	0	6.819482	1.645324	-2.245826
29	8	0	4.888528	5.051204	0.477290
30	6	0	-2.675351	-0.397433	0.088111
31	8	0	-3.452210	0.070894	-1.039706
32	6	0	-4.315024	1.114240	-0.789452
33	6	0	-4.753687	1.412470	0.511863
34	6	0	-4.301227	0.584800	1.698524
35	6	0	-3.650042	-0.727780	1.238100
36	6	0	-4.750020	1.825170	-1.908820
37	6	0	-5.647443	2.878827	-1.728566
38	6	0	-6.094930	3.225154	-0.450665
39	6	0	-5.644254	2.492330	0.649487
40	8	0	-6.124460	2.877044	1.869772
41	8	0	-6.050372	3.552358	-2.846432
42	8	0	-4.616144	-1.695586	0.844741
43	1	0	0.473354	0.341116	0.325484
44	1	0	6.561893	4.125048	-1.236590
45	1	0	3.189080	3.088277	1.247216
46	1	0	4.699183	-0.429302	-2.385786
47	1	0	6.096810	-0.694214	-1.357887
48	1	0	4.054298	-2.221886	-0.943717
49	1	0	2.434555	-0.326958	-1.145711
50	1	0	5.037024	-0.759457	1.260790
51	1	0	3.129660	-2.283567	2.259641
52	1	0	-3.413053	-2.583096	-1.419740
53	1	0	-1.461060	-5.312141	-2.520795
54	1	0	1.420218	-4.726857	-1.421015
55	1	0	0.426921	-1.055085	4.542972
56	1	0	7.407288	2.379453	-2.473256
57	1	0	4.183383	5.183752	1.126475
58	1	0	-2.029750	0.420458	0.429098
59	1	0	-5.147829	0.323388	2.346478
60	1	0	-3.579308	1.135831	2.316526
61	1	0	-3.092647	-1.173003	2.063787
62	1	0	-4.389818	1.563352	-2.896424
63	1	0	-6.782625	4.050426	-0.295242
64	1	0	-5.727548	2.338132	2.567497
65	1	0	-6.663063	4.256764	-2.592673
66	1	0	-5.077442	-1.346788	0.067874

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11H at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.078435	-3.694421	-0.019510
2	6	0	-6.040489	-3.278730	-0.948107
3	6	0	-6.042721	-1.949063	-1.375800
4	6	0	-5.106855	-1.013482	-0.902850
5	6	0	-4.154693	-1.480163	0.013245
6	6	0	-4.125256	-2.799870	0.466888
7	6	0	-5.136970	0.433184	-1.347460
8	6	0	-4.280362	1.312176	-0.425996
9	6	0	-2.956083	0.577097	-0.173025
10	8	0	-3.207536	-0.634212	0.554329
11	8	0	-4.954085	1.626254	0.792094
12	6	0	-1.888321	1.345157	0.625396
13	6	0	-2.245633	1.706941	2.045035
14	6	0	-1.335313	1.234841	2.916199
15	6	0	-0.257850	0.503969	2.221388
16	6	0	-0.520435	0.583643	0.720088
17	6	0	0.426385	1.489983	-0.041194
18	6	0	-0.309484	2.590873	-0.479118
19	8	0	-1.636963	2.568400	-0.147568
20	6	0	1.781854	1.383462	-0.369775
21	6	0	2.356062	2.408729	-1.142961
22	6	0	1.604292	3.508231	-1.564906
23	6	0	0.246240	3.619405	-1.226443
24	8	0	2.196456	4.476175	-2.320209
25	8	0	-0.437797	4.714364	-1.681654
26	8	0	0.663958	-0.048988	2.803371
27	8	0	-1.310665	1.345268	4.254294
28	8	0	-6.957919	-1.482233	-2.275270
29	8	0	-5.021367	-4.978184	0.440875
30	6	0	2.631578	0.228280	0.109412
31	8	0	3.420466	-0.212311	-1.013428
32	6	0	4.436863	-1.098727	-0.771062
33	6	0	4.908523	-1.363158	0.519475
34	6	0	4.329559	-0.656953	1.722208
35	6	0	3.542521	0.584169	1.308476
36	6	0	4.986378	-1.708604	-1.906339
37	6	0	6.032954	-2.614387	-1.744311
38	6	0	6.525552	-2.917790	-0.469856
39	6	0	5.959791	-2.288787	0.639438
40	8	0	6.402923	-2.537116	1.909824
41	8	0	6.618714	-3.252430	-2.802292
42	8	0	4.481916	1.603259	0.978752
43	1	0	-0.572242	-0.430712	0.309922
44	1	0	-6.777173	-3.980000	-1.331817
45	1	0	-3.372678	-3.119710	1.177380
46	1	0	-4.775442	0.527368	-2.379891
47	1	0	-6.162360	0.815309	-1.343711
48	1	0	-4.072821	2.270647	-0.906258
49	1	0	-2.513537	0.328335	-1.147831
50	1	0	-5.084300	0.798500	1.278302
51	1	0	-3.138424	2.268612	2.280069
52	1	0	3.389533	2.339395	-1.460367
53	1	0	1.528829	5.149188	-2.526863
54	1	0	-1.360962	4.661682	-1.394539
55	1	0	-0.514167	0.872806	4.559178
56	1	0	-7.570801	-2.191851	-2.513510
57	1	0	-5.724226	-5.501144	0.030341
58	1	0	1.983765	-0.597061	0.431704
59	1	0	5.125484	-0.356457	2.410431
60	1	0	3.665553	-1.322971	2.288016
61	1	0	2.896501	0.900520	2.135395
62	1	0	4.585199	-1.471331	-2.886394
63	1	0	7.335814	-3.631755	-0.360551
64	1	0	7.146638	-3.154820	1.874317
65	1	0	6.197986	-2.960138	-3.623058
66	1	0	3.981108	2.403596	0.763592

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11I at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.880798	3.750305	0.067583
2	6	0	5.849511	3.384784	-0.874891
3	6	0	5.888627	2.068379	-1.332751
4	6	0	4.983513	1.092115	-0.875738
5	6	0	4.023128	1.507826	0.053131
6	6	0	3.956544	2.817782	0.537473
7	6	0	5.056973	-0.343289	-1.350768
8	6	0	4.232221	-1.267457	-0.444308
9	6	0	2.886537	-0.579929	-0.171178
10	8	0	3.102988	0.624411	0.579372
11	8	0	4.920750	-1.585636	0.764566
12	6	0	1.846852	-1.396913	0.615106
13	6	0	2.215473	-1.766187	2.030142
14	6	0	1.277719	-1.358308	2.904840
15	6	0	0.169308	-0.666714	2.218465
16	6	0	0.452874	-0.687108	0.718923
17	6	0	-0.457648	-1.605245	-0.069281
18	6	0	0.312805	-2.678803	-0.513305
19	8	0	1.639235	-2.617433	-0.175535
20	6	0	-1.818088	-1.539689	-0.388001
21	6	0	-2.363988	-2.578326	-1.159237
22	6	0	-1.579226	-3.648734	-1.591439
23	6	0	-0.213728	-3.716588	-1.267739
24	8	0	-2.146628	-4.637601	-2.341505
25	8	0	0.500594	-4.787936	-1.734115
26	8	0	-0.791086	-0.187491	2.804059
27	8	0	1.249121	-1.501829	4.239869
28	8	0	6.811263	1.648730	-2.247956
29	8	0	4.886105	5.049852	0.485142
30	6	0	-2.673864	-0.392482	0.090840
31	8	0	-3.441727	0.089419	-1.037761
32	6	0	-4.309710	1.126447	-0.781454
33	6	0	-4.758629	1.411656	0.517010
34	6	0	-4.311009	0.575595	1.699503
35	6	0	-3.656074	-0.732405	1.231731
36	6	0	-4.739739	1.847938	-1.898850
37	6	0	-5.642435	2.896353	-1.714935
38	6	0	-6.101470	3.228140	-0.437265
39	6	0	-5.656087	2.488327	0.657538
40	8	0	-6.145003	2.857851	1.879263
41	8	0	-6.107144	3.649072	-2.755688
42	8	0	-4.619503	-1.697337	0.825088
43	1	0	0.474813	0.340656	0.340888
44	1	0	6.554914	4.127020	-1.234844
45	1	0	3.190450	3.084681	1.257939
46	1	0	4.694723	-0.427549	-2.383789
47	1	0	6.093914	-0.692867	-1.358118
48	1	0	4.052167	-2.221870	-0.943241
49	1	0	2.432556	-0.325050	-1.139148
50	1	0	5.036092	-0.762929	1.262904
51	1	0	3.131959	-2.290869	2.259490
52	1	0	-3.410746	-2.566555	-1.433097
53	1	0	-1.460585	-5.292346	-2.545886
54	1	0	1.418454	-4.719553	-1.433770
55	1	0	0.426492	-1.079379	4.548661
56	1	0	7.397173	2.383853	-2.477079
57	1	0	4.183153	5.181059	1.136972
58	1	0	-2.028629	0.420445	0.444090
59	1	0	-5.160592	0.307567	2.340813
60	1	0	-3.593519	1.123006	2.325798
61	1	0	-3.103037	-1.184403	2.056694
62	1	0	-4.360679	1.585722	-2.881246
63	1	0	-6.793566	4.049854	-0.295886
64	1	0	-5.749151	2.313947	2.573597
65	1	0	-5.721001	3.326343	-3.581994
66	1	0	-5.084181	-1.338202	0.055014

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11J at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.842905	3.759845	0.081454
2	6	0	5.813585	3.403570	-0.862760
3	6	0	5.865604	2.084831	-1.320213
4	6	0	4.972065	1.102064	-0.861001
5	6	0	4.008518	1.510435	0.070928
6	6	0	3.929831	2.817510	0.554085
7	6	0	5.057162	-0.332573	-1.336829
8	6	0	4.235724	-1.264501	-0.434994
9	6	0	2.886888	-0.584003	-0.160579
10	8	0	3.099409	0.615642	0.598218
11	8	0	4.923825	-1.583559	0.773921
12	6	0	1.847944	-1.409141	0.617995
13	6	0	2.215551	-1.791261	2.029808
14	6	0	1.275080	-1.395086	2.906976
15	6	0	0.165745	-0.699714	2.225736
16	6	0	0.453289	-0.701677	0.726782
17	6	0	-0.454417	-1.609865	-0.075805
18	6	0	0.317173	-2.678895	-0.528718
19	8	0	1.642086	-2.622777	-0.184052
20	6	0	-1.813270	-1.539186	-0.400011
21	6	0	-2.356548	-2.568056	-1.186050
22	6	0	-1.570677	-3.633883	-1.627433
23	6	0	-0.206781	-3.706954	-1.298129
24	8	0	-2.135351	-4.612961	-2.392306
25	8	0	0.508817	-4.773327	-1.773944
26	8	0	-0.797793	-0.230755	2.814363
27	8	0	1.244375	-1.552748	4.240322
28	8	0	6.790963	1.675206	-2.237017
29	8	0	4.738064	5.029852	0.570712
30	6	0	-2.670045	-0.396608	0.088074
31	8	0	-3.431704	0.099385	-1.038700
32	6	0	-4.298861	1.135220	-0.774778
33	6	0	-4.754078	1.405881	0.524592
34	6	0	-4.314370	0.554916	1.699382
35	6	0	-3.658504	-0.748425	1.219940
36	6	0	-4.721453	1.870841	-1.885776
37	6	0	-5.622718	2.919109	-1.694109
38	6	0	-6.087682	3.236755	-0.415004
39	6	0	-5.649685	2.482997	0.673261
40	8	0	-6.144124	2.839233	1.896711
41	8	0	-6.080244	3.685264	-2.728244
42	8	0	-4.620772	-1.707647	0.797406
43	1	0	0.476311	0.330847	0.362076
44	1	0	6.518136	4.142433	-1.236088
45	1	0	3.170167	3.091549	1.276070
46	1	0	4.698746	-0.417842	-2.371138
47	1	0	6.096505	-0.675109	-1.341478
48	1	0	4.061588	-2.217861	-0.938078
49	1	0	2.433743	-0.324281	-1.127672
50	1	0	5.021693	-0.764119	1.281382
51	1	0	3.133048	-2.315748	2.255584
52	1	0	-3.401946	-2.551825	-1.464796
53	1	0	-1.448605	-5.265120	-2.602465
54	1	0	1.426650	-4.706241	-1.473223
55	1	0	0.420352	-1.135210	4.552084
56	1	0	7.370477	2.414841	-2.467674
57	1	0	5.416593	5.589244	0.167479
58	1	0	-2.025525	0.411280	0.453998
59	1	0	-5.167919	0.280546	2.332693
60	1	0	-3.599676	1.093786	2.336201
61	1	0	-3.110203	-1.210380	2.042529
62	1	0	-4.337800	1.619515	-2.869231
63	1	0	-6.778421	4.058524	-0.267418
64	1	0	-5.751717	2.287589	2.586864
65	1	0	-5.690017	3.371943	-3.556258
66	1	0	-5.080435	-1.339702	0.028495

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11K at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.089326	-3.696808	-0.034505
2	6	0	-6.051166	-3.277857	-0.961635
3	6	0	-6.050037	-1.950183	-1.387651
4	6	0	-5.110227	-1.015248	-0.914701
5	6	0	-4.159105	-1.483541	-0.001493
6	6	0	-4.132824	-2.806024	0.451539
7	6	0	-5.138247	0.432155	-1.356758
8	6	0	-4.282104	1.308111	-0.431938
9	6	0	-2.957649	0.572648	-0.180569
10	8	0	-3.207977	-0.643129	0.540064
11	8	0	-4.956825	1.618952	0.786410
12	6	0	-1.891712	1.336951	0.623969
13	6	0	-2.251053	1.686861	2.046126
14	6	0	-1.341637	1.208026	2.914527
15	6	0	-0.262882	0.483574	2.215090
16	6	0	-0.522717	0.576763	0.714105
17	6	0	0.423910	1.491888	-0.036838
18	6	0	-0.313290	2.595053	-0.466692
19	8	0	-1.641689	2.566361	-0.139101
20	6	0	1.780332	1.391067	-0.363301
21	6	0	2.354314	2.424635	-1.125455
22	6	0	1.601373	3.526690	-1.538647
23	6	0	0.242204	3.631863	-1.202648
24	8	0	2.193483	4.503108	-2.282946
25	8	0	-0.442831	4.729729	-1.649208
26	8	0	0.657820	-0.074649	2.793876
27	8	0	-1.319028	1.306808	4.253624
28	8	0	-6.964689	-1.478836	-2.285527
29	8	0	-5.133689	-5.004931	0.352778
30	6	0	2.631016	0.232897	0.106949
31	8	0	3.423922	-0.195280	-1.017463
32	6	0	4.439971	-1.084357	-0.782051
33	6	0	4.907245	-1.360438	0.509865
34	6	0	4.323773	-0.665516	1.717034
35	6	0	3.537703	0.578949	1.312062
36	6	0	4.992942	-1.681894	-1.919538
37	6	0	6.038910	-2.589410	-1.762838
38	6	0	6.526675	-2.905388	-0.489306
39	6	0	5.956866	-2.285277	0.625748
40	8	0	6.396843	-2.545951	1.894641
41	8	0	6.551838	-3.155882	-2.896733
42	8	0	4.477700	1.601306	0.994572
43	1	0	-0.571822	-0.433765	0.294233
44	1	0	-6.782862	-3.987715	-1.334392
45	1	0	-3.372744	-3.114863	1.161531
46	1	0	-4.775563	0.528260	-2.388581
47	1	0	-6.163298	0.815186	-1.353292
48	1	0	-4.073761	2.267992	-0.909014
49	1	0	-2.513768	0.329282	-1.156100
50	1	0	-5.096967	0.788857	1.265759
51	1	0	-3.144629	2.245862	2.284509
52	1	0	3.388576	2.360127	-1.441352
53	1	0	1.524969	5.176636	-2.485042
54	1	0	-1.366176	4.673573	-1.363346
55	1	0	-0.522348	0.832665	4.555421
56	1	0	-7.578209	-2.187913	-2.524016
57	1	0	-4.430039	-5.173557	0.995230
58	1	0	1.983600	-0.596468	0.419757
59	1	0	5.117068	-0.371459	2.411057
60	1	0	3.657670	-1.336848	2.274048
61	1	0	2.888925	0.887538	2.139752
62	1	0	4.607540	-1.443569	-2.903743
63	1	0	7.336400	-3.620485	-0.367663
64	1	0	7.144490	-3.158646	1.856664
65	1	0	7.267120	-3.761669	-2.657607
66	1	0	3.977267	2.402998	0.783594

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11L at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.078349	-3.697536	-0.025617
2	6	0	-6.042039	-3.280558	-0.951929
3	6	0	-6.045579	-1.950085	-1.377101
4	6	0	-5.109394	-1.014963	-0.903873
5	6	0	-4.155614	-1.482901	0.009892
6	6	0	-4.124864	-2.803450	0.461014
7	6	0	-5.140750	0.432489	-1.345826
8	6	0	-4.283327	1.310247	-0.423940
9	6	0	-2.958340	0.575449	-0.173990
10	8	0	-3.208077	-0.637552	0.551153
11	8	0	-4.955689	1.622013	0.795515
12	6	0	-1.890178	1.342383	0.625010
13	6	0	-2.246318	1.700208	2.045969
14	6	0	-1.335557	1.225208	2.915070
15	6	0	-0.258774	0.496189	2.217304
16	6	0	-0.521720	0.581428	0.716382
17	6	0	0.424169	1.491457	-0.041780
18	6	0	-0.312952	2.592855	-0.476273
19	8	0	-1.640477	2.567726	-0.144995
20	6	0	1.779770	1.387557	-0.370758
21	6	0	2.352858	2.415987	-1.140511
22	6	0	1.599817	3.515995	-1.558932
23	6	0	0.241629	3.624486	-1.220174
24	8	0	2.190906	4.487141	-2.310951
25	8	0	-0.443660	4.720213	-1.671718
26	8	0	0.662791	-0.059442	2.797160
27	8	0	-1.310050	1.331305	4.253522
28	8	0	-6.962461	-1.481991	-2.274198
29	8	0	-5.020005	-4.982146	0.432271
30	6	0	2.630848	0.231969	0.105108
31	8	0	3.422811	-0.202407	-1.017587
32	6	0	4.439129	-1.090078	-0.778076
33	6	0	4.907433	-1.358954	0.514988
34	6	0	4.325102	-0.657118	1.718715
35	6	0	3.538702	0.585012	1.307283
36	6	0	4.991311	-1.693831	-1.912660
37	6	0	6.037417	-2.600442	-1.751719
38	6	0	6.525985	-2.909554	-0.476814
39	6	0	5.956904	-2.283404	0.635236
40	8	0	6.397576	-2.537312	1.905257
41	8	0	6.549684	-3.172977	-2.882887
42	8	0	4.478365	1.605486	0.982679
43	1	0	-0.572787	-0.431350	0.302238
44	1	0	-6.778934	-3.981488	-1.335845
45	1	0	-3.371022	-3.124270	1.169721
46	1	0	-4.780648	0.528687	-2.378567
47	1	0	-6.166305	0.814147	-1.340024
48	1	0	-4.076839	2.269639	-0.902821
49	1	0	-2.516764	0.329032	-1.149819
50	1	0	-5.085655	0.793341	1.280217
51	1	0	-3.138874	2.261288	2.283286
52	1	0	3.386327	2.348625	-1.458388
53	1	0	1.522249	5.159532	-2.516289
54	1	0	-1.367177	4.664589	-1.386305
55	1	0	-0.513512	0.857561	4.556315
56	1	0	-7.575349	-2.191473	-2.512832
57	1	0	-5.723171	-5.504660	0.021696
58	1	0	1.983760	-0.595647	0.423162
59	1	0	5.119070	-0.359130	2.410290
60	1	0	3.659464	-1.325202	2.280152
61	1	0	2.890871	0.898527	2.133847
62	1	0	4.605192	-1.460940	-2.897885
63	1	0	7.335647	-3.624137	-0.351765
64	1	0	7.143860	-3.151846	1.870307
65	1	0	7.265402	-3.777129	-2.640959
66	1	0	3.977576	2.405578	0.766491

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11M at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.475107	3.488677	0.085075
2	6	0	5.446212	3.106212	-0.848167
3	6	0	5.490387	1.780157	-1.276912
4	6	0	4.587263	0.811266	-0.800758
5	6	0	3.624350	1.243513	0.117998
6	6	0	3.553124	2.563566	0.573640
7	6	0	4.665843	-0.633718	-1.244726
8	6	0	3.846646	-1.541020	-0.316732
9	6	0	2.497431	-0.854850	-0.057695
10	8	0	2.706670	0.369173	0.662531
11	8	0	4.539269	-1.829550	0.897416
12	6	0	1.464021	-1.658130	0.750314
13	6	0	1.834348	-1.988238	2.173920
14	6	0	0.876476	-1.595172	3.032646
15	6	0	-0.245028	-0.945076	2.326223
16	6	0	0.061825	-0.960181	0.829350
17	6	0	-0.825634	-1.884504	0.021650
18	6	0	-0.048481	-2.968087	-0.375924
19	8	0	1.268217	-2.905381	-0.004128
20	6	0	-2.174858	-1.811222	-0.348058
21	6	0	-2.704316	-2.867451	-1.104881
22	6	0	-1.917641	-3.964709	-1.468412
23	6	0	-0.562926	-4.029548	-1.109311
24	8	0	-2.475750	-4.974655	-2.197564
25	8	0	0.156840	-5.120469	-1.516060
26	8	0	-1.225757	-0.497061	2.902656
27	8	0	0.835795	-1.720374	4.369075
28	8	0	6.416468	1.343434	-2.180619
29	8	0	4.475618	4.796848	0.475014
30	6	0	-2.989606	-0.598527	0.046721
31	8	0	-2.598147	0.482059	-0.855078
32	6	0	-3.175262	1.705786	-0.586287
33	6	0	-4.377918	1.802454	0.123384
34	6	0	-5.105088	0.570522	0.617344
35	6	0	-4.519502	-0.705841	-0.003680
36	6	0	-2.509446	2.824977	-1.097817
37	6	0	-3.060782	4.087456	-0.882579
38	6	0	-4.252343	4.233476	-0.162549
39	6	0	-4.892483	3.095726	0.328367
40	8	0	-6.062421	3.173828	1.030629
41	8	0	-2.473702	5.231841	-1.343405
42	8	0	-4.987567	-0.893749	-1.341063
43	1	0	0.078132	0.067268	0.451862
44	1	0	6.149866	3.842636	-1.223220
45	1	0	2.785388	2.843565	1.287371
46	1	0	4.302107	-0.742056	-2.274987
47	1	0	5.704209	-0.979097	-1.246498
48	1	0	3.670319	-2.507168	-0.793888
49	1	0	2.041077	-0.626514	-1.031207
50	1	0	4.661322	-0.994592	1.373218
51	1	0	2.762962	-2.483691	2.418824
52	1	0	-3.734479	-2.838390	-1.436409
53	1	0	-1.790807	-5.641197	-2.363833
54	1	0	1.065735	-5.047856	-1.190241
55	1	0	-0.002831	-1.316935	4.660509
56	1	0	7.004038	2.073836	-2.420242
57	1	0	3.773435	4.938603	1.125487
58	1	0	-2.705541	-0.299465	1.061638
59	1	0	-6.169038	0.626281	0.365606
60	1	0	-5.048873	0.502155	1.712076
61	1	0	-4.849306	-1.580809	0.564070
62	1	0	-1.580208	2.692876	-1.642424
63	1	0	-4.661999	5.224815	0.003187
64	1	0	-6.340943	4.098567	1.089815
65	1	0	-1.665304	5.006119	-1.824776
66	1	0	-4.423845	-0.351599	-1.914017

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11N at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.424827	3.506525	0.064316
2	6	0	5.403880	3.126388	-0.861720
3	6	0	5.468717	1.793431	-1.274065
4	6	0	4.578652	0.820191	-0.788738
5	6	0	3.607042	1.251642	0.124338
6	6	0	3.516278	2.573504	0.563397
7	6	0	4.675205	-0.628006	-1.218758
8	6	0	3.856529	-1.536739	-0.291489
9	6	0	2.501832	-0.857856	-0.042706
10	8	0	2.701931	0.368124	0.676360
11	8	0	4.543860	-1.815203	0.928109
12	6	0	1.467156	-1.665132	0.759630
13	6	0	1.832323	-1.999093	2.183656
14	6	0	0.869410	-1.612097	3.039463
15	6	0	-0.251118	-0.963087	2.330322
16	6	0	0.063330	-0.970247	0.834993
17	6	0	-0.818107	-1.891646	0.017663
18	6	0	-0.037312	-2.972340	-0.380646
19	8	0	1.276811	-2.910572	0.000471
20	6	0	-2.165030	-1.817737	-0.360068
21	6	0	-2.688553	-2.870249	-1.126130
22	6	0	-1.898334	-3.964568	-1.490893
23	6	0	-0.545923	-4.030134	-1.123345
24	8	0	-2.450638	-4.970824	-2.229591
25	8	0	0.177779	-5.117833	-1.531855
26	8	0	-1.236412	-0.521722	2.904052
27	8	0	0.822827	-1.742563	4.375204
28	8	0	6.403700	1.360000	-2.170024
29	8	0	4.307741	4.791626	0.509601
30	6	0	-2.983607	-0.608242	0.037023
31	8	0	-2.583434	0.479501	-0.851730
32	6	0	-3.160994	1.702249	-0.577953
33	6	0	-4.372942	1.791886	0.120854
34	6	0	-5.104703	0.555434	0.596549
35	6	0	-4.512825	-0.715295	-0.029908
36	6	0	-2.490317	2.823901	-1.070964
37	6	0	-3.043518	4.084803	-0.850841
38	6	0	-4.242925	4.224905	-0.142386
39	6	0	-4.889441	3.081016	0.332517
40	8	0	-6.066395	3.154200	1.023292
41	8	0	-2.361975	5.161497	-1.343563
42	8	0	-4.966693	-0.890776	-1.373842
43	1	0	0.079901	0.059192	0.463012
44	1	0	6.104454	3.857955	-1.256267
45	1	0	2.750357	2.865630	1.271551
46	1	0	4.321451	-0.747989	-2.251255
47	1	0	5.716778	-0.963613	-1.209056
48	1	0	3.690005	-2.506130	-0.765665
49	1	0	2.050214	-0.633610	-1.019358
50	1	0	4.645116	-0.979153	1.406937
51	1	0	2.761323	-2.492561	2.431084
52	1	0	-3.716473	-2.840353	-1.464505
53	1	0	-1.763768	-5.635412	-2.395712
54	1	0	1.084286	-5.046219	-1.199226
55	1	0	-0.018170	-1.342229	4.664136
56	1	0	6.984787	2.093758	-2.414938
57	1	0	4.984278	5.341946	0.090781
58	1	0	-2.709582	-0.318103	1.057296
59	1	0	-6.166260	0.613291	0.335334
60	1	0	-5.058750	0.477121	1.691123
61	1	0	-4.848572	-1.595230	0.526603
62	1	0	-1.555579	2.712688	-1.607354
63	1	0	-4.667752	5.209581	0.035794
64	1	0	-6.345660	4.078108	1.090322
65	1	0	-2.838324	5.973627	-1.121382
66	1	0	-4.394073	-0.346366	-1.935780

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11O at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.003293	-3.695297	0.132783
2	6	0	-5.950158	-3.329757	-0.831116
3	6	0	-5.926965	-2.033065	-1.344297
4	6	0	-4.981162	-1.080319	-0.925259
5	6	0	-4.044752	-1.493489	0.028758
6	6	0	-4.042354	-2.784377	0.569017
7	6	0	-4.991118	0.335053	-1.454881
8	6	0	-4.176623	1.266314	-0.547662
9	6	0	-2.856535	0.566957	-0.215294
10	8	0	-3.076879	-0.646433	0.510904
11	8	0	-4.854671	1.535652	0.678566
12	6	0	-1.838962	1.375930	0.610864
13	6	0	-2.239683	1.707763	2.026014
14	6	0	-1.311271	1.296544	2.908767
15	6	0	-0.181267	0.634213	2.229682
16	6	0	-0.443211	0.671260	0.726274
17	6	0	0.475686	1.600491	-0.037705
18	6	0	-0.289477	2.683499	-0.467840
19	8	0	-1.619325	2.616764	-0.144849
20	6	0	1.838946	1.538660	-0.344587
21	6	0	2.393281	2.591602	-1.090412
22	6	0	1.614271	3.671931	-1.507870
23	6	0	0.245706	3.735220	-1.196392
24	8	0	2.190105	4.675326	-2.232489
25	8	0	-0.462949	4.817012	-1.648131
26	8	0	0.777771	0.161380	2.822728
27	8	0	-1.307924	1.413525	4.247423
28	8	0	-6.827602	-1.613448	-2.283388
29	8	0	-5.066085	-4.975331	0.606001
30	6	0	2.688293	0.378995	0.115806
31	8	0	3.437913	-0.098768	-1.028139
32	6	0	4.313618	-1.132856	-0.791783
33	6	0	4.776112	-1.429596	0.496820
34	6	0	4.336434	-0.619128	1.696934
35	6	0	3.681108	0.694815	1.255305
36	6	0	4.737052	-1.841161	-1.922882
37	6	0	5.646439	-2.884690	-1.759191
38	6	0	6.123440	-3.225344	-0.487749
39	6	0	5.685124	-2.497039	0.617610
40	8	0	6.119258	-2.777052	1.882917
41	8	0	6.106640	-3.626500	-2.809906
42	8	0	4.644838	1.666313	0.856884
43	1	0	-0.457260	-0.352490	0.337229
44	1	0	-6.686159	-4.054599	-1.164224
45	1	0	-3.293998	-3.053831	1.307081
46	1	0	-4.584720	0.377670	-2.474278
47	1	0	-6.019010	0.707816	-1.527052
48	1	0	-3.944604	2.197127	-1.079229
49	1	0	-2.371675	0.329728	-1.173326
50	1	0	-5.668796	2.010798	0.463623
51	1	0	-3.171759	2.207401	2.247142
52	1	0	3.443087	2.583721	-1.352289
53	1	0	1.506660	5.334976	-2.429573
54	1	0	-1.383820	4.742831	-1.358688
55	1	0	-0.484558	0.996185	4.561121
56	1	0	-7.444316	-2.332063	-2.481707
57	1	0	-4.366797	-5.109164	1.261171
58	1	0	2.037842	-0.431465	0.465294
59	1	0	5.191873	-0.391769	2.340896
60	1	0	3.625902	-1.186780	2.311804
61	1	0	3.132446	1.138424	2.088227
62	1	0	4.347017	-1.571374	-2.898950
63	1	0	6.825013	-4.046266	-0.378763
64	1	0	6.760312	-3.501055	1.850140
65	1	0	5.711184	-3.299389	-3.630097
66	1	0	5.135332	1.297255	0.107985

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11P at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.908208	3.744520	0.126916
2	6	0	5.857826	3.400227	-0.842568
3	6	0	5.883822	2.095969	-1.334767
4	6	0	4.984886	1.110688	-0.884927
5	6	0	4.043339	1.505524	0.072013
6	6	0	3.990085	2.802936	0.590646
7	6	0	5.045348	-0.312894	-1.396180
8	6	0	4.235645	-1.256640	-0.496197
9	6	0	2.896524	-0.573172	-0.183423
10	8	0	3.129967	0.611875	0.592605
11	8	0	4.944854	-1.602102	0.693068
12	6	0	1.867689	-1.406164	0.600392
13	6	0	2.257652	-1.807960	2.000694
14	6	0	1.333025	-1.420829	2.898303
15	6	0	0.215540	-0.711246	2.245172
16	6	0	0.477053	-0.695765	0.741367
17	6	0	-0.447034	-1.591247	-0.057620
18	6	0	0.314139	-2.657060	-0.535929
19	8	0	1.645432	-2.608243	-0.213501
20	6	0	-1.810255	-1.513280	-0.360359
21	6	0	-2.368702	-2.529860	-1.151908
22	6	0	-1.593668	-3.593119	-1.616636
23	6	0	-0.224632	-3.673518	-1.309981
24	8	0	-2.172514	-4.563364	-2.383334
25	8	0	0.480558	-4.736816	-1.808778
26	8	0	-0.733780	-0.243628	2.857263
27	8	0	1.323282	-1.595855	4.229966
28	8	0	6.786978	1.697773	-2.278584
29	8	0	4.925606	5.033239	0.576531
30	6	0	-2.658501	-0.364445	0.136329
31	8	0	-3.350909	0.185672	-1.005498
32	6	0	-4.287613	1.154286	-0.758933
33	6	0	-4.791915	1.399056	0.524535
34	6	0	-4.348538	0.572353	1.708635
35	6	0	-3.663169	-0.718087	1.244738
36	6	0	-4.721313	1.873849	-1.880220
37	6	0	-5.679446	2.871518	-1.711548
38	6	0	-6.198941	3.158068	-0.443844
39	6	0	-5.750923	2.419280	0.651395
40	8	0	-6.226582	2.645881	1.914217
41	8	0	-6.148544	3.619178	-2.755750
42	8	0	-4.597488	-1.650004	0.705402
43	1	0	0.497488	0.341081	0.389109
44	1	0	6.558834	4.149361	-1.196586
45	1	0	3.238539	3.053412	1.332029
46	1	0	4.662672	-0.371314	-2.423610
47	1	0	6.081091	-0.664310	-1.432187
48	1	0	4.045087	-2.199339	-1.013146
49	1	0	2.426865	-0.293318	-1.136923
50	1	0	5.064650	-0.790993	1.209029
51	1	0	3.177155	-2.338184	2.203851
52	1	0	-3.419942	-2.501822	-1.406166
53	1	0	-1.489624	-5.213027	-2.612734
54	1	0	1.404495	-4.671674	-1.527001
55	1	0	0.506019	-1.178871	4.559899
56	1	0	7.366667	2.438851	-2.504488
57	1	0	4.233399	5.151017	1.242242
58	1	0	-2.003542	0.411719	0.550320
59	1	0	-5.206962	0.323825	2.343175
60	1	0	-3.654904	1.134835	2.348018
61	1	0	-3.102575	-1.159647	2.077419
62	1	0	-4.300169	1.647676	-2.854561
63	1	0	-6.938773	3.943967	-0.329291
64	1	0	-6.900869	3.338931	1.882964
65	1	0	-5.718911	3.329498	-3.572823
66	1	0	-5.178356	-1.928454	1.426032

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11Q at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.007494	3.687458	0.143432
2	6	0	5.955091	3.322070	-0.820081
3	6	0	5.929646	2.024362	-1.337127
4	6	0	4.982347	1.074860	-0.921192
5	6	0	4.044808	1.489440	0.034142
6	6	0	4.044162	2.777166	0.575981
7	6	0	4.988851	-0.339291	-1.454279
8	6	0	4.173112	-1.270863	-0.548623
9	6	0	2.854083	-0.570058	-0.215280
10	8	0	3.075722	0.641572	0.512942
11	8	0	4.850967	-1.543186	0.677059
12	6	0	1.835388	-1.379063	0.609552
13	6	0	2.235645	-1.713522	2.024203
14	6	0	1.307831	-1.302300	2.907567
15	6	0	0.178571	-0.637715	2.229439
16	6	0	0.440537	-0.672791	0.725976
17	6	0	-0.479553	-1.599749	-0.039339
18	6	0	0.284211	-2.683170	-0.470948
19	8	0	1.614147	-2.618561	-0.148001
20	6	0	-1.842746	-1.535808	-0.346104
21	6	0	-2.398478	-2.587127	-1.093194
22	6	0	-1.620886	-3.667943	-1.512011
23	6	0	-0.252384	-3.733312	-1.200744
24	8	0	-2.198049	-4.669777	-2.237785
25	8	0	0.454932	-4.815419	-1.653915
26	8	0	-0.780061	-0.164912	2.823139
27	8	0	1.304308	-1.421264	4.246049
28	8	0	6.830847	1.606179	-2.276148
29	8	0	4.975140	4.938554	0.691378
30	6	0	-2.690640	-0.375634	0.115698
31	8	0	-3.440166	0.103939	-1.027573
32	6	0	-4.314908	1.138559	-0.790018
33	6	0	-4.776729	1.434578	0.498988
34	6	0	-4.337235	0.622759	1.698253
35	6	0	-3.683395	-0.691450	1.255248
36	6	0	-4.738158	1.848171	-1.920371
37	6	0	-5.646589	2.892336	-1.755468
38	6	0	-6.122893	3.232290	-0.483582
39	6	0	-5.684794	2.502683	0.621010
40	8	0	-6.118285	2.781942	1.886698
41	8	0	-6.106548	3.635424	-2.805410
42	8	0	-4.648259	-1.661626	0.856266
43	1	0	0.455928	0.351552	0.338565
44	1	0	6.701005	4.035505	-1.161140
45	1	0	3.302763	3.060939	1.313187
46	1	0	4.581009	-0.378554	-2.473257
47	1	0	6.015815	-0.714141	-1.528615
48	1	0	3.939827	-2.200461	-1.081777
49	1	0	2.369491	-0.331120	-1.173079
50	1	0	5.664074	-2.019667	0.461216
51	1	0	3.167100	-2.214625	2.244624
52	1	0	-3.448292	-2.577579	-1.354990
53	1	0	-1.515491	-5.330178	-2.435419
54	1	0	1.375622	-4.743286	-1.363382
55	1	0	0.481812	-1.002686	4.560384
56	1	0	7.450049	2.323030	-2.472778
57	1	0	5.680664	5.477266	0.306873
58	1	0	-2.039185	0.433807	0.465661
59	1	0	-5.192572	0.395720	2.342464
60	1	0	-3.625828	1.189232	2.313192
61	1	0	-3.134907	-1.136347	2.087586
62	1	0	-4.348651	1.578918	-2.896797
63	1	0	-6.823695	4.053748	-0.373662
64	1	0	-6.758392	3.506820	1.854829
65	1	0	-5.711374	3.308889	-3.625964
66	1	0	-5.138645	-1.291332	0.107911

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11R at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.804863	3.784907	0.105339
2	6	0	5.766464	3.449490	-0.851434
3	6	0	5.831907	2.136057	-1.321933
4	6	0	4.959175	1.135075	-0.858017
5	6	0	3.999240	1.525376	0.089379
6	6	0	3.908610	2.825839	0.581855
7	6	0	5.051868	-0.300381	-1.337875
8	6	0	4.243882	-1.245441	-0.433528
9	6	0	2.892898	-0.575338	-0.149094
10	8	0	3.108486	0.614563	0.622459
11	8	0	4.942709	-1.561117	0.767537
12	6	0	1.861185	-1.415678	0.622976
13	6	0	2.234580	-1.815212	2.028318
14	6	0	1.291782	-1.440491	2.912368
15	6	0	0.175976	-0.742912	2.243051
16	6	0	0.463633	-0.716310	0.744179
17	6	0	-0.439939	-1.613027	-0.075761
18	6	0	0.335279	-2.672871	-0.543921
19	8	0	1.659687	-2.619043	-0.195119
20	6	0	-1.798072	-1.539640	-0.402399
21	6	0	-2.336416	-2.556978	-1.206866
22	6	0	-1.547264	-3.614090	-1.662798
23	6	0	-0.183976	-3.689444	-1.331348
24	8	0	-2.107730	-4.582218	-2.444805
25	8	0	0.535450	-4.746390	-1.822654
26	8	0	-0.790981	-0.292597	2.839875
27	8	0	1.263190	-1.619977	4.242680
28	8	0	6.797257	1.875542	-2.252300
29	8	0	4.687317	5.048924	0.606546
30	6	0	-2.659706	-0.405693	0.097775
31	8	0	-3.394364	0.120007	-1.034711
32	6	0	-4.276849	1.140417	-0.765538
33	6	0	-4.761411	1.375803	0.527522
34	6	0	-4.338414	0.512024	1.695913
35	6	0	-3.668613	-0.777458	1.206240
36	6	0	-4.683445	1.899624	-1.869362
37	6	0	-5.597393	2.933354	-1.672139
38	6	0	-6.096101	3.213680	-0.394309
39	6	0	-5.674431	2.435303	0.683119
40	8	0	-6.129173	2.655370	1.953041
41	8	0	-6.041487	3.722895	-2.694625
42	8	0	-4.619510	-1.735778	0.750059
43	1	0	0.482926	0.322959	0.398997
44	1	0	6.462938	4.187221	-1.237117
45	1	0	3.153257	3.083715	1.314205
46	1	0	4.684994	-0.395112	-2.369187
47	1	0	6.090282	-0.655182	-1.333806
48	1	0	4.077710	-2.196486	-0.943035
49	1	0	2.435025	-0.305998	-1.111141
50	1	0	4.997946	-0.751936	1.297778
51	1	0	3.155325	-2.337705	2.245687
52	1	0	-3.381593	-2.538529	-1.485938
53	1	0	-1.419144	-5.229887	-2.662595
54	1	0	1.452068	-4.682652	-1.517599
55	1	0	0.436137	-1.214014	4.561776
56	1	0	6.748101	0.952809	-2.536634
57	1	0	5.353333	5.620139	0.198855
58	1	0	-2.018610	0.390642	0.493995
59	1	0	-5.203517	0.251177	2.313750
60	1	0	-3.641513	1.053614	2.348720
61	1	0	-3.130624	-1.254756	2.027421
62	1	0	-4.277226	1.676114	-2.850460
63	1	0	-6.800459	4.028337	-0.259066
64	1	0	-6.770046	3.380211	1.944569
65	1	0	-5.630776	3.435838	-3.522319
66	1	0	-5.099224	-1.337879	0.009021

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11S at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.189774	-3.643983	0.007103
2	6	0	-6.136283	-3.217612	-0.931826
3	6	0	-6.080422	-1.904861	-1.399745
4	6	0	-5.100945	-0.996001	-0.961359
5	6	0	-4.166970	-1.469035	-0.033176
6	6	0	-4.197160	-2.777289	0.462427
7	6	0	-5.073815	0.436043	-1.443036
8	6	0	-4.225922	1.311771	-0.511529
9	6	0	-2.922779	0.564978	-0.217333
10	8	0	-3.169422	-0.667496	0.466551
11	8	0	-4.885431	1.554940	0.730114
12	6	0	-1.876512	1.315611	0.628431
13	6	0	-2.263205	1.620334	2.053313
14	6	0	-1.358581	1.134193	2.922449
15	6	0	-0.259094	0.444055	2.221904
16	6	0	-0.504599	0.560724	0.719949
17	6	0	0.446059	1.489635	-0.007249
18	6	0	-0.288028	2.603303	-0.414515
19	8	0	-1.617487	2.569103	-0.092760
20	6	0	1.803608	1.394066	-0.329812
21	6	0	2.382381	2.443289	-1.066636
22	6	0	1.632580	3.555430	-1.457973
23	6	0	0.272216	3.655282	-1.125012
24	8	0	2.228944	4.547146	-2.178529
25	8	0	-0.409316	4.764226	-1.549445
26	8	0	0.665358	-0.109023	2.799990
27	8	0	-1.356578	1.199544	4.264435
28	8	0	-6.980109	-1.425816	-2.310877
29	8	0	-5.285047	-4.936992	0.437546
30	6	0	2.649280	0.223896	0.118688
31	8	0	3.439950	-0.187891	-1.013888
32	6	0	4.448754	-1.088544	-0.793041
33	6	0	4.915368	-1.390627	0.491058
34	6	0	4.338589	-0.713029	1.711235
35	6	0	3.557953	0.542406	1.329857
36	6	0	4.995967	-1.672864	-1.942775
37	6	0	6.034499	-2.591459	-1.802421
38	6	0	6.522002	-2.931979	-0.535392
39	6	0	5.959429	-2.326937	0.588756
40	8	0	6.398622	-2.610826	1.853032
41	8	0	6.616799	-3.206850	-2.875619
42	8	0	4.502833	1.566436	1.032063
43	1	0	-0.547073	-0.443617	0.284844
44	1	0	-6.897657	-3.908083	-1.280879
45	1	0	-3.449518	-3.094231	1.182186
46	1	0	-4.673583	0.501469	-2.463643
47	1	0	-6.091009	0.840076	-1.494436
48	1	0	-3.973123	2.254360	-1.012085
49	1	0	-2.452336	0.350379	-1.187729
50	1	0	-5.686863	2.061609	0.540947
51	1	0	-3.172722	2.152929	2.290529
52	1	0	3.417863	2.384523	-1.379719
53	1	0	1.561976	5.225638	-2.368728
54	1	0	-1.335445	4.699415	-1.274685
55	1	0	-0.557258	0.729321	4.565226
56	1	0	-7.625966	-2.115592	-2.518200
57	1	0	-4.583342	-5.112723	1.080121
58	1	0	1.998311	-0.608262	0.416188
59	1	0	5.135150	-0.434562	2.407922
60	1	0	3.670950	-1.390638	2.258698
61	1	0	2.910164	0.838092	2.162998
62	1	0	4.599096	-1.406699	-2.917127
63	1	0	7.325693	-3.655729	-0.443115
64	1	0	7.140411	-3.229782	1.802681
65	1	0	6.199418	-2.890447	-3.689108
66	1	0	4.006359	2.375758	0.842169

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11T at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.003577	-3.696879	0.128761
2	6	0	-5.951933	-3.330881	-0.833492
3	6	0	-5.929131	-2.034128	-1.346573
4	6	0	-4.982286	-1.081770	-0.929012
5	6	0	-4.044471	-1.495391	0.023401
6	6	0	-4.041605	-2.786352	0.563495
7	6	0	-4.992479	0.333746	-1.458243
8	6	0	-4.177578	1.264710	-0.551041
9	6	0	-2.856837	0.565839	-0.220400
10	8	0	-3.075644	-0.648794	0.504257
11	8	0	-4.854733	1.532835	0.675940
12	6	0	-1.839446	1.373892	0.606931
13	6	0	-2.239955	1.701761	2.023108
14	6	0	-1.312354	1.286325	2.904700
15	6	0	-0.183113	0.624786	2.223659
16	6	0	-0.443298	0.669517	0.720198
17	6	0	0.475798	1.603988	-0.037278
18	6	0	-0.290177	2.687683	-0.464187
19	8	0	-1.620834	2.616792	-0.145380
20	6	0	1.839834	1.545718	-0.341546
21	6	0	2.394289	2.603476	-1.080361
22	6	0	1.614487	3.684619	-1.494322
23	6	0	0.245030	3.743979	-1.186076
24	8	0	2.190438	4.692549	-2.212496
25	8	0	-0.464397	4.826740	-1.634330
26	8	0	0.774266	0.147138	2.815569
27	8	0	-1.309356	1.398367	4.243809
28	8	0	-6.831231	-1.614109	-2.284076
29	8	0	-5.066060	-4.976928	0.602024
30	6	0	2.689310	0.383916	0.113276
31	8	0	3.448624	-0.079942	-1.029661
32	6	0	4.318819	-1.120470	-0.799058
33	6	0	4.770664	-1.430434	0.492370
34	6	0	4.326219	-0.627964	1.696241
35	6	0	3.674210	0.690249	1.262006
36	6	0	4.747499	-1.818042	-1.931895
37	6	0	5.650930	-2.867399	-1.771921
38	6	0	6.115476	-3.223451	-0.499853
39	6	0	5.671964	-2.501878	0.610897
40	8	0	6.095672	-2.796919	1.876190
41	8	0	6.047387	-3.528838	-2.899534
42	8	0	4.640219	1.665101	0.877514
43	1	0	-0.455670	-0.352032	0.325365
44	1	0	-6.688764	-4.055421	-1.165424
45	1	0	-3.292149	-3.056112	1.300332
46	1	0	-4.586535	0.376717	-2.477803
47	1	0	-6.020401	0.706528	-1.529798
48	1	0	-3.946439	2.196023	-1.082141
49	1	0	-2.372282	0.330440	-1.179017
50	1	0	-5.669589	2.007161	0.461967
51	1	0	-3.171525	2.201715	2.245638
52	1	0	3.444465	2.598204	-1.340952
53	1	0	1.506033	5.351266	-2.409366
54	1	0	-1.386435	4.748198	-1.349803
55	1	0	-0.486657	0.978745	4.556211
56	1	0	-7.448412	-2.332561	-2.481528
57	1	0	-4.365627	-5.111075	1.255907
58	1	0	2.038491	-0.431621	0.450172
59	1	0	5.178714	-0.406723	2.346263
60	1	0	3.611706	-1.199189	2.303151
61	1	0	3.120808	1.126561	2.095604
62	1	0	4.377017	-1.547946	-2.913480
63	1	0	6.811637	-4.049139	-0.376328
64	1	0	6.735182	-3.522167	1.842549
65	1	0	6.667075	-4.231807	-2.659462
66	1	0	5.126805	1.307313	0.120612

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11U at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.435842	3.484707	0.048430
2	6	0	5.416065	3.094079	-0.871979
3	6	0	5.475475	1.758392	-1.276182
4	6	0	4.578626	0.792668	-0.788364
5	6	0	3.606121	1.234463	0.118786
6	6	0	3.520717	2.559340	0.549782
7	6	0	4.669191	-0.658508	-1.209550
8	6	0	3.843350	-1.557593	-0.279305
9	6	0	2.491174	-0.870777	-0.038854
10	8	0	2.694485	0.358917	0.672832
11	8	0	4.525680	-1.832120	0.943976
12	6	0	1.450463	-1.668087	0.765635
13	6	0	1.809971	-1.994998	2.192730
14	6	0	0.846501	-1.598137	3.043439
15	6	0	-0.269285	-0.949062	2.327031
16	6	0	0.049849	-0.966089	0.832834
17	6	0	-0.833580	-1.887982	0.018429
18	6	0	-0.057105	-2.974905	-0.371067
19	8	0	1.256032	-2.917320	0.013523
20	6	0	-2.179055	-1.810002	-0.363456
21	6	0	-2.706002	-2.864491	-1.124298
22	6	0	-1.920160	-3.964998	-1.480055
23	6	0	-0.569124	-4.034939	-1.108355
24	8	0	-2.475589	-4.972888	-2.213868
25	8	0	0.149912	-5.128848	-1.507831
26	8	0	-1.255140	-0.501076	2.894721
27	8	0	0.795742	-1.720237	4.379798
28	8	0	6.411461	1.314879	-2.166134
29	8	0	4.323990	4.772961	0.485836
30	6	0	-2.992210	-0.594610	0.026264
31	8	0	-2.573145	0.492363	-0.853141
32	6	0	-3.138520	1.720584	-0.577086
33	6	0	-4.360496	1.821023	0.107623
34	6	0	-5.112056	0.584089	0.558317
35	6	0	-4.520079	-0.689937	-0.067207
36	6	0	-2.447820	2.835621	-1.051430
37	6	0	-2.987867	4.103674	-0.828166
38	6	0	-4.190916	4.254548	-0.133552
39	6	0	-4.859438	3.117357	0.325829
40	8	0	-6.033879	3.333661	0.990619
41	8	0	-2.284547	5.173392	-1.304701
42	8	0	-4.953369	-0.850489	-1.417259
43	1	0	0.072250	0.061117	0.455038
44	1	0	6.121761	3.819681	-1.268365
45	1	0	2.753926	2.859556	1.253600
46	1	0	4.317797	-0.782887	-2.242325
47	1	0	5.709041	-0.999202	-1.194833
48	1	0	3.673534	-2.529008	-0.748150
49	1	0	2.043426	-0.650954	-1.018288
50	1	0	4.631426	-0.993526	1.417340
51	1	0	2.735926	-2.491288	2.445865
52	1	0	-3.732438	-2.832730	-1.466963
53	1	0	-1.791624	-5.641813	-2.374554
54	1	0	1.056107	-5.059735	-1.173801
55	1	0	-0.044241	-1.314599	4.664177
56	1	0	6.997577	2.044098	-2.412598
57	1	0	5.005073	5.317246	0.066470
58	1	0	-2.730985	-0.309996	1.051479
59	1	0	-6.167836	0.631966	0.261799
60	1	0	-5.089981	0.486841	1.652992
61	1	0	-4.875042	-1.567353	0.480657
62	1	0	-1.507748	2.715522	-1.576413
63	1	0	-4.616548	5.234881	0.056180
64	1	0	-6.401846	2.493443	1.296058
65	1	0	-2.752724	5.990092	-1.081430
66	1	0	-4.357683	-0.319479	-1.968250

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11V at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.877041	3.749982	0.142940
2	6	0	5.829286	3.413899	-0.827065
3	6	0	5.865173	2.107958	-1.321290
4	6	0	4.974892	1.117624	-0.872033
5	6	0	4.029911	1.506060	0.087127
6	6	0	3.966809	2.800256	0.606013
7	6	0	5.044521	-0.304922	-1.385383
8	6	0	4.237148	-1.255422	-0.490134
9	6	0	2.895184	-0.578106	-0.176912
10	8	0	3.124852	0.602675	0.606368
11	8	0	4.945444	-1.601784	0.699439
12	6	0	1.866564	-1.417794	0.599947
13	6	0	2.255168	-1.830079	1.997525
14	6	0	1.328672	-1.451464	2.896859
15	6	0	0.210963	-0.738392	2.247759
16	6	0	0.475544	-0.709132	0.744658
17	6	0	-0.446720	-1.597288	-0.064312
18	6	0	0.315137	-2.659519	-0.549403
19	8	0	1.645669	-2.613985	-0.223283
20	6	0	-1.809121	-1.515896	-0.369624
21	6	0	-2.366445	-2.525746	-1.170551
22	6	0	-1.590884	-3.585737	-1.641861
23	6	0	-0.222540	-3.669357	-1.332843
24	8	0	-2.168496	-4.549574	-2.417561
25	8	0	0.483160	-4.729026	-1.838670
26	8	0	-0.740612	-0.278300	2.861979
27	8	0	1.317137	-1.637533	4.226972
28	8	0	6.771195	1.718873	-2.265970
29	8	0	4.788175	5.006946	0.667818
30	6	0	-2.656982	-0.369933	0.134223
31	8	0	-3.342004	0.193881	-1.005435
32	6	0	-4.275532	1.164118	-0.753195
33	6	0	-4.784697	1.397865	0.530430
34	6	0	-4.350884	0.556813	1.707968
35	6	0	-3.668383	-0.731435	1.233895
36	6	0	-4.700794	1.897246	-1.868929
37	6	0	-5.655053	2.897601	-1.694232
38	6	0	-6.178962	3.173503	-0.425985
39	6	0	-5.739350	2.421373	0.663572
40	8	0	-6.219495	2.637216	1.926582
41	8	0	-6.116033	3.658226	-2.732697
42	8	0	-4.603840	-1.653915	0.680319
43	1	0	0.496792	0.330944	0.402190
44	1	0	6.532659	4.158290	-1.191368
45	1	0	3.221030	3.058945	1.347857
46	1	0	4.664887	-0.363272	-2.413979
47	1	0	6.082193	-0.650880	-1.419345
48	1	0	4.051876	-2.197056	-1.010994
49	1	0	2.426605	-0.294224	-1.129765
50	1	0	5.048939	-0.794034	1.224202
51	1	0	3.174980	-2.360826	2.197972
52	1	0	-3.417148	-2.495151	-1.426769
53	1	0	-1.485561	-5.198115	-2.649949
54	1	0	1.406142	-4.667546	-1.552967
55	1	0	0.499101	-1.223923	4.559222
56	1	0	7.345139	2.463988	-2.493032
57	1	0	5.460305	5.574299	0.264998
58	1	0	-2.002027	0.400070	0.559484
59	1	0	-5.213660	0.305080	2.335317
60	1	0	-3.658296	1.109565	2.356876
61	1	0	-3.113648	-1.184039	2.064599
62	1	0	-4.276076	1.679359	-2.843610
63	1	0	-6.915437	3.961855	-0.306683
64	1	0	-6.889838	3.334258	1.899746
65	1	0	-5.684233	3.375008	-3.550887
66	1	0	-5.189932	-1.936675	1.395018

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11W at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.835630	3.779382	0.094823
2	6	0	5.792745	3.437764	-0.864353
3	6	0	5.846689	2.126878	-1.336534
4	6	0	4.966258	1.129791	-0.871982
5	6	0	4.011400	1.524648	0.075457
6	6	0	3.931627	2.827394	0.570548
7	6	0	5.049972	-0.306302	-1.351228
8	6	0	4.241024	-1.245884	-0.442270
9	6	0	2.892877	-0.570525	-0.156277
10	8	0	3.112878	0.622582	0.609433
11	8	0	4.942085	-1.561498	0.757475
12	6	0	1.861743	-1.405228	0.622716
13	6	0	2.237305	-1.794758	2.030338
14	6	0	1.296302	-1.412983	2.913264
15	6	0	0.179825	-0.719590	2.240809
16	6	0	0.464280	-0.705060	0.741179
17	6	0	-0.440916	-1.608840	-0.069281
18	6	0	0.333787	-2.671806	-0.531184
19	8	0	1.659112	-2.614172	-0.186514
20	6	0	-1.800004	-1.539197	-0.392819
21	6	0	-2.339665	-2.563365	-1.187690
22	6	0	-1.550967	-3.623522	-1.637268
23	6	0	-0.186728	-3.695126	-1.308950
24	8	0	-2.112816	-4.598381	-2.409811
25	8	0	0.532192	-4.755405	-1.793675
26	8	0	-0.785456	-0.263625	2.836121
27	8	0	1.269935	-1.582424	4.244964
28	8	0	6.807645	1.857356	-2.269197
29	8	0	4.824611	5.074388	0.525766
30	6	0	-2.661588	-0.402285	0.100666
31	8	0	-3.399787	0.113518	-1.034003
32	6	0	-4.284724	1.133265	-0.770699
33	6	0	-4.766401	1.378039	0.521716
34	6	0	-4.337489	0.525336	1.696067
35	6	0	-3.666885	-0.766853	1.214821
36	6	0	-4.696931	1.881856	-1.879707
37	6	0	-5.613831	2.914125	-1.688651
38	6	0	-6.109924	3.203548	-0.411818
39	6	0	-5.682709	2.435625	0.670891
40	8	0	-6.134877	2.664757	1.940130
41	8	0	-6.063459	3.693493	-2.716476
42	8	0	-4.617546	-1.730154	0.768829
43	1	0	0.482303	0.331326	0.387287
44	1	0	6.486594	4.180940	-1.239034
45	1	0	3.171479	3.075504	1.303909
46	1	0	4.679016	-0.400510	-2.381098
47	1	0	6.086718	-0.665954	-1.350365
48	1	0	4.069573	-2.197602	-0.948685
49	1	0	2.433023	-0.304042	-1.118152
50	1	0	5.011217	-0.749317	1.281374
51	1	0	3.158182	-2.316175	2.249688
52	1	0	-3.385637	-2.548028	-1.463955
53	1	0	-1.424389	-5.247430	-2.623993
54	1	0	1.449284	-4.689242	-1.490571
55	1	0	0.443303	-1.174189	4.562268
56	1	0	6.747166	0.936202	-2.556233
57	1	0	4.130046	5.186885	1.189871
58	1	0	-2.020426	0.397990	0.488785
59	1	0	-5.199879	0.268079	2.319160
60	1	0	-3.639369	1.073875	2.341741
61	1	0	-3.125781	-1.236790	2.038205
62	1	0	-4.292814	1.651309	-2.860051
63	1	0	-6.816796	4.016819	-0.281435
64	1	0	-6.779172	3.386485	1.927019
65	1	0	-5.654571	3.400459	-3.542979
66	1	0	-5.101406	-1.338031	0.027404

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11X at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.007009	3.689263	0.139704
2	6	0	5.956060	3.323643	-0.822285
3	6	0	5.931164	2.025915	-1.339344
4	6	0	4.983022	1.076618	-0.924872
5	6	0	4.044105	1.491425	0.028983
6	6	0	4.042837	2.779179	0.570772
7	6	0	4.989933	-0.337629	-1.457703
8	6	0	4.173960	-1.269109	-0.552118
9	6	0	2.854219	-0.568978	-0.220337
10	8	0	3.074238	0.643826	0.506495
11	8	0	4.851035	-1.540284	0.674245
12	6	0	1.835831	-1.377272	0.605616
13	6	0	2.235982	-1.707943	2.021229
14	6	0	1.308947	-1.292796	2.903537
15	6	0	0.180340	-0.629029	2.223602
16	6	0	0.440536	-0.671422	0.720061
17	6	0	-0.479699	-1.603517	-0.038957
18	6	0	0.284918	-2.687541	-0.467485
19	8	0	1.615665	-2.618761	-0.148699
20	6	0	-1.843668	-1.543124	-0.343131
21	6	0	-2.399493	-2.599192	-1.083350
22	6	0	-1.621074	-3.680757	-1.498791
23	6	0	-0.251671	-3.742187	-1.190766
24	8	0	-2.198328	-4.687067	-2.218244
25	8	0	0.456450	-4.825186	-1.640598
26	8	0	-0.776694	-0.151684	2.816287
27	8	0	1.305824	-1.407073	4.242456
28	8	0	6.833804	1.607549	-2.276900
29	8	0	4.974085	4.940371	0.687624
30	6	0	-2.691668	-0.380818	0.113161
31	8	0	-3.450788	0.085028	-1.029123
32	6	0	-4.319746	1.126309	-0.797266
33	6	0	-4.770882	1.435518	0.494585
34	6	0	-4.326974	0.631374	1.697537
35	6	0	-3.676650	-0.687173	1.261807
36	6	0	-4.747966	1.825456	-1.929309
37	6	0	-5.650125	2.875703	-1.768046
38	6	0	-6.113894	3.231056	-0.495503
39	6	0	-5.670874	2.507911	0.614426
40	8	0	-6.093896	2.802186	1.880121
41	8	0	-6.046194	3.538677	-2.894915
42	8	0	-4.643921	-1.660478	0.876481
43	1	0	0.454187	0.350826	0.327101
44	1	0	6.702677	4.036916	-1.162143
45	1	0	3.300362	3.063085	1.306844
46	1	0	4.582501	-0.377202	-2.476830
47	1	0	6.016977	-0.712350	-1.531509
48	1	0	3.941631	-2.199175	-1.084899
49	1	0	2.369855	-0.331792	-1.178665
50	1	0	5.664890	-2.015878	0.459267
51	1	0	3.167009	-2.209271	2.242933
52	1	0	-3.449676	-2.592253	-1.343879
53	1	0	-1.514793	-5.346502	-2.415724
54	1	0	1.378307	-4.748710	-1.354928
55	1	0	0.483948	-0.986383	4.555593
56	1	0	7.453298	2.324370	-2.472712
57	1	0	5.680236	5.478964	0.304108
58	1	0	-2.039823	0.433638	0.450667
59	1	0	-5.179512	0.410508	2.347634
60	1	0	-3.611568	1.201166	2.304734
61	1	0	-3.123591	-1.125000	2.094825
62	1	0	-4.378028	1.555925	-2.911254
63	1	0	-6.809048	4.057445	-0.370983
64	1	0	-6.732142	3.528589	1.847435
65	1	0	-6.664782	4.242295	-2.653918
66	1	0	-5.130038	-1.301357	0.119912

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11Y at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.801327	3.788603	0.103538
2	6	0	5.763606	3.453985	-0.852831
3	6	0	5.830172	2.140660	-1.323483
4	6	0	4.957949	1.138998	-0.860066
5	6	0	3.997312	1.528506	0.086936
6	6	0	3.905541	2.828853	0.579526
7	6	0	5.051869	-0.296370	-1.339948
8	6	0	4.244778	-1.242133	-0.435524
9	6	0	2.893029	-0.573487	-0.151399
10	8	0	3.107068	0.617046	0.619642
11	8	0	4.943852	-1.556926	0.765648
12	6	0	1.862319	-1.414423	0.621381
13	6	0	2.236101	-1.811460	2.027349
14	6	0	1.293158	-1.435891	2.910860
15	6	0	0.176880	-0.740098	2.240506
16	6	0	0.463860	-0.716619	0.741467
17	6	0	-0.438837	-1.616768	-0.075732
18	6	0	0.337787	-2.676389	-0.542044
19	8	0	1.662502	-2.619224	-0.194867
20	6	0	-1.797326	-1.546332	-0.401596
21	6	0	-2.334681	-2.566716	-1.202813
22	6	0	-1.544150	-3.623687	-1.656741
23	6	0	-0.180428	-3.695852	-1.326411
24	8	0	-2.103710	-4.594744	-2.435740
25	8	0	0.540366	-4.752841	-1.815660
26	8	0	-0.789939	-0.288849	2.836871
27	8	0	1.264811	-1.613027	4.241514
28	8	0	6.796185	1.880925	-2.253379
29	8	0	4.682702	5.052480	0.604881
30	6	0	-2.659983	-0.411660	0.095264
31	8	0	-3.399269	0.106333	-1.037495
32	6	0	-4.277794	1.131659	-0.772269
33	6	0	-4.757740	1.373318	0.523526
34	6	0	-4.333995	0.512362	1.693847
35	6	0	-3.665717	-0.779368	1.207772
36	6	0	-4.684980	1.885748	-1.876413
37	6	0	-5.594949	2.923487	-1.681336
38	6	0	-6.087791	3.211822	-0.402795
39	6	0	-5.665068	2.434990	0.678447
40	8	0	-6.115639	2.662931	1.948319
41	8	0	-5.969332	3.642116	-2.781171
42	8	0	-4.617575	-1.739362	0.757088
43	1	0	0.481431	0.321797	0.393642
44	1	0	6.459706	4.192270	-1.238129
45	1	0	3.149657	3.086105	1.311549
46	1	0	4.684999	-0.391443	-2.371226
47	1	0	6.090600	-0.650234	-1.335944
48	1	0	4.079655	-2.193436	-0.944896
49	1	0	2.434846	-0.305186	-1.113578
50	1	0	4.998813	-0.747469	1.295492
51	1	0	3.157237	-2.332957	2.245451
52	1	0	-3.379936	-2.550475	-1.481778
53	1	0	-1.413904	-5.241046	-2.653722
54	1	0	1.457895	-4.684969	-1.514264
55	1	0	0.437506	-1.207008	4.559892
56	1	0	6.747281	0.958403	-2.538440
57	1	0	5.348331	5.624250	0.197338
58	1	0	-2.019231	0.387877	0.485630
59	1	0	-5.198383	0.254413	2.313931
60	1	0	-3.635408	1.055243	2.343790
61	1	0	-3.126233	-1.253413	2.029838
62	1	0	-4.292967	1.667848	-2.862594
63	1	0	-6.789363	4.028381	-0.252028
64	1	0	-6.755986	3.388155	1.939812
65	1	0	-6.594785	4.331554	-2.517912
66	1	0	-5.091430	-1.347938	0.008843

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11Z at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.835722	3.781769	0.092059
2	6	0	5.793572	3.440179	-0.866390
3	6	0	5.847689	2.129359	-1.338753
4	6	0	4.966759	1.132311	-0.875052
5	6	0	4.011203	1.527150	0.071685
6	6	0	3.931206	2.829845	0.566900
7	6	0	5.050669	-0.303778	-1.354284
8	6	0	4.241960	-1.243401	-0.445162
9	6	0	2.893375	-0.568717	-0.159767
10	8	0	3.112266	0.625208	0.604998
11	8	0	4.942997	-1.558319	0.754815
12	6	0	1.862830	-1.403195	0.620281
13	6	0	2.238577	-1.789634	2.028726
14	6	0	1.297904	-1.405521	2.910967
15	6	0	0.181468	-0.713448	2.237170
16	6	0	0.464762	-0.703874	0.737296
17	6	0	-0.440212	-1.611817	-0.068889
18	6	0	0.335475	-2.675099	-0.528373
19	8	0	1.661362	-2.613870	-0.186471
20	6	0	-1.799887	-1.545368	-0.390740
21	6	0	-2.339213	-2.573427	-1.180732
22	6	0	-1.549535	-3.633982	-1.627734
23	6	0	-0.184623	-3.702110	-1.301547
24	8	0	-2.111129	-4.612583	-2.395699
25	8	0	0.535246	-4.762993	-1.783586
26	8	0	-0.783032	-0.254979	2.831851
27	8	0	1.271945	-1.571547	4.243128
28	8	0	6.809423	1.859845	-2.270620
29	8	0	4.824534	5.076713	0.523234
30	6	0	-2.662058	-0.407062	0.098604
31	8	0	-3.406384	0.098878	-1.036222
32	6	0	-4.287571	1.123543	-0.777679
33	6	0	-4.762947	1.376946	0.517579
34	6	0	-4.331408	0.529418	1.694836
35	6	0	-3.662659	-0.765710	1.218676
36	6	0	-4.702467	1.864447	-1.887874
37	6	0	-5.615792	2.900532	-1.699820
38	6	0	-6.104163	3.200491	-0.422225
39	6	0	-5.673882	2.436571	0.665205
40	8	0	-6.120121	2.675998	1.934493
41	8	0	-5.997886	3.605860	-2.805562
42	8	0	-4.614629	-1.731667	0.781146
43	1	0	0.481221	0.331170	0.379436
44	1	0	6.487784	4.183329	-1.240445
45	1	0	3.170522	3.077935	1.299710
46	1	0	4.679669	-0.398135	-2.384113
47	1	0	6.087476	-0.663252	-1.353437
48	1	0	4.071032	-2.195387	-0.951256
49	1	0	2.433359	-0.303460	-1.121895
50	1	0	5.012608	-0.745733	1.278012
51	1	0	3.159420	-2.310680	2.249082
52	1	0	-3.385456	-2.560523	-1.456159
53	1	0	-1.421671	-5.260477	-2.610054
54	1	0	1.453524	-4.692347	-1.485124
55	1	0	0.445472	-1.162361	4.559612
56	1	0	6.748412	0.939020	-2.558590
57	1	0	4.129156	5.189265	1.186478
58	1	0	-2.020909	0.397139	0.478644
59	1	0	-5.192163	0.276007	2.321789
60	1	0	-3.630894	1.080590	2.335665
61	1	0	-3.118922	-1.230815	2.043051
62	1	0	-4.314051	1.637517	-2.873443
63	1	0	-6.808192	4.015911	-0.276865
64	1	0	-6.764431	3.397617	1.920768
65	1	0	-6.626495	4.294264	-2.547179
66	1	0	-5.093728	-1.347475	0.032489

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11AA at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.105324	-3.683343	-0.045366
2	6	0	-6.067413	-3.257550	-0.969111
3	6	0	-6.060656	-1.928994	-1.392282
4	6	0	-5.114828	-0.999865	-0.919845
5	6	0	-4.163805	-1.474871	-0.009999
6	6	0	-4.143097	-2.798456	0.440139
7	6	0	-5.136573	0.448622	-1.358663
8	6	0	-4.275974	1.318414	-0.432210
9	6	0	-2.953943	0.577226	-0.184782
10	8	0	-3.207090	-0.640660	0.531117
11	8	0	-4.948130	1.628390	0.787724
12	6	0	-1.885005	1.334357	0.622605
13	6	0	-2.242487	1.677811	2.046811
14	6	0	-1.335347	1.189730	2.912516
15	6	0	-0.259507	0.465415	2.208781
16	6	0	-0.518415	0.569375	0.708384
17	6	0	0.431511	1.487407	-0.034637
18	6	0	-0.302251	2.595143	-0.458446
19	8	0	-1.631331	2.566870	-0.134170
20	6	0	1.788556	1.386551	-0.358135
21	6	0	2.367317	2.424487	-1.110474
22	6	0	1.617652	3.530969	-1.517801
23	6	0	0.257580	3.636199	-1.185162
24	8	0	2.213888	4.511596	-2.252908
25	8	0	-0.423619	4.738625	-1.625632
26	8	0	0.659568	-0.099656	2.783765
27	8	0	-1.312850	1.280573	4.252161
28	8	0	-6.975238	-1.451107	-2.286742
29	8	0	-5.155325	-4.992015	0.339284
30	6	0	2.634808	0.222743	0.105786
31	8	0	3.437205	-0.193976	-1.014917
32	6	0	4.449447	-1.087339	-0.780290
33	6	0	4.906606	-1.383974	0.511211
34	6	0	4.312680	-0.694319	1.719586
35	6	0	3.534081	0.557934	1.318455
36	6	0	5.010017	-1.670707	-1.921594
37	6	0	6.053933	-2.583798	-1.769605
38	6	0	6.528806	-2.920876	-0.499587
39	6	0	5.951700	-2.320594	0.619550
40	8	0	6.463988	-2.687043	1.834170
41	8	0	6.648551	-3.194762	-2.838377
42	8	0	4.482126	1.575119	1.015102
43	1	0	-0.569805	-0.438007	0.281271
44	1	0	-6.803757	-3.962847	-1.341353
45	1	0	-3.383058	-3.112619	1.147839
46	1	0	-4.774019	0.545579	-2.390449
47	1	0	-6.159885	0.836227	-1.353717
48	1	0	-4.064338	2.278886	-0.906662
49	1	0	-2.511604	0.336664	-1.161721
50	1	0	-5.095259	0.797091	1.262853
51	1	0	-3.133583	2.239364	2.288436
52	1	0	3.402450	2.360421	-1.423643
53	1	0	1.547608	5.188369	-2.451599
54	1	0	-1.347443	4.683908	-1.341002
55	1	0	-0.518231	0.801701	4.551773
56	1	0	-7.593168	-2.156479	-2.524843
57	1	0	-4.450776	-5.165602	0.979422
58	1	0	1.985005	-0.609265	0.406263
59	1	0	5.094947	-0.378695	2.421908
60	1	0	3.636818	-1.360868	2.271607
61	1	0	2.883301	0.860943	2.146070
62	1	0	4.620153	-1.408270	-2.899768
63	1	0	7.333256	-3.637209	-0.381678
64	1	0	5.981200	-2.244208	2.544840
65	1	0	6.236778	-2.879764	-3.655219
66	1	0	3.989044	2.382835	0.809729

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11AB at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.948630	3.734289	0.103585
2	6	0	5.899770	3.378554	-0.860266
3	6	0	5.917233	2.072189	-1.347305
4	6	0	5.008017	1.096111	-0.898046
5	6	0	4.065610	1.502225	0.053287
6	6	0	4.020844	2.802010	0.566785
7	6	0	5.058545	-0.329802	-1.403801
8	6	0	4.240939	-1.263746	-0.500869
9	6	0	2.905188	-0.570726	-0.194779
10	8	0	3.142884	0.618366	0.573746
11	8	0	4.945662	-1.607659	0.691510
12	6	0	1.871086	-1.392531	0.594008
13	6	0	2.257681	-1.783171	1.998513
14	6	0	1.338069	-1.376139	2.892393
15	6	0	0.227369	-0.662950	2.231970
16	6	0	0.483558	-0.674045	0.727364
17	6	0	-0.446633	-1.580835	-0.052232
18	6	0	0.310842	-2.653719	-0.520682
19	8	0	1.644473	-2.600682	-0.208799
20	6	0	-1.811800	-1.506694	-0.347639
21	6	0	-2.375712	-2.534776	-1.120074
22	6	0	-1.604286	-3.605063	-1.574511
23	6	0	-0.233272	-3.681267	-1.276112
24	8	0	-2.188665	-4.586237	-2.322886
25	8	0	0.468537	-4.751674	-1.764509
26	8	0	-0.713958	-0.174168	2.839962
27	8	0	1.328376	-1.534448	4.226198
28	8	0	6.821528	1.662895	-2.285266
29	8	0	4.974435	5.024471	0.548601
30	6	0	-2.657817	-0.350358	0.135737
31	8	0	-3.374710	0.164918	-1.006769
32	6	0	-4.316721	1.131300	-0.770991
33	6	0	-4.799631	1.405698	0.516902
34	6	0	-4.326087	0.614847	1.713791
35	6	0	-3.639202	-0.682280	1.271402
36	6	0	-4.778471	1.813663	-1.901512
37	6	0	-5.743944	2.805930	-1.742606
38	6	0	-6.241480	3.123339	-0.473146
39	6	0	-5.764949	2.418114	0.635049
40	8	0	-6.219928	2.675761	1.899407
41	8	0	-6.168438	3.452906	-2.869974
42	8	0	-4.575410	-1.635244	0.773847
43	1	0	0.505358	0.356252	0.356425
44	1	0	6.608437	4.120589	-1.214068
45	1	0	3.268394	3.061414	1.304153
46	1	0	4.676593	-0.389499	-2.431414
47	1	0	6.091675	-0.688983	-1.437137
48	1	0	4.045502	-2.207876	-1.013387
49	1	0	2.438406	-0.295175	-1.150923
50	1	0	5.072693	-0.794275	1.202111
51	1	0	3.172241	-2.319850	2.206909
52	1	0	-3.428331	-2.509374	-1.368889
53	1	0	-1.507390	-5.239108	-2.547934
54	1	0	1.393885	-4.683715	-1.488119
55	1	0	0.515872	-1.104982	4.551838
56	1	0	7.408914	2.398053	-2.510560
57	1	0	4.279878	5.150279	1.210411
58	1	0	-2.000139	0.440178	0.517322
59	1	0	-5.169630	0.377043	2.371939
60	1	0	-3.624431	1.199665	2.323718
61	1	0	-3.060248	-1.097159	2.105080
62	1	0	-4.383964	1.575262	-2.882093
63	1	0	-6.987302	3.904444	-0.349293
64	1	0	-6.903644	3.359164	1.862864
65	1	0	-6.832291	4.114087	-2.629508
66	1	0	-5.139027	-1.901067	1.512719

Cartesian coordinates of the optimized geometry of (1‴*R*,5‴*R*)-11AC at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.103690	-3.687557	-0.049752
2	6	0	-6.067497	-3.260967	-0.971328
3	6	0	-6.062538	-1.931643	-1.392107
4	6	0	-5.116873	-1.002521	-0.919344
5	6	0	-4.164155	-1.478278	-0.011663
6	6	0	-4.141605	-2.802669	0.436023
7	6	0	-5.140448	0.446689	-1.355673
8	6	0	-4.279349	1.315667	-0.428934
9	6	0	-2.956374	0.575234	-0.184374
10	8	0	-3.207495	-0.644171	0.529666
11	8	0	-4.950282	1.623246	0.792306
12	6	0	-1.887188	1.331970	0.623084
13	6	0	-2.243451	1.672482	2.048314
14	6	0	-1.335223	1.183144	2.912153
15	6	0	-0.259609	0.460949	2.205920
16	6	0	-0.519762	0.568128	0.705976
17	6	0	0.428558	1.488714	-0.036050
18	6	0	-0.306869	2.596283	-0.457371
19	8	0	-1.635601	2.566049	-0.131767
20	6	0	1.785405	1.389943	-0.361084
21	6	0	2.362185	2.429615	-1.112524
22	6	0	1.610809	3.535850	-1.517433
23	6	0	0.251024	3.639102	-1.183050
24	8	0	2.205130	4.518271	-2.251690
25	8	0	-0.431892	4.741558	-1.620877
26	8	0	0.660112	-0.105000	2.779043
27	8	0	-1.311526	1.271098	4.251989
28	8	0	-6.978858	-1.452965	-2.284364
29	8	0	-5.151946	-4.996979	0.332606
30	6	0	2.633745	0.227012	0.101334
31	8	0	3.437466	-0.186622	-1.019169
32	6	0	4.450601	-1.079956	-0.786515
33	6	0	4.907108	-1.376484	0.507578
34	6	0	4.310968	-0.688586	1.715885
35	6	0	3.531489	0.562984	1.314896
36	6	0	5.011546	-1.661111	-1.926239
37	6	0	6.056173	-2.573427	-1.774078
38	6	0	6.530578	-2.910397	-0.503851
39	6	0	5.951682	-2.310269	0.616987
40	8	0	6.465697	-2.678236	1.830213
41	8	0	6.577161	-3.121848	-2.912921
42	8	0	4.478684	1.581327	1.012805
43	1	0	-0.570516	-0.438315	0.276573
44	1	0	-6.803728	-3.966258	-1.343796
45	1	0	-3.380242	-3.117437	1.142033
46	1	0	-4.779379	0.545680	-2.387784
47	1	0	-6.164078	0.833421	-1.348680
48	1	0	-4.069085	2.277058	-0.902130
49	1	0	-2.515001	0.336809	-1.162262
50	1	0	-5.096619	0.791090	1.266176
51	1	0	-3.134682	2.232960	2.291923
52	1	0	3.396969	2.366964	-1.427163
53	1	0	1.537602	5.194058	-2.449538
54	1	0	-1.355913	4.684068	-1.337438
55	1	0	-0.516384	0.791931	4.549749
56	1	0	-7.596350	-2.158534	-2.523021
57	1	0	-4.446148	-5.171114	0.971213
58	1	0	1.985189	-0.606371	0.400858
59	1	0	5.091897	-0.373056	2.419753
60	1	0	3.634821	-1.356338	2.266085
61	1	0	2.879797	0.864877	2.142206
62	1	0	4.633941	-1.407457	-2.909598
63	1	0	7.336495	-3.624923	-0.369846
64	1	0	5.983355	-2.236832	2.542155
65	1	0	7.286613	-3.735495	-2.676048
66	1	0	3.984805	2.387997	0.805174

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11A at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.815997	-2.950048	0.495209
2	6	0	6.367548	-2.667313	-0.759848
3	6	0	5.889364	-1.570785	-1.476991
4	6	0	4.871644	-0.738125	-0.978761
5	6	0	4.359484	-1.049237	0.285517
6	6	0	4.811270	-2.144808	1.029918
7	6	0	4.327242	0.420302	-1.781708
8	6	0	2.965194	0.870298	-1.237976
9	6	0	3.073737	0.968915	0.286199
10	8	0	3.362942	-0.306052	0.869888
11	8	0	1.936813	-0.069142	-1.551086
12	6	0	1.838111	1.502377	1.036442
13	6	0	2.084442	1.669678	2.515452
14	6	0	1.133652	1.062443	3.246840
15	6	0	0.138994	0.398881	2.377265
16	6	0	0.526395	0.655408	0.923952
17	6	0	-0.419061	1.592974	0.200510
18	6	0	0.248931	2.800439	0.011721
19	8	0	1.548115	2.816868	0.448166
20	6	0	-1.732313	1.443874	-0.255749
21	6	0	-2.346218	2.542306	-0.874182
22	6	0	-1.671908	3.756630	-1.025811
23	6	0	-0.346175	3.901601	-0.587657
24	8	0	-2.308096	4.807814	-1.621482
25	8	0	0.266680	5.111582	-0.787781
26	8	0	-0.811634	-0.232810	2.815663
27	8	0	1.001826	0.994089	4.580948
28	8	0	6.382307	-1.245921	-2.710145
29	8	0	6.315923	-4.034278	1.159324
30	6	0	-2.425620	0.105389	-0.157464
31	8	0	-3.849331	0.336829	-0.073479
32	6	0	-4.648013	-0.783748	-0.053138
33	6	0	-4.193388	-2.020026	-0.527271
34	6	0	-2.797425	-2.184808	-1.085541
35	6	0	-2.151262	-0.821384	-1.362372
36	6	0	-5.947817	-0.596172	0.430949
37	6	0	-6.819425	-1.684024	0.448954
38	6	0	-6.402437	-2.942645	-0.000587
39	6	0	-5.101769	-3.093453	-0.480317
40	8	0	-4.636932	-4.293947	-0.939072
41	8	0	-8.102522	-1.586322	0.907212
42	8	0	-2.616962	-0.237639	-2.575087
43	1	0	0.693188	-0.289362	0.403594
44	1	0	7.154229	-3.300723	-1.157580
45	1	0	4.379867	-2.342626	2.005797
46	1	0	5.020907	1.271803	-1.767758
47	1	0	4.222399	0.137808	-2.835162
48	1	0	2.718916	1.864485	-1.629454
49	1	0	3.901340	1.660387	0.501865
50	1	0	1.827292	-0.076293	-2.511371
51	1	0	2.931910	2.226704	2.896825
52	1	0	-1.694662	5.559076	-1.639587
53	1	0	-3.365022	2.469377	-1.233430
54	1	0	1.155861	5.088263	-0.405633
55	1	0	0.199803	0.466589	4.753513
56	1	0	7.050714	-1.895150	-2.970175
57	1	0	5.863384	-4.125475	2.009555
58	1	0	-2.104444	-0.408127	0.756277
59	1	0	-2.820836	-2.761507	-2.015608
60	1	0	-2.166374	-2.750228	-0.386651
61	1	0	-1.070550	-0.936493	-1.486480
62	1	0	-6.249704	0.383318	0.787445
63	1	0	-7.092457	-3.780130	0.028811
64	1	0	-5.344106	-4.952415	-0.891434
65	1	0	-8.275528	-0.674837	1.181658
66	1	0	-3.544184	0.007343	-2.440905

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11B at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.288841	3.533163	0.875536
2	6	0	5.593498	3.394834	0.388004
3	6	0	5.946354	2.221063	-0.278029
4	6	0	5.032015	1.172017	-0.479696
5	6	0	3.735177	1.360386	0.010093
6	6	0	3.348046	2.521500	0.688099
7	6	0	5.439609	-0.118597	-1.153181
8	6	0	4.421682	-1.223725	-0.867770
9	6	0	3.013175	-0.638518	-1.081410
10	8	0	2.758746	0.403496	-0.132710
11	8	0	4.627113	-1.658963	0.469665
12	6	0	1.840776	-1.623581	-0.972800
13	6	0	1.831579	-2.676232	-2.054072
14	6	0	0.671708	-2.669415	-2.735819
15	6	0	-0.244832	-1.627983	-2.221196
16	6	0	0.434044	-0.935385	-1.041590
17	6	0	-0.181823	-1.273711	0.301692
18	6	0	0.728654	-2.064384	1.000344
19	8	0	1.911055	-2.290156	0.342374
20	6	0	-1.411528	-0.945422	0.882902
21	6	0	-1.696064	-1.455269	2.157408
22	6	0	-0.787831	-2.278405	2.826329
23	6	0	0.454730	-2.594677	2.253002
24	8	0	-1.108631	-2.773902	4.055302
25	8	0	1.308728	-3.379430	2.985466
26	8	0	-1.346903	-1.414879	-2.702034
27	8	0	0.289224	-3.445630	-3.758490
28	8	0	7.207267	2.022962	-0.768152
29	8	0	3.991409	4.698810	1.523440
30	6	0	-2.377124	-0.015223	0.184862
31	8	0	-3.718273	-0.413962	0.547442
32	6	0	-4.740808	0.371091	0.066629
33	6	0	-4.521913	1.686775	-0.358487
34	6	0	-3.144726	2.310508	-0.309642
35	6	0	-2.191816	1.473381	0.553608
36	6	0	-6.011353	-0.215995	0.069736
37	6	0	-7.097707	0.535183	-0.376162
38	6	0	-6.922575	1.849408	-0.825909
39	6	0	-5.643811	2.405231	-0.811324
40	8	0	-5.409003	3.684108	-1.231836
41	8	0	-8.368723	0.035992	-0.407798
42	8	0	-2.391207	1.689872	1.946264
43	1	0	0.506317	0.140237	-1.228488
44	1	0	6.311126	4.195630	0.535929
45	1	0	2.328567	2.616081	1.047568
46	1	0	5.539658	0.014366	-2.238025
47	1	0	6.418990	-0.445141	-0.789798
48	1	0	4.571728	-2.048890	-1.579740
49	1	0	2.974968	-0.220243	-2.097695
50	1	0	3.813686	-2.098002	0.762276
51	1	0	2.663100	-3.348948	-2.221700
52	1	0	-0.381841	-3.349666	4.342650
53	1	0	-2.641755	-1.234470	2.635360
54	1	0	1.964672	-3.786507	2.401976
55	1	0	-0.608601	-3.158467	-4.009175
56	1	0	7.760369	2.785759	-0.548661
57	1	0	3.070219	4.675427	1.818372
58	1	0	-2.269074	-0.118372	-0.900759
59	1	0	-3.195525	3.323861	0.100972
60	1	0	-2.728071	2.406877	-1.321216
61	1	0	-1.156761	1.766104	0.354636
62	1	0	-6.126465	-1.239870	0.410228
63	1	0	-7.778575	2.416437	-1.177889
64	1	0	-6.244985	4.095870	-1.492106
65	1	0	-8.364438	-0.871680	-0.072740
66	1	0	-3.269581	1.348954	2.169626

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11C at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.805643	-2.949221	0.509594
2	6	0	6.360529	-2.670253	-0.745120
3	6	0	5.885905	-1.571564	-1.466136
4	6	0	4.871096	-0.737025	-0.970958
5	6	0	4.355735	-1.045920	0.294805
6	6	0	4.802522	-2.139518	1.040645
7	6	0	4.331266	0.422376	-1.775738
8	6	0	2.968393	0.875101	-1.236266
9	6	0	3.073083	0.975586	0.287991
10	8	0	3.359472	-0.298414	0.874458
11	8	0	1.939369	-0.062993	-1.551137
12	6	0	1.835473	1.509931	1.034467
13	6	0	2.079171	1.681232	2.513449
14	6	0	1.129041	1.073034	3.244881
15	6	0	0.137116	0.405335	2.375354
16	6	0	0.525398	0.660411	0.922027
17	6	0	-0.421146	1.595389	0.196726
18	6	0	0.245108	2.803538	0.006100
19	8	0	1.544253	2.822537	0.442475
20	6	0	-1.734162	1.443617	-0.259277
21	6	0	-2.349888	2.540315	-0.879038
22	6	0	-1.677519	3.755521	-1.032131
23	6	0	-0.351884	3.903007	-0.594506
24	8	0	-2.315469	4.805147	-1.628735
25	8	0	0.259159	5.113666	-0.796302
26	8	0	-0.812458	-0.227946	2.813761
27	8	0	0.995668	1.007034	4.578951
28	8	0	6.382693	-1.251144	-2.698801
29	8	0	6.220975	-4.007073	1.267876
30	6	0	-2.425143	0.104050	-0.159414
31	8	0	-3.849237	0.332958	-0.074201
32	6	0	-4.645655	-0.789214	-0.051910
33	6	0	-4.189224	-2.024935	-0.525765
34	6	0	-2.793602	-2.187460	-1.085554
35	6	0	-2.150352	-0.823001	-1.364017
36	6	0	-5.945151	-0.603937	0.433915
37	6	0	-6.814531	-1.693529	0.453963
38	6	0	-6.395674	-2.951612	0.004645
39	6	0	-5.095387	-3.100146	-0.476809
40	8	0	-4.628812	-4.300016	-0.935438
41	8	0	-8.097173	-1.598102	0.914004
42	8	0	-2.618629	-0.240992	-2.576576
43	1	0	0.694255	-0.284804	0.403168
44	1	0	7.148032	-3.297998	-1.154757
45	1	0	4.379330	-2.346842	2.016160
46	1	0	5.026306	1.272738	-1.759252
47	1	0	4.229398	0.140249	-2.829565
48	1	0	2.724834	1.869193	-1.629710
49	1	0	3.900243	1.667310	0.504761
50	1	0	1.832296	-0.070835	-2.511692
51	1	0	2.924853	2.241001	2.894776
52	1	0	-1.703582	5.557682	-1.646614
53	1	0	-3.368662	2.465367	-1.237963
54	1	0	1.146875	5.093426	-0.410590
55	1	0	0.195324	0.476992	4.751534
56	1	0	7.048470	-1.903079	-2.958546
57	1	0	6.920565	-4.484056	0.800041
58	1	0	-2.102242	-0.408292	0.754351
59	1	0	-2.816995	-2.764836	-2.015203
60	1	0	-2.160691	-2.751182	-0.386980
61	1	0	-1.069559	-0.936130	-1.489227
62	1	0	-6.248457	0.375175	0.790238
63	1	0	-7.083960	-3.790468	0.035650
64	1	0	-5.334476	-4.959961	-0.885921
65	1	0	-8.271477	-0.686881	1.188503
66	1	0	-3.546158	0.002286	-2.441381

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11D at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.805278	-2.965091	0.485381
2	6	0	6.363754	-2.673660	-0.764629
3	6	0	5.892276	-1.569868	-1.475041
4	6	0	4.874128	-0.738681	-0.975183
5	6	0	4.355019	-1.058620	0.284013
6	6	0	4.800141	-2.161449	1.021702
7	6	0	4.337172	0.427942	-1.771264
8	6	0	2.974555	0.879303	-1.229885
9	6	0	3.076110	0.963770	0.295581
10	8	0	3.357612	-0.317424	0.869420
11	8	0	1.942919	-0.051940	-1.556403
12	6	0	1.838579	1.494866	1.044403
13	6	0	2.079771	1.652560	2.525322
14	6	0	1.126209	1.041012	3.249443
15	6	0	0.134342	0.383580	2.372094
16	6	0	0.526043	0.650447	0.921848
17	6	0	-0.416095	1.594731	0.202745
18	6	0	0.254704	2.802075	0.023307
19	8	0	1.552745	2.813404	0.463330
20	6	0	-1.728794	1.451400	-0.257012
21	6	0	-2.339134	2.555153	-0.869570
22	6	0	-1.661930	3.768957	-1.012093
23	6	0	-0.336819	3.908266	-0.570269
24	8	0	-2.294645	4.825362	-1.602176
25	8	0	0.279098	5.118185	-0.761295
26	8	0	-0.817351	-0.251457	2.803318
27	8	0	0.989711	0.963586	4.582569
28	8	0	6.392537	-1.235907	-2.702794
29	8	0	6.299038	-4.056044	1.143075
30	6	0	-2.426034	0.114330	-0.167360
31	8	0	-3.849123	0.349215	-0.084209
32	6	0	-4.649867	-0.770303	-0.060173
33	6	0	-4.196206	-2.006873	-0.540281
34	6	0	-2.802928	-2.170213	-1.105950
35	6	0	-2.154742	-0.806518	-1.377346
36	6	0	-5.944618	-0.583718	0.430854
37	6	0	-6.816266	-1.671582	0.453498
38	6	0	-6.401709	-2.929674	-0.000466
39	6	0	-5.102020	-3.079555	-0.490183
40	8	0	-4.640969	-4.279483	-0.953884
41	8	0	-8.073504	-1.455224	0.942042
42	8	0	-2.622264	-0.215467	-2.585811
43	1	0	0.692996	-0.290542	0.394718
44	1	0	7.150711	-3.305965	-1.163589
45	1	0	4.363357	-2.365954	1.993804
46	1	0	5.034066	1.276609	-1.747906
47	1	0	4.235584	0.153935	-2.827261
48	1	0	2.735085	1.878217	-1.613440
49	1	0	3.905294	1.650076	0.521409
50	1	0	1.835409	-0.047040	-2.516929
51	1	0	2.926271	2.206602	2.913150
52	1	0	-1.680007	5.575783	-1.612974
53	1	0	-3.357649	2.487070	-1.230573
54	1	0	1.166181	5.091427	-0.374518
55	1	0	0.186695	0.435458	4.748579
56	1	0	7.062123	-1.883474	-2.963923
57	1	0	5.842214	-4.152818	1.990391
58	1	0	-2.107154	-0.405409	0.743650
59	1	0	-2.831028	-2.741528	-2.039229
60	1	0	-2.169933	-2.740644	-0.412884
61	1	0	-1.074517	-0.923432	-1.504211
62	1	0	-6.258664	0.388187	0.792037
63	1	0	-7.080024	-3.778910	0.026712
64	1	0	-5.347400	-4.938612	-0.905841
65	1	0	-8.576647	-2.280982	0.913730
66	1	0	-3.544911	0.041989	-2.443260

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11E at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.386208	-2.608343	0.401705
2	6	0	6.054117	-2.132211	-0.733293
3	6	0	5.604147	-0.959497	-1.343796
4	6	0	4.499811	-0.240997	-0.853722
5	6	0	3.872008	-0.748180	0.293305
6	6	0	4.293013	-1.919816	0.926025
7	6	0	3.993669	1.008506	-1.542973
8	6	0	2.558011	1.317158	-1.101065
9	6	0	2.509852	1.215362	0.431632
10	8	0	2.770149	-0.133665	0.845385
11	8	0	1.614714	0.451397	-1.729863
12	6	0	1.196775	1.627726	1.123719
13	6	0	1.309738	1.573843	2.625787
14	6	0	0.300456	0.872500	3.168982
15	6	0	-0.621676	0.380923	2.127115
16	6	0	-0.092080	0.815068	0.761191
17	6	0	-0.945214	1.826845	0.016198
18	6	0	-0.270875	3.050076	0.083212
19	8	0	0.946618	3.012087	0.711763
20	6	0	-2.146856	1.752755	-0.699440
21	6	0	-2.640546	2.931700	-1.285006
22	6	0	-1.972827	4.150005	-1.165560
23	6	0	-0.754564	4.223303	-0.473823
24	8	0	-2.493744	5.266131	-1.751770
25	8	0	-0.116117	5.434772	-0.422100
26	8	0	-1.619173	-0.272038	2.411152
27	8	0	0.049749	0.605058	4.459621
28	8	0	6.211145	-0.447384	-2.454450
29	8	0	5.771305	-3.748461	1.045713
30	6	0	-2.963534	0.493795	-0.921304
31	8	0	-2.135369	-0.644270	-0.628429
32	6	0	-2.730319	-1.882408	-0.618646
33	6	0	-4.118676	-2.036975	-0.549112
34	6	0	-5.037224	-0.839644	-0.485304
35	6	0	-4.270074	0.435044	-0.103825
36	6	0	-1.854004	-2.974013	-0.651082
37	6	0	-2.385603	-4.261997	-0.618531
38	6	0	-3.769633	-4.463700	-0.562185
39	6	0	-4.613426	-3.353867	-0.529316
40	8	0	-5.972978	-3.485223	-0.472186
41	8	0	-1.599193	-5.379142	-0.648905
42	8	0	-4.032341	0.530992	1.289402
43	1	0	0.124760	-0.068304	0.161953
44	1	0	6.910154	-2.667171	-1.136436
45	1	0	3.779852	-2.280531	1.809190
46	1	0	4.639629	1.867761	-1.320571
47	1	0	4.010962	0.880984	-2.629540
48	1	0	2.279249	2.330295	-1.398656
49	1	0	3.296085	1.872587	0.831044
50	1	0	1.916016	-0.459415	-1.596676
51	1	0	2.119125	2.056340	3.160534
52	1	0	-1.887282	6.004741	-1.585167
53	1	0	-3.558661	2.913698	-1.863967
54	1	0	0.720125	5.335243	0.055681
55	1	0	-0.771757	0.079471	4.479673
56	1	0	6.936189	-1.028290	-2.724760
57	1	0	6.535850	-4.133175	0.594773
58	1	0	-3.241696	0.446899	-1.984124
59	1	0	-5.829351	-1.002029	0.251892
60	1	0	-5.539908	-0.687673	-1.450486
61	1	0	-4.873901	1.307862	-0.373502
62	1	0	-0.784163	-2.801822	-0.707576
63	1	0	-4.166310	-5.473904	-0.546054
64	1	0	-6.203127	-4.424216	-0.435052
65	1	0	-0.669155	-5.114487	-0.681592
66	1	0	-3.244831	0.005354	1.521414

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11F at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.395988	-2.613035	0.396729
2	6	0	6.059646	-2.138368	-0.741180
3	6	0	5.607178	-0.969917	-1.352265
4	6	0	4.501345	-0.250308	-0.861109
5	6	0	3.877401	-0.754460	0.286807
6	6	0	4.302772	-1.925839	0.922430
7	6	0	3.992442	0.997007	-1.552163
8	6	0	2.558058	1.306079	-1.106483
9	6	0	2.514165	1.206888	0.426648
10	8	0	2.776504	-0.141468	0.842033
11	8	0	1.613273	0.438816	-1.730966
12	6	0	1.203135	1.620740	1.121449
13	6	0	1.318190	1.564601	2.623307
14	6	0	0.307818	0.865246	3.167022
15	6	0	-0.616811	0.376881	2.125790
16	6	0	-0.088529	0.811995	0.759742
17	6	0	-0.940163	1.827478	0.017786
18	6	0	-0.262185	3.048656	0.085336
19	8	0	0.956230	3.006268	0.711808
20	6	0	-2.143272	1.758089	-0.695923
21	6	0	-2.634422	2.939375	-1.278878
22	6	0	-1.962944	4.155550	-1.158845
23	6	0	-0.743299	4.224169	-0.469087
24	8	0	-2.481539	5.274028	-1.742566
25	8	0	-0.100947	5.433524	-0.416818
26	8	0	-1.614821	-0.275029	2.410514
27	8	0	0.058080	0.596641	4.457620
28	8	0	6.209574	-0.458509	-2.465913
29	8	0	5.876472	-3.761177	0.956836
30	6	0	-2.964527	0.502193	-0.917943
31	8	0	-2.139406	-0.639123	-0.628989
32	6	0	-2.738508	-1.875267	-0.620864
33	6	0	-4.127150	-2.025350	-0.547580
34	6	0	-5.041574	-0.825130	-0.478779
35	6	0	-4.269190	0.446428	-0.097216
36	6	0	-1.866036	-2.969770	-0.658905
37	6	0	-2.401821	-4.256041	-0.628264
38	6	0	-3.786334	-4.453237	-0.568038
39	6	0	-4.626265	-3.340641	-0.529661
40	8	0	-5.986053	-3.467614	-0.468696
41	8	0	-1.619087	-5.375626	-0.664135
42	8	0	-4.027535	0.539524	1.295487
43	1	0	0.124923	-0.070648	0.158198
44	1	0	6.912899	-2.683420	-1.131979
45	1	0	3.782337	-2.272066	1.809229
46	1	0	4.638937	1.857043	-1.334476
47	1	0	4.006134	0.866356	-2.638409
48	1	0	2.278035	2.318627	-1.404890
49	1	0	3.301433	1.864707	0.822904
50	1	0	1.917712	-0.471409	-1.600883
51	1	0	2.129559	2.044470	3.157421
52	1	0	-1.872960	6.010774	-1.575440
53	1	0	-3.553589	2.924857	-1.856252
54	1	0	0.734713	5.331202	0.061379
55	1	0	-0.765015	0.073517	4.477900
56	1	0	6.935336	-1.039132	-2.735129
57	1	0	5.339992	-3.991294	1.728565
58	1	0	-3.245515	0.457938	-1.980118
59	1	0	-5.832189	-0.986298	0.260296
60	1	0	-5.546425	-0.669712	-1.442286
61	1	0	-4.870843	1.321628	-0.363938
62	1	0	-0.795814	-2.801032	-0.718358
63	1	0	-4.186452	-5.462112	-0.553595
64	1	0	-6.219209	-4.405936	-0.433311
65	1	0	-0.688400	-5.113716	-0.700514
66	1	0	-3.242190	0.009557	1.524787

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11G at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.776825	3.053846	-1.993376
2	6	0	-4.976390	3.286288	-1.310944
3	6	0	-5.277570	2.513822	-0.189133
4	6	0	-4.411987	1.510769	0.281968
5	6	0	-3.216979	1.324344	-0.421558
6	6	0	-2.885715	2.075722	-1.554445
7	6	0	-4.772743	0.641535	1.465504
8	6	0	-3.891596	-0.607392	1.509759
9	6	0	-2.434826	-0.167899	1.269194
10	8	0	-2.294961	0.376024	-0.047623
11	8	0	-4.357562	-1.495801	0.502693
12	6	0	-1.361043	-1.255921	1.416377
13	6	0	-1.219034	-1.764056	2.828378
14	6	0	0.054156	-1.671986	3.251394
15	6	0	0.927301	-1.111743	2.199025
16	6	0	0.068768	-0.792320	0.974928
17	6	0	0.345597	-1.621729	-0.265864
18	6	0	-0.716255	-2.521810	-0.401537
19	8	0	-1.707546	-2.388173	0.537457
20	6	0	1.356808	-1.611894	-1.234844
21	6	0	1.282608	-2.552453	-2.276514
22	6	0	0.248016	-3.483834	-2.353658
23	6	0	-0.785923	-3.475661	-1.404113
24	8	0	0.225344	-4.387137	-3.372941
25	8	0	-1.811493	-4.371949	-1.571757
26	8	0	2.127650	-0.953942	2.378390
27	8	0	0.578128	-2.021367	4.433384
28	8	0	-6.437431	2.686896	0.514011
29	8	0	-3.526436	3.833658	-3.087131
30	6	0	2.530561	-0.651755	-1.272667
31	8	0	2.242667	0.454328	-0.401566
32	6	0	3.240427	1.378109	-0.199131
33	6	0	4.578023	1.096762	-0.494220
34	6	0	4.991932	-0.240634	-1.061826
35	6	0	3.883206	-1.291493	-0.898662
36	6	0	2.831454	2.600147	0.347824
37	6	0	3.794117	3.575264	0.603594
38	6	0	5.143380	3.341687	0.312926
39	6	0	5.515482	2.112282	-0.230201
40	8	0	6.816461	1.823284	-0.534016
41	8	0	3.478486	4.794595	1.133157
42	8	0	3.859489	-1.863824	0.397021
43	1	0	0.117481	0.280041	0.777603
44	1	0	-5.654575	4.057456	-1.662140
45	1	0	-1.945229	1.891016	-2.063220
46	1	0	-4.670157	1.193483	2.408457
47	1	0	-5.819596	0.328320	1.402794
48	1	0	-3.962791	-1.067461	2.506532
49	1	0	-2.192021	0.609164	2.009002
50	1	0	-3.641659	-2.122492	0.315343
51	1	0	-2.050712	-2.161749	3.396099
52	1	0	-0.546590	-4.961439	-3.243503
53	1	0	2.038792	-2.569234	-3.054964
54	1	0	-2.261660	-4.517570	-0.727416
55	1	0	1.532174	-1.823175	4.387627
56	1	0	-6.971631	3.372739	0.089397
57	1	0	-2.676658	3.579157	-3.473386
58	1	0	2.623941	-0.263432	-2.297107
59	1	0	5.893377	-0.608002	-0.562050
60	1	0	5.247410	-0.142766	-2.125900
61	1	0	4.070151	-2.115782	-1.594750
62	1	0	1.779831	2.770736	0.553868
63	1	0	5.878443	4.115371	0.511166
64	1	0	7.377984	2.572459	-0.290123
65	1	0	2.525612	4.836328	1.295637
66	1	0	3.376008	-1.273886	1.003342

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11H at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.391597	-2.622348	0.399597
2	6	0	6.056921	-2.150159	-0.738372
3	6	0	5.606791	-0.981816	-1.351369
4	6	0	4.501969	-0.259614	-0.861809
5	6	0	3.876570	-0.761181	0.286442
6	6	0	4.299343	-1.932522	0.923774
7	6	0	3.995356	0.987477	-1.554953
8	6	0	2.561825	1.300964	-1.109362
9	6	0	2.517994	1.203385	0.423852
10	8	0	2.776750	-0.145202	0.840470
11	8	0	1.614213	0.436267	-1.732904
12	6	0	1.208331	1.621235	1.118843
13	6	0	1.324636	1.567074	2.620695
14	6	0	0.313445	0.870477	3.166351
15	6	0	-0.613357	0.382858	2.126712
16	6	0	-0.085391	0.814679	0.759508
17	6	0	-0.935647	1.831003	0.017100
18	6	0	-0.255119	3.050884	0.082458
19	8	0	0.963979	3.006714	0.707461
20	6	0	-2.139741	1.763278	-0.695118
21	6	0	-2.629301	2.944923	-1.278687
22	6	0	-1.955251	4.159875	-1.160765
23	6	0	-0.734594	4.226760	-0.472623
24	8	0	-2.472309	5.278820	-1.745041
25	8	0	-0.089709	5.434892	-0.422479
26	8	0	-1.612805	-0.265918	2.413540
27	8	0	0.064306	0.604203	4.457573
28	8	0	6.210792	-0.472995	-2.465417
29	8	0	5.869818	-3.770562	0.961529
30	6	0	-2.963000	0.508342	-0.915354
31	8	0	-2.139192	-0.633270	-0.625405
32	6	0	-2.737884	-1.869866	-0.618957
33	6	0	-4.128759	-2.017399	-0.543930
34	6	0	-5.041356	-0.815733	-0.474320
35	6	0	-4.267147	0.455019	-0.093779
36	6	0	-1.868017	-2.963379	-0.659765
37	6	0	-2.404814	-4.249382	-0.630872
38	6	0	-3.789659	-4.445097	-0.568301
39	6	0	-4.629713	-3.329738	-0.526606
40	8	0	-5.989340	-3.456416	-0.463579
41	8	0	-1.525894	-5.294920	-0.674870
42	8	0	-4.024541	0.548270	1.298720
43	1	0	0.125189	-0.069547	0.159266
44	1	0	6.909406	-2.697249	-1.127974
45	1	0	3.777307	-2.276958	1.810319
46	1	0	4.643896	1.846501	-1.339276
47	1	0	4.008228	0.854705	-2.640964
48	1	0	2.284900	2.314127	-1.408645
49	1	0	3.307160	1.859505	0.819224
50	1	0	1.914335	-0.475059	-1.600451
51	1	0	2.137498	2.046056	3.153336
52	1	0	-1.861845	6.014399	-1.579659
53	1	0	-3.549127	2.931551	-1.855048
54	1	0	0.746303	5.331364	0.054845
55	1	0	-0.759630	0.082450	4.479163
56	1	0	6.934938	-1.055922	-2.734010
57	1	0	5.331013	-3.999951	1.731854
58	1	0	-3.244776	0.463695	-1.977353
59	1	0	-5.831875	-0.975642	0.265138
60	1	0	-5.546434	-0.659687	-1.437633
61	1	0	-4.868024	1.330760	-0.360591
62	1	0	-0.796998	-2.811559	-0.719764
63	1	0	-4.206765	-5.448943	-0.553993
64	1	0	-6.224696	-4.394057	-0.426696
65	1	0	-2.016272	-6.128650	-0.657560
66	1	0	-3.238434	0.019063	1.527353

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11l at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.408798	-2.592062	0.407698
2	6	0	6.062894	-2.127589	-0.739908
3	6	0	5.601335	-0.968211	-1.361383
4	6	0	4.496427	-0.247038	-0.870448
5	6	0	3.882010	-0.740945	0.287016
6	6	0	4.316218	-1.903429	0.932842
7	6	0	3.979125	0.991605	-1.570815
8	6	0	2.546644	1.300978	-1.119298
9	6	0	2.512061	1.216620	0.415002
10	8	0	2.781962	-0.126454	0.842311
11	8	0	1.600643	0.425080	-1.729738
12	6	0	1.203392	1.631812	1.113380
13	6	0	1.325990	1.586705	2.615006
14	6	0	0.319309	0.889985	3.169043
15	6	0	-0.610358	0.394122	2.136113
16	6	0	-0.087806	0.817116	0.764252
17	6	0	-0.944993	1.823738	0.017129
18	6	0	-0.270968	3.047690	0.073314
19	8	0	0.950049	3.013701	0.695014
20	6	0	-2.150836	1.745348	-0.690806
21	6	0	-2.649056	2.920572	-1.279908
22	6	0	-1.981273	4.139847	-1.171175
23	6	0	-0.758802	4.217550	-0.487239
24	8	0	-2.506289	5.252252	-1.760335
25	8	0	-0.121015	5.429496	-0.446265
26	8	0	-1.608942	-0.252966	2.430166
27	8	0	0.076493	0.631379	4.462962
28	8	0	6.193638	-0.467642	-2.485325
29	8	0	5.897732	-3.731777	0.977564
30	6	0	-2.966859	0.484237	-0.902550
31	8	0	-2.140439	-0.651457	-0.601217
32	6	0	-2.733949	-1.890555	-0.602609
33	6	0	-4.124488	-2.048164	-0.536556
34	6	0	-5.040384	-0.846279	-0.461256
35	6	0	-4.269087	0.429281	-0.079403
36	6	0	-1.857299	-2.979001	-0.642384
37	6	0	-2.387105	-4.269830	-0.622321
38	6	0	-3.768495	-4.474616	-0.573154
39	6	0	-4.616105	-3.368033	-0.534257
40	8	0	-5.956765	-3.631234	-0.486143
41	8	0	-1.595395	-5.382830	-0.660534
42	8	0	-4.028145	0.519110	1.311221
43	1	0	0.125362	-0.070740	0.170334
44	1	0	6.916430	-2.672982	-1.129597
45	1	0	3.803010	-2.241740	1.826869
46	1	0	4.624349	1.855705	-1.365818
47	1	0	3.986347	0.850126	-2.655757
48	1	0	2.262034	2.309837	-1.425873
49	1	0	3.298827	1.881454	0.800392
50	1	0	1.909382	-0.482929	-1.594390
51	1	0	2.139179	2.071730	3.141620
52	1	0	-1.899511	5.992315	-1.601423
53	1	0	-3.570424	2.898798	-1.853527
54	1	0	0.717623	5.333919	0.028126
55	1	0	-0.746309	0.108319	4.492206
56	1	0	6.916214	-1.051504	-2.756114
57	1	0	5.366781	-3.955744	1.754908
58	1	0	-3.248064	0.429771	-1.964150
59	1	0	-5.819881	-0.986695	0.298622
60	1	0	-5.553831	-0.681938	-1.419362
61	1	0	-4.876172	1.300154	-0.346770
62	1	0	-0.787821	-2.803578	-0.695473
63	1	0	-4.178223	-5.477745	-0.568141
64	1	0	-6.456173	-2.803423	-0.493141
65	1	0	-0.666603	-5.113792	-0.691740
66	1	0	-3.228769	0.008712	1.538787

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11J at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.399929	-2.603790	0.406715
2	6	0	6.056785	-2.140094	-0.739629
3	6	0	5.599507	-0.978665	-1.360421
4	6	0	4.496335	-0.254574	-0.869948
5	6	0	3.879319	-0.747659	0.286490
6	6	0	4.309090	-1.912194	0.931518
7	6	0	3.982904	0.985835	-1.570059
8	6	0	2.551022	1.299271	-1.119253
9	6	0	2.515346	1.214080	0.414927
10	8	0	2.781077	-0.129933	0.841680
11	8	0	1.602447	0.427157	-1.730897
12	6	0	1.207564	1.632361	1.113172
13	6	0	1.330483	1.587755	2.614800
14	6	0	0.322410	0.893565	3.169446
15	6	0	-0.608901	0.399718	2.137055
16	6	0	-0.085256	0.819999	0.764770
17	6	0	-0.940473	1.827622	0.016824
18	6	0	-0.264387	3.050445	0.072550
19	8	0	0.956562	3.014631	0.694302
20	6	0	-2.146408	1.750864	-0.691105
21	6	0	-2.642751	2.926636	-1.280695
22	6	0	-1.972909	4.144832	-1.172482
23	6	0	-0.750297	4.220831	-0.488594
24	8	0	-2.496040	5.257901	-1.762176
25	8	0	-0.110584	5.431835	-0.448092
26	8	0	-1.609683	-0.243597	2.431922
27	8	0	0.079257	0.636301	4.463591
28	8	0	6.194694	-0.478786	-2.483229
29	8	0	5.884801	-3.745573	0.975954
30	6	0	-2.963460	0.490340	-0.902947
31	8	0	-2.138170	-0.645233	-0.599694
32	6	0	-2.730453	-1.885167	-0.601734
33	6	0	-4.123381	-2.041068	-0.536321
34	6	0	-5.038321	-0.838203	-0.463564
35	6	0	-4.266604	0.436920	-0.081266
36	6	0	-1.855427	-2.972100	-0.640657
37	6	0	-2.385641	-4.262831	-0.620436
38	6	0	-3.767096	-4.466904	-0.571357
39	6	0	-4.615686	-3.358329	-0.533177
40	8	0	-5.955723	-3.623854	-0.485440
41	8	0	-1.499010	-5.301684	-0.661232
42	8	0	-4.027226	0.526776	1.309660
43	1	0	0.125807	-0.069199	0.172106
44	1	0	6.908734	-2.687999	-1.129244
45	1	0	3.793390	-2.250145	1.824237
46	1	0	4.630455	1.848066	-1.364479
47	1	0	3.990251	0.844655	-2.655043
48	1	0	2.269946	2.309326	-1.425208
49	1	0	3.303868	1.876462	0.801028
50	1	0	1.906766	-0.482229	-1.594711
51	1	0	2.144903	2.071201	3.140964
52	1	0	-1.887513	5.996737	-1.604273
53	1	0	-3.564035	2.906120	-1.854503
54	1	0	0.728853	5.334620	0.024546
55	1	0	-0.744602	0.114940	4.493226
56	1	0	6.915768	-1.064649	-2.753697
57	1	0	5.350947	-3.969904	1.751199
58	1	0	-3.243571	0.435785	-1.964887
59	1	0	-5.819655	-0.977223	0.294696
60	1	0	-5.549468	-0.673965	-1.422920
61	1	0	-4.872881	1.308082	-0.349636
62	1	0	-0.785066	-2.813127	-0.692729
63	1	0	-4.192832	-5.465325	-0.564924
64	1	0	-6.456413	-2.796740	-0.491353
65	1	0	-1.985369	-6.137992	-0.650802
66	1	0	-3.226953	0.017967	1.537866

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11K at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.440695	-2.567254	0.426437
2	6	0	6.086459	-2.107761	-0.728014
3	6	0	5.608008	-0.959124	-1.362206
4	6	0	4.498232	-0.246969	-0.875282
5	6	0	3.891978	-0.737728	0.290295
6	6	0	4.340463	-1.886245	0.945941
7	6	0	3.967024	0.980561	-1.584961
8	6	0	2.534812	1.284802	-1.128899
9	6	0	2.507926	1.210384	0.406053
10	8	0	2.785112	-0.128989	0.839352
11	8	0	1.591085	0.399350	-1.729089
12	6	0	1.201677	1.625864	1.108558
13	6	0	1.328784	1.581035	2.609784
14	6	0	0.321553	0.887843	3.167289
15	6	0	-0.612786	0.394312	2.137520
16	6	0	-0.092012	0.813331	0.763776
17	6	0	-0.948782	1.820233	0.016651
18	6	0	-0.273197	3.043418	0.071032
19	8	0	0.948836	3.008217	0.690481
20	6	0	-2.156133	1.742989	-0.688814
21	6	0	-2.654054	2.918539	-1.277548
22	6	0	-1.984634	4.137076	-1.170563
23	6	0	-0.760754	4.213626	-0.489039
24	8	0	-2.509514	5.249884	-1.759108
25	8	0	-0.121536	5.424890	-0.449613
26	8	0	-1.613433	-0.248093	2.434768
27	8	0	0.081714	0.631340	4.462185
28	8	0	6.191492	-0.465184	-2.493519
29	8	0	5.855084	-3.682913	1.094571
30	6	0	-2.974024	0.482738	-0.898521
31	8	0	-2.149457	-0.653799	-0.595624
32	6	0	-2.744951	-1.892001	-0.598008
33	6	0	-4.135797	-2.047161	-0.532763
34	6	0	-5.049658	-0.843791	-0.456165
35	6	0	-4.275989	0.430522	-0.074874
36	6	0	-1.870167	-2.981891	-0.638130
37	6	0	-2.402274	-4.271810	-0.619467
38	6	0	-3.784072	-4.474183	-0.571607
39	6	0	-4.629750	-3.366144	-0.532139
40	8	0	-5.970934	-3.626984	-0.485198
41	8	0	-1.612532	-5.386162	-0.658144
42	8	0	-4.034114	0.520082	1.315634
43	1	0	0.117730	-0.076304	0.171353
44	1	0	6.949024	-2.635783	-1.126470
45	1	0	3.843791	-2.234210	1.843531
46	1	0	4.607006	1.851244	-1.391560
47	1	0	3.969545	0.828927	-2.668556
48	1	0	2.243083	2.289739	-1.441658
49	1	0	3.293866	1.880751	0.783602
50	1	0	1.899886	-0.506325	-1.579112
51	1	0	2.145030	2.063763	3.133735
52	1	0	-1.901647	5.989313	-1.601412
53	1	0	-3.576565	2.897674	-1.849362
54	1	0	0.717897	5.328453	0.023204
55	1	0	-0.742296	0.110403	4.494440
56	1	0	6.915389	-1.046676	-2.765623
57	1	0	6.623383	-4.062763	0.645869
58	1	0	-3.255570	0.427179	-1.959989
59	1	0	-5.828582	-0.983251	0.304486
60	1	0	-5.563867	-0.678376	-1.413685
61	1	0	-4.881744	1.302363	-0.342152
62	1	0	-0.800349	-2.808329	-0.690334
63	1	0	-4.195586	-5.476585	-0.567694
64	1	0	-6.468790	-2.798229	-0.490684
65	1	0	-0.683146	-5.118795	-0.686012
66	1	0	-3.233371	0.011443	1.542508

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11L at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.810962	-2.949682	0.487429
2	6	0	6.368198	-2.657379	-0.762932
3	6	0	5.893356	-1.555342	-1.473828
4	6	0	4.872955	-0.726809	-0.974134
5	6	0	4.355083	-1.047604	0.285335
6	6	0	4.803611	-2.148670	1.023556
7	6	0	4.332659	0.438026	-1.770541
8	6	0	2.968811	0.885649	-1.229281
9	6	0	3.070222	0.971037	0.296173
10	8	0	3.355607	-0.308997	0.870576
11	8	0	1.939789	-0.048757	-1.555459
12	6	0	1.831018	1.498449	1.044811
13	6	0	2.070927	1.656573	2.525858
14	6	0	1.118559	1.042464	3.249499
15	6	0	0.128784	0.382767	2.371598
16	6	0	0.521168	0.650150	0.921637
17	6	0	-0.423206	1.591296	0.201640
18	6	0	0.243819	2.800784	0.022722
19	8	0	1.541300	2.816163	0.463657
20	6	0	-1.735259	1.444367	-0.258571
21	6	0	-2.349077	2.546112	-0.871157
22	6	0	-1.675421	3.761957	-1.013473
23	6	0	-0.350863	3.905180	-0.571187
24	8	0	-2.311319	4.816215	-1.603447
25	8	0	0.261162	5.116831	-0.761773
26	8	0	-0.822330	-0.254029	2.801514
27	8	0	0.981840	0.964970	4.582552
28	8	0	6.392271	-1.220606	-2.701892
29	8	0	6.308059	-4.038778	1.145628
30	6	0	-2.428362	0.105071	-0.168350
31	8	0	-3.852335	0.333609	-0.097085
32	6	0	-4.647614	-0.789921	-0.067981
33	6	0	-4.189856	-2.029135	-0.538219
34	6	0	-2.792283	-2.183695	-1.101980
35	6	0	-2.148801	-0.815381	-1.375823
36	6	0	-5.944355	-0.603669	0.418386
37	6	0	-6.814377	-1.694894	0.444412
38	6	0	-6.395714	-2.952954	0.002854
39	6	0	-5.096026	-3.105784	-0.478592
40	8	0	-4.748067	-4.358071	-0.901436
41	8	0	-8.095966	-1.594233	0.905841
42	8	0	-2.617744	-0.232807	-2.585325
43	1	0	0.691573	-0.290602	0.395189
44	1	0	7.156905	-3.287582	-1.161743
45	1	0	4.367852	-2.353794	1.995981
46	1	0	5.027092	1.288705	-1.747411
47	1	0	4.231924	0.163542	-2.826503
48	1	0	2.726372	1.883680	-1.613286
49	1	0	3.897218	1.660057	0.521698
50	1	0	1.834036	-0.046235	-2.516198
51	1	0	2.915693	2.212847	2.914248
52	1	0	-1.699104	5.568628	-1.614541
53	1	0	-3.367594	2.475801	-1.231774
54	1	0	1.148678	5.092756	-0.375766
55	1	0	0.180138	0.435006	4.748833
56	1	0	7.063850	-1.866203	-2.962790
57	1	0	5.852089	-4.136121	1.993344
58	1	0	-2.112951	-0.411533	0.745629
59	1	0	-2.804857	-2.735399	-2.050843
60	1	0	-2.148976	-2.747422	-0.411759
61	1	0	-1.068499	-0.931770	-1.499785
62	1	0	-6.246802	0.377105	0.770778
63	1	0	-7.070043	-3.800652	0.032807
64	1	0	-3.825594	-4.365960	-1.190666
65	1	0	-8.268710	-0.680988	1.174406
66	1	0	-3.531923	0.050260	-2.435819

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11M at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.441686	-2.572532	0.431701
2	6	0	6.086604	-2.117345	-0.724932
3	6	0	5.607839	-0.971003	-1.363009
4	6	0	4.498762	-0.256721	-0.877669
5	6	0	3.893390	-0.743170	0.290159
6	6	0	4.342082	-1.889371	0.949637
7	6	0	3.967326	0.968457	-1.591233
8	6	0	2.536180	1.276372	-1.134021
9	6	0	2.511381	1.206420	0.401180
10	8	0	2.787125	-0.132075	0.837845
11	8	0	1.589918	0.391224	-1.730426
12	6	0	1.206951	1.625903	1.104636
13	6	0	1.336185	1.583348	2.605770
14	6	0	0.328175	0.893495	3.165933
15	6	0	-0.609032	0.400696	2.138412
16	6	0	-0.089186	0.815779	0.763158
17	6	0	-0.944778	1.823526	0.015751
18	6	0	-0.266478	3.045326	0.067510
19	8	0	0.956642	3.008167	0.684668
20	6	0	-2.153561	1.748144	-0.687490
21	6	0	-2.650157	2.924165	-1.276406
22	6	0	-1.978009	4.141406	-1.171854
23	6	0	-0.752641	4.216006	-0.492787
24	8	0	-2.501649	5.254814	-1.760468
25	8	0	-0.110713	5.425950	-0.455836
26	8	0	-1.611155	-0.238092	2.438472
27	8	0	0.089477	0.639803	4.461619
28	8	0	6.190551	-0.481322	-2.496649
29	8	0	5.856686	-3.685669	1.103681
30	6	0	-2.973600	0.488915	-0.895210
31	8	0	-2.150234	-0.647915	-0.591684
32	6	0	-2.745267	-1.886609	-0.595863
33	6	0	-4.138455	-2.039176	-0.528303
34	6	0	-5.050482	-0.834375	-0.450646
35	6	0	-4.274824	0.439065	-0.070332
36	6	0	-1.872964	-2.975500	-0.639428
37	6	0	-2.406330	-4.264987	-0.622013
38	6	0	-3.788217	-4.465763	-0.571095
39	6	0	-4.633995	-3.355221	-0.528112
40	8	0	-5.974629	-3.617544	-0.478808
41	8	0	-1.522350	-5.305856	-0.667744
42	8	0	-4.031589	0.528533	1.319892
43	1	0	0.117129	-0.075610	0.172168
44	1	0	6.948733	-2.647020	-1.122129
45	1	0	3.845653	-2.234229	1.848551
46	1	0	4.608574	1.839254	-1.402474
47	1	0	3.967734	0.812537	-2.674229
48	1	0	2.245963	2.280995	-1.449275
49	1	0	3.298909	1.876675	0.775671
50	1	0	1.895222	-0.514875	-1.575847
51	1	0	2.154385	2.065023	3.127641
52	1	0	-1.891877	5.993069	-1.604650
53	1	0	-3.573697	2.904568	-1.846604
54	1	0	0.729123	5.328264	0.016001
55	1	0	-0.735517	0.120534	4.495701
56	1	0	6.913242	-1.064693	-2.767935
57	1	0	6.623267	-4.068352	0.654457
58	1	0	-3.256311	0.433082	-1.956403
59	1	0	-5.829240	-0.972612	0.310420
60	1	0	-5.564975	-0.668147	-1.407894
61	1	0	-4.879843	1.311517	-0.337403
62	1	0	-0.802313	-2.818982	-0.692912
63	1	0	-4.216431	-5.463141	-0.566846
64	1	0	-6.473241	-2.789162	-0.481301
65	1	0	-2.010641	-6.141037	-0.657633
66	1	0	-3.230004	0.020701	1.545754

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11N at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.802456	-2.962881	0.479183
2	6	0	6.365114	-2.663786	-0.767143
3	6	0	5.895656	-1.555966	-1.472615
4	6	0	4.875133	-0.728413	-0.971520
5	6	0	4.351810	-1.056113	0.283895
6	6	0	4.794950	-2.162989	1.016676
7	6	0	4.340725	0.442898	-1.762392
8	6	0	2.976452	0.891525	-1.222918
9	6	0	3.072493	0.965932	0.303425
10	8	0	3.351862	-0.318914	0.870078
11	8	0	1.945045	-0.036566	-1.559416
12	6	0	1.831980	1.491759	1.051077
13	6	0	2.067971	1.641804	2.533614
14	6	0	1.113300	1.024410	3.251372
15	6	0	0.125461	0.370180	2.367277
16	6	0	0.521122	0.646113	0.919831
17	6	0	-0.420344	1.593209	0.203714
18	6	0	0.249428	2.802292	0.032459
19	8	0	1.546094	2.812853	0.475981
20	6	0	-1.732082	1.451634	-0.259185
21	6	0	-2.342615	2.558050	-0.866660
22	6	0	-1.666126	3.773178	-1.001437
23	6	0	-0.341956	3.911141	-0.556375
24	8	0	-2.298873	4.832017	-1.586548
25	8	0	0.273062	5.122453	-0.739455
26	8	0	-0.826575	-0.269108	2.791429
27	8	0	0.973032	0.939365	4.583587
28	8	0	6.400268	-1.214150	-2.696386
29	8	0	6.294562	-4.057371	1.132177
30	6	0	-2.429013	0.113828	-0.176096
31	8	0	-3.852313	0.345940	-0.105932
32	6	0	-4.650095	-0.776197	-0.073582
33	6	0	-4.193251	-2.016130	-0.549074
34	6	0	-2.797719	-2.170232	-1.118239
35	6	0	-2.151985	-0.801983	-1.387588
36	6	0	-5.942197	-0.590230	0.418642
37	6	0	-6.812425	-1.681295	0.448528
38	6	0	-6.396417	-2.938724	0.002772
39	6	0	-5.097508	-3.091372	-0.487187
40	8	0	-4.755008	-4.343824	-0.913374
41	8	0	-8.068780	-1.463334	0.938036
42	8	0	-2.622100	-0.213349	-2.593712
43	1	0	0.691163	-0.291501	0.387693
44	1	0	7.153915	-3.293229	-1.166980
45	1	0	4.354965	-2.373365	1.986072
46	1	0	5.037664	1.291300	-1.731835
47	1	0	4.242559	0.175156	-2.820312
48	1	0	2.739167	1.893155	-1.600693
49	1	0	3.900785	1.650780	0.536764
50	1	0	1.840750	-0.024646	-2.520244
51	1	0	2.912156	2.195308	2.927198
52	1	0	-1.685403	5.583470	-1.591590
53	1	0	-3.360981	2.492172	-1.228529
54	1	0	1.158828	5.095157	-0.349658
55	1	0	0.170362	0.409222	4.744620
56	1	0	7.072432	-1.858706	-2.958344
57	1	0	5.835420	-4.158938	1.977680
58	1	0	-2.115849	-0.407920	0.735732
59	1	0	-2.813942	-2.717784	-2.069458
60	1	0	-2.153340	-2.738032	-0.432324
61	1	0	-1.072100	-0.920224	-1.513639
62	1	0	-6.256809	0.383082	0.775416
63	1	0	-7.059808	-3.797407	0.029285
64	1	0	-3.834679	-4.352967	-1.209544
65	1	0	-8.569072	-2.291135	0.915958
66	1	0	-3.532294	0.079102	-2.437695

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11O at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.979681	-2.842595	0.514427
2	6	0	6.514431	-2.547258	-0.742500
3	6	0	5.978548	-1.489075	-1.479467
4	6	0	4.910949	-0.709982	-0.996193
5	6	0	4.419561	-1.032907	0.280288
6	6	0	4.930600	-2.085354	1.038773
7	6	0	4.296563	0.412420	-1.810811
8	6	0	2.914865	0.788171	-1.256841
9	6	0	3.050363	0.927454	0.268107
10	8	0	3.368313	-0.344870	0.845893
11	8	0	1.923170	-0.166702	-1.630813
12	6	0	1.820340	1.452683	1.029508
13	6	0	2.071179	1.603821	2.509072
14	6	0	1.119232	0.993766	3.236872
15	6	0	0.118405	0.344641	2.363592
16	6	0	0.501800	0.616711	0.911795
17	6	0	-0.439685	1.569558	0.203371
18	6	0	0.236182	2.774217	0.025442
19	8	0	1.539030	2.774351	0.452012
20	6	0	-1.756338	1.434930	-0.248181
21	6	0	-2.365691	2.545761	-0.848214
22	6	0	-1.683910	3.757511	-0.987306
23	6	0	-0.354543	3.887575	-0.555427
24	8	0	-2.316361	4.820609	-1.564768
25	8	0	0.265334	5.095596	-0.743368
26	8	0	-0.833655	-0.287865	2.796866
27	8	0	0.991214	0.912810	4.570264
28	8	0	6.543945	-1.257666	-2.700812
29	8	0	6.455449	-3.862749	1.285837
30	6	0	-2.458029	0.099881	-0.166265
31	8	0	-3.878458	0.339835	-0.055024
32	6	0	-4.684896	-0.775407	-0.044879
33	6	0	-4.246519	-2.005240	-0.550241
34	6	0	-2.860427	-2.168625	-1.133073
35	6	0	-2.209762	-0.804296	-1.394193
36	6	0	-5.975849	-0.588364	0.462525
37	6	0	-6.855002	-1.670231	0.472283
38	6	0	-6.454013	-2.922561	-0.008278
39	6	0	-5.162041	-3.072920	-0.511016
40	8	0	-4.713285	-4.267109	-1.001187
41	8	0	-8.130285	-1.572759	0.951831
42	8	0	-2.692908	-0.193992	-2.586642
43	1	0	0.655262	-0.323479	0.379371
44	1	0	7.337899	-3.119960	-1.157081
45	1	0	4.521261	-2.303248	2.017734
46	1	0	4.939353	1.302848	-1.812307
47	1	0	4.159710	0.115197	-2.858198
48	1	0	2.588233	1.741157	-1.677430
49	1	0	3.871495	1.631398	0.466812
50	1	0	2.248494	-1.045328	-1.384932
51	1	0	2.922331	2.152874	2.893541
52	1	0	-1.697395	5.567424	-1.578956
53	1	0	-3.386614	2.484526	-1.203499
54	1	0	1.157888	5.060610	-0.370049
55	1	0	0.187259	0.387697	4.740960
56	1	0	6.143059	-0.480944	-3.113889
57	1	0	7.177784	-4.308318	0.821246
58	1	0	-2.126946	-0.434532	0.731781
59	1	0	-2.902102	-2.727280	-2.073428
60	1	0	-2.222579	-2.751231	-0.454756
61	1	0	-1.132144	-0.923535	-1.539874
62	1	0	-6.265151	0.386009	0.842710
63	1	0	-7.149673	-3.755538	0.014980
64	1	0	-5.424924	-4.921058	-0.957530
65	1	0	-8.292707	-0.665624	1.246424
66	1	0	-3.617782	0.048716	-2.433356

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11P at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.807208	-2.958167	0.498417
2	6	0	6.370461	-2.671235	-0.747624
3	6	0	5.901136	-1.570400	-1.468236
4	6	0	4.875570	-0.741957	-0.979965
5	6	0	4.353811	-1.057730	0.284563
6	6	0	4.798080	-2.151897	1.027392
7	6	0	4.324755	0.418088	-1.781454
8	6	0	2.960720	0.869148	-1.235820
9	6	0	3.072301	0.963466	0.287709
10	8	0	3.352810	-0.315471	0.863307
11	8	0	1.934016	-0.068305	-1.552550
12	6	0	1.838505	1.500563	1.038576
13	6	0	2.087553	1.669254	2.516854
14	6	0	1.136147	1.065579	3.250462
15	6	0	0.138512	0.403175	2.383210
16	6	0	0.525748	0.654968	0.928925
17	6	0	-0.418610	1.591419	0.202855
18	6	0	0.250169	2.798113	0.011870
19	8	0	1.549697	2.814223	0.448059
20	6	0	-1.731957	1.442305	-0.253215
21	6	0	-2.345240	2.540241	-0.873075
22	6	0	-1.670429	3.754149	-1.026034
23	6	0	-0.344400	3.898914	-0.588638
24	8	0	-2.306293	4.804973	-1.622523
25	8	0	0.269405	5.107962	-0.791423
26	8	0	-0.813868	-0.224275	2.823552
27	8	0	1.005880	1.000182	4.584660
28	8	0	6.489229	-1.349864	-2.682736
29	8	0	6.218783	-4.017970	1.255663
30	6	0	-2.426071	0.104277	-0.152954
31	8	0	-3.849848	0.336615	-0.074373
32	6	0	-4.649533	-0.783319	-0.054432
33	6	0	-4.194307	-2.020898	-0.524442
34	6	0	-2.796416	-2.188084	-1.076993
35	6	0	-2.147921	-0.825918	-1.354392
36	6	0	-5.950862	-0.593650	0.424691
37	6	0	-6.823455	-1.680742	0.441766
38	6	0	-6.406015	-2.940573	-0.003951
39	6	0	-5.103765	-3.093461	-0.478670
40	8	0	-4.638305	-4.295216	-0.933406
41	8	0	-8.108055	-1.581067	0.895340
42	8	0	-2.607862	-0.244503	-2.570428
43	1	0	0.691382	-0.291897	0.412065
44	1	0	7.164294	-3.282068	-1.165734
45	1	0	4.369263	-2.362993	1.999606
46	1	0	5.011515	1.275898	-1.773690
47	1	0	4.188054	0.139298	-2.835060
48	1	0	2.719237	1.863889	-1.626900
49	1	0	3.903841	1.649604	0.505599
50	1	0	1.764109	-0.012740	-2.502377
51	1	0	2.936867	2.224757	2.896296
52	1	0	-1.693922	5.557180	-1.637973
53	1	0	-3.364238	2.467479	-1.231794
54	1	0	1.153069	5.089830	-0.396420
55	1	0	0.203259	0.474373	4.759602
56	1	0	6.147705	-0.535252	-3.075390
57	1	0	6.923221	-4.490049	0.789935
58	1	0	-2.107938	-0.406599	0.763352
59	1	0	-2.816723	-2.766777	-2.005893
60	1	0	-2.168534	-2.752526	-0.374481
61	1	0	-1.066876	-0.942737	-1.473847
62	1	0	-6.253187	0.386789	0.778190
63	1	0	-7.096869	-3.777398	0.024610
64	1	0	-5.346038	-4.953130	-0.886454
65	1	0	-8.281077	-0.669035	1.167942
66	1	0	-3.535290	0.002070	-2.440682

Cartesian coordinates of the optimized geometry of (1‴*S*,5‴*S*)-11Q at the B3LYP/6-31G(d,p) level in MeOH (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.439305	-2.603407	0.412074
2	6	0	6.103814	-2.126941	-0.721152
3	6	0	5.638620	-0.968714	-1.347656
4	6	0	4.515613	-0.265329	-0.874028
5	6	0	3.891292	-0.773583	0.277713
6	6	0	4.329315	-1.928865	0.923849
7	6	0	3.982990	0.970802	-1.572786
8	6	0	2.546678	1.273465	-1.120238
9	6	0	2.513890	1.176520	0.412328
10	8	0	2.774352	-0.173672	0.818214
11	8	0	1.605676	0.400963	-1.738494
12	6	0	1.209040	1.595859	1.115486
13	6	0	1.332698	1.533875	2.616349
14	6	0	0.317752	0.844461	3.164314
15	6	0	-0.617961	0.368218	2.127295
16	6	0	-0.091535	0.799070	0.758949
17	6	0	-0.937162	1.822540	0.021300
18	6	0	-0.249474	3.038200	0.089189
19	8	0	0.971218	2.984400	0.710778
20	6	0	-2.143677	1.764218	-0.687616
21	6	0	-2.627959	2.950859	-1.265351
22	6	0	-1.946875	4.161618	-1.144446
23	6	0	-0.723720	4.218995	-0.459750
24	8	0	-2.459522	5.285620	-1.722556
25	8	0	-0.071794	5.423114	-0.407178
26	8	0	-1.622136	-0.272148	2.415662
27	8	0	0.072488	0.576510	4.455659
28	8	0	6.331677	-0.561602	-2.451570
29	8	0	5.840668	-3.728622	1.071734
30	6	0	-2.975232	0.515104	-0.909525
31	8	0	-2.158979	-0.632971	-0.622530
32	6	0	-2.768064	-1.864442	-0.618980
33	6	0	-4.157797	-2.003169	-0.544729
34	6	0	-5.062250	-0.795811	-0.469177
35	6	0	-4.278708	0.468634	-0.086441
36	6	0	-1.904707	-2.965849	-0.662708
37	6	0	-2.451078	-4.247799	-0.637292
38	6	0	-3.837143	-4.433688	-0.576882
39	6	0	-4.667773	-3.314370	-0.532374
40	8	0	-6.028494	-3.430476	-0.470428
41	8	0	-1.677629	-5.373537	-0.678949
42	8	0	-4.033269	0.556831	1.305910
43	1	0	0.109139	-0.086341	0.157283
44	1	0	6.973352	-2.636139	-1.124404
45	1	0	3.818076	-2.288182	1.808668
46	1	0	4.616998	1.845275	-1.373604
47	1	0	3.958971	0.834071	-2.661214
48	1	0	2.263661	2.283442	-1.423239
49	1	0	3.306012	1.831138	0.804018
50	1	0	1.881364	-0.509634	-1.556642
51	1	0	2.152137	2.003755	3.146941
52	1	0	-1.846364	6.018070	-1.553270
53	1	0	-3.549620	2.945116	-1.838870
54	1	0	0.761051	5.315166	0.074667
55	1	0	-0.755621	0.061595	4.480227
56	1	0	5.957375	0.259169	-2.799330
57	1	0	6.616062	-4.102212	0.629846
58	1	0	-3.258293	0.474016	-1.971290
59	1	0	-5.851677	-0.952922	0.272052
60	1	0	-5.569099	-0.633529	-1.430500
61	1	0	-4.873878	1.349190	-0.350058
62	1	0	-0.833163	-2.805871	-0.722215
63	1	0	-4.245771	-5.439197	-0.566793
64	1	0	-6.269134	-4.367026	-0.438126
65	1	0	-0.744733	-5.119163	-0.712631
66	1	0	-3.250267	0.022131	1.532155

Cartesian coordinates of the optimized geometry of (4‴*S*)-12A at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.920485	3.108810	0.474613
2	6	0	5.819442	2.753227	-0.538466
3	6	0	5.674412	1.517680	-1.172784
4	6	0	4.652218	0.617644	-0.825363
5	6	0	3.768469	1.022839	0.185357
6	6	0	3.887160	2.248330	0.843738
7	6	0	4.517858	-0.731026	-1.500936
8	6	0	3.636810	-1.665963	-0.664744
9	6	0	2.383142	-0.880892	-0.248285
10	8	0	2.742886	0.208516	0.613734
11	8	0	4.342082	-2.196736	0.456988
12	6	0	1.287558	-1.669585	0.493417
13	6	0	1.667265	-2.163699	1.898207
14	6	0	0.655090	-1.555436	2.844836
15	6	0	-0.578806	-1.031571	2.063779
16	6	0	-0.032043	-0.817356	0.623029
17	6	0	-0.861176	-1.333956	-0.528341
18	6	0	-0.232305	-2.476488	-1.010980
19	8	0	0.942036	-2.793423	-0.375322
20	6	0	-2.069729	-0.902904	-1.088600
21	6	0	-2.607657	-1.656004	-2.144058
22	6	0	-1.972664	-2.814516	-2.602161
23	6	0	-0.763063	-3.246829	-2.034953
24	8	0	-2.534254	-3.525391	-3.622798
25	8	0	-0.205102	-4.403168	-2.514429
26	8	0	0.761867	-1.404983	4.042899
27	8	0	6.520358	1.114216	-2.165888
28	8	0	5.005390	4.300216	1.135056
29	6	0	-2.735550	0.341642	-0.541240
30	8	0	-1.982834	1.484546	-1.045375
31	6	0	-2.394828	2.713341	-0.571249
32	6	0	-3.695802	2.904045	-0.085764
33	6	0	-4.706040	1.777479	-0.065460
34	6	0	-4.213300	0.574405	-0.881817
35	6	0	-1.458733	3.747206	-0.645633
36	6	0	-1.830176	5.018834	-0.210509
37	6	0	-3.112874	5.252844	0.299650
38	6	0	-4.025450	4.196486	0.354343
39	8	0	-5.294250	4.366070	0.833140
40	8	0	-0.891492	6.007939	-0.295616
41	8	0	-4.398633	0.783951	-2.283285
42	1	0	0.196456	0.248955	0.548792
43	8	0	-1.024563	0.188777	2.596602
44	6	0	-1.705522	-2.086257	2.123351
45	8	0	-1.224236	-3.309718	1.873809
46	6	0	-2.187199	-4.402357	1.796259
47	8	0	-2.863863	-1.827107	2.364897
48	6	0	-1.441654	-5.630836	1.317722
49	1	0	6.619687	3.428354	-0.830182
50	1	0	3.183745	2.524204	1.619921
51	1	0	4.088140	-0.622332	-2.505286
52	1	0	5.500456	-1.193767	-1.634101
53	1	0	3.327711	-2.529649	-1.257209
54	1	0	1.925900	-0.476598	-1.163243
55	1	0	4.767860	-1.457175	0.915186
56	1	0	2.679670	-1.892389	2.193231
57	1	0	1.590127	-3.254195	1.944975
58	1	0	-3.521620	-1.340387	-2.630775
59	1	0	-1.952441	-4.275164	-3.823815
60	1	0	0.672986	-4.522900	-2.124274
61	1	0	7.197210	1.790283	-2.310615
62	1	0	5.747366	4.813260	0.785446
63	1	0	-2.641180	0.341445	0.551103
64	1	0	-4.907522	1.459045	0.966184
65	1	0	-5.663292	2.112442	-0.477682
66	1	0	-4.796748	-0.314047	-0.623451
67	1	0	-0.462537	3.559189	-1.027626
68	1	0	-3.397698	6.242344	0.648724
69	1	0	-5.425118	5.292079	1.080396
70	1	0	-1.263951	6.835861	0.038499
71	1	0	-3.645865	1.312097	-2.590409
72	1	0	-1.062400	0.080494	3.561203
73	1	0	-2.624853	-4.542189	2.788391
74	1	0	-2.982072	-4.105927	1.107594
75	1	0	-1.004723	-5.462875	0.329489
76	1	0	-2.137197	-6.472243	1.248618
77	1	0	-0.643263	-5.902684	2.013861

Cartesian coordinates of the optimized geometry of (4‴*S*)-12B at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.893994	3.068699	0.538845
2	6	0	5.773921	2.745736	-0.497683
3	6	0	5.632168	1.525029	-1.156097
4	6	0	4.628056	0.599748	-0.806337
5	6	0	3.757428	0.975889	0.227443
6	6	0	3.875392	2.188792	0.908993
7	6	0	4.493050	-0.745199	-1.495330
8	6	0	3.617131	-1.697122	-0.667561
9	6	0	2.369405	-0.916895	-0.228530
10	8	0	2.746251	0.144826	0.659273
11	8	0	4.331409	-2.247489	0.436019
12	6	0	1.269732	-1.716840	0.495608
13	6	0	1.644134	-2.251176	1.885268
14	6	0	0.642378	-1.662218	2.860641
15	6	0	-0.600108	-1.119841	2.085256
16	6	0	-0.037399	-0.860175	0.652313
17	6	0	-0.863975	-1.316579	-0.526517
18	6	0	-0.251675	-2.455263	-1.040151
19	8	0	0.911521	-2.812827	-0.404400
20	6	0	-2.051935	-0.838339	-1.092108
21	6	0	-2.591719	-1.545730	-2.178571
22	6	0	-1.978238	-2.704661	-2.662871
23	6	0	-0.785336	-3.180938	-2.094351
24	8	0	-2.542430	-3.371708	-3.711135
25	8	0	-0.246143	-4.333290	-2.603394
26	8	0	0.767960	-1.572678	4.059712
27	8	0	6.526781	1.270141	-2.156371
28	8	0	5.073063	4.275179	1.150990
29	6	0	-2.685903	0.416220	-0.531163
30	8	0	-1.945364	1.549827	-1.073164
31	6	0	-2.327337	2.782486	-0.583608
32	6	0	-3.602815	2.986905	-0.044741
33	6	0	-4.623657	1.871210	0.018023
34	6	0	-4.174687	0.660979	-0.813139
35	6	0	-1.382531	3.807980	-0.696121
36	6	0	-1.722513	5.082812	-0.245063
37	6	0	-2.980924	5.329937	0.316330
38	6	0	-3.899926	4.285074	0.408836
39	8	0	-5.146050	4.466205	0.939979
40	8	0	-0.859020	6.139165	-0.313636
41	8	0	-4.413841	0.869501	-2.206505
42	1	0	0.203889	0.205723	0.625526
43	8	0	-1.098899	0.058983	2.662526
44	6	0	-1.705785	-2.186306	2.131986
45	8	0	-1.285350	-3.382904	1.745560
46	6	0	-2.273960	-4.459923	1.693798
47	8	0	-2.830422	-1.915370	2.513047
48	6	0	-1.580789	-5.681199	1.128464
49	1	0	6.556887	3.434932	-0.790899
50	1	0	3.174162	2.424762	1.702433
51	1	0	4.058718	-0.635900	-2.498326
52	1	0	5.470500	-1.227879	-1.621357
53	1	0	3.306493	-2.548616	-1.276046
54	1	0	1.912550	-0.483882	-1.130371
55	1	0	4.716364	-1.513224	0.937013
56	1	0	2.660587	-2.003545	2.186745
57	1	0	1.552875	-3.341786	1.901297
58	1	0	-3.493057	-1.194930	-2.664855
59	1	0	-1.977113	-4.130218	-3.925885
60	1	0	0.617601	-4.492356	-2.195561
61	1	0	6.319157	0.430270	-2.587475
62	1	0	4.408023	4.386497	1.844948
63	1	0	-2.544108	0.427068	0.555731
64	1	0	-4.789823	1.558641	1.057723
65	1	0	-5.592195	2.215079	-0.359024
66	1	0	-4.755228	-0.221945	-0.530776
67	1	0	-0.407637	3.592868	-1.121219
68	1	0	-3.225247	6.326672	0.670112
69	1	0	-5.254775	5.392920	1.195685
70	1	0	-0.029010	5.849219	-0.717470
71	1	0	-3.679776	1.407723	-2.540308
72	1	0	-1.982615	-0.160895	3.008666
73	1	0	-2.648219	-4.623350	2.707422
74	1	0	-3.102722	-4.124227	1.066173
75	1	0	-0.750003	-5.993103	1.767316
76	1	0	-1.198487	-5.485703	0.122959
77	1	0	-2.296992	-6.505823	1.070630

Cartesian coordinates of the optimized geometry of (4‴*S*)-12C at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.303275	2.423305	-0.184652
2	6	0	4.375539	3.431192	0.781114
3	6	0	3.200723	4.086472	1.166764
4	6	0	1.949845	3.752152	0.619263
5	6	0	1.938461	2.736414	-0.343502
6	6	0	3.090499	2.080070	-0.775419
7	6	0	0.669281	4.425513	1.077474
8	6	0	-0.558758	3.960815	0.266873
9	6	0	-0.375142	2.464844	-0.018328
10	8	0	0.748073	2.329079	-0.908168
11	8	0	-0.720767	4.710139	-0.936683
12	6	0	-1.534223	1.660254	-0.632689
13	6	0	-2.067925	2.126255	-1.991874
14	6	0	-1.973375	0.932227	-2.927469
15	6	0	-1.728944	-0.374991	-2.105051
16	6	0	-1.111268	0.160688	-0.776896
17	6	0	-1.594230	-0.425378	0.523882
18	6	0	-2.482089	0.489356	1.080751
19	8	0	-2.602738	1.662439	0.372832
20	6	0	-1.291508	-1.619922	1.184645
21	6	0	-1.958883	-1.887937	2.389085
22	6	0	-2.901142	-0.989850	2.902686
23	6	0	-3.169453	0.229828	2.257071
24	8	0	-3.540377	-1.290252	4.070649
25	8	0	-4.094248	1.066663	2.826978
26	8	0	-2.032576	0.956901	-4.134588
27	8	0	3.201505	5.074547	2.106449
28	8	0	5.406819	1.699816	-0.572655
29	6	0	-0.197720	-2.494507	0.608644
30	8	0	1.046098	-1.771363	0.853428
31	6	0	2.178770	-2.341743	0.308620
32	6	0	2.234808	-3.711559	0.033149
33	6	0	1.058164	-4.622157	0.315251
34	6	0	-0.018089	-3.915071	1.156371
35	6	0	3.256345	-1.476961	0.091671
36	6	0	4.435882	-1.994051	-0.447117
37	6	0	4.532974	-3.360602	-0.746443
38	6	0	3.442040	-4.195632	-0.503885
39	8	0	3.486186	-5.535248	-0.775803
40	8	0	5.526312	-1.222690	-0.712431
41	8	0	0.329044	-3.894618	2.541774
42	1	0	-0.030583	0.085347	-0.910132
43	8	0	-0.849058	-1.246862	-2.766142
44	6	0	-3.075664	-1.094860	-1.928538
45	8	0	-4.029398	-0.301020	-1.461373
46	6	0	-5.340201	-0.899501	-1.210360
47	8	0	-3.209218	-2.268339	-2.225678
48	6	0	-6.198496	0.155795	-0.545832
49	1	0	5.325075	3.693307	1.240473
50	1	0	3.028170	1.295882	-1.519428
51	1	0	0.504470	4.212698	2.141364
52	1	0	0.748315	5.514498	0.992637
53	1	0	-1.472068	4.123240	0.844124
54	1	0	-0.130759	1.966680	0.930131
55	1	0	0.057058	4.537741	-1.488475
56	1	0	-1.523003	2.976573	-2.401139
57	1	0	-3.116723	2.426467	-1.902025
58	1	0	-1.731715	-2.779932	2.959263
59	1	0	-4.114748	-0.543114	4.301008
60	1	0	-4.069068	1.925827	2.381057
61	1	0	4.103709	5.227990	2.420476
62	1	0	6.193403	2.015063	-0.104277
63	1	0	-0.329081	-2.560954	-0.478724
64	1	0	0.611123	-4.972370	-0.624985
65	1	0	1.383863	-5.518427	0.853062
66	1	0	-0.962013	-4.463663	1.084823
67	1	0	3.150116	-0.424300	0.327518
68	1	0	5.451633	-3.751214	-1.173322
69	1	0	4.363193	-5.764354	-1.114072
70	1	0	5.335682	-0.277329	-0.563380
71	1	0	0.938766	-3.151322	2.666867
72	1	0	-1.362984	-2.051348	-2.961732
73	1	0	-5.749456	-1.226872	-2.169513
74	1	0	-5.194556	-1.777222	-0.576675
75	1	0	-6.312889	1.031768	-1.190132
76	1	0	-5.765492	0.472397	0.406844
77	1	0	-7.191693	-0.259337	-0.351914

Cartesian coordinates of the optimized geometry of (4‴*S*)-12D at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.035930	2.929704	0.716316
2	6	0	5.951117	2.615778	-0.296060
3	6	0	5.787757	1.430310	-1.015856
4	6	0	4.731745	0.540141	-0.754841
5	6	0	3.833142	0.903340	0.259045
6	6	0	3.968959	2.078307	1.000821
7	6	0	4.578294	-0.757640	-1.520442
8	6	0	3.662165	-1.722583	-0.759406
9	6	0	2.414948	-0.936843	-0.324200
10	8	0	2.774664	0.093603	0.607682
11	8	0	4.334223	-2.331111	0.342983
12	6	0	1.285879	-1.740751	0.346978
13	6	0	1.622988	-2.318670	1.731198
14	6	0	0.652901	-1.675693	2.697183
15	6	0	-0.564002	-1.085366	1.935899
16	6	0	-0.016624	-0.862921	0.496902
17	6	0	-0.854556	-1.328328	-0.670007
18	6	0	-0.230037	-2.446181	-1.212752
19	8	0	0.938331	-2.806928	-0.588725
20	6	0	-2.051488	-0.851874	-1.218548
21	6	0	-2.584819	-1.537969	-2.321197
22	6	0	-1.950518	-2.668039	-2.845343
23	6	0	-0.748206	-3.142046	-2.295526
24	8	0	-2.502745	-3.307542	-3.917197
25	8	0	-0.176510	-4.248876	-2.863836
26	8	0	0.778865	-1.543701	3.895461
27	8	0	6.647338	1.068453	-2.013240
28	8	0	5.137398	4.070810	1.458071
29	6	0	-2.704084	0.375437	-0.619483
30	8	0	-1.965729	1.533911	-1.110340
31	6	0	-2.366636	2.747507	-0.589877
32	6	0	-3.654241	2.921329	-0.063589
33	6	0	-4.662126	1.792384	-0.048127
34	6	0	-4.190510	0.616508	-0.915128
35	6	0	-1.434581	3.785344	-0.659947
36	6	0	-1.795967	5.043196	-0.178790
37	6	0	-3.064745	5.259743	0.372234
38	6	0	-3.973864	4.200115	0.421531
39	8	0	-5.229605	4.353272	0.938847
40	8	0	-0.861137	6.036229	-0.260784
41	8	0	-4.412874	0.872565	-2.303589
42	1	0	0.237112	0.199164	0.444086
43	8	0	-0.950870	0.142379	2.497542
44	6	0	-1.736618	-2.088441	1.986321
45	8	0	-1.307646	-3.333387	1.738614
46	6	0	-2.305365	-4.399686	1.709834
47	8	0	-2.882320	-1.773767	2.222924
48	6	0	-2.552375	-4.952600	3.102047
49	1	0	6.778215	3.284135	-0.520921
50	1	0	3.253760	2.322584	1.776815
51	1	0	4.167530	-0.573921	-2.521784
52	1	0	5.552317	-1.233689	-1.668587
53	1	0	3.349029	-2.543497	-1.408058
54	1	0	1.987440	-0.471276	-1.224360
55	1	0	4.772718	-1.628130	0.844740
56	1	0	2.653181	-2.147677	2.037974
57	1	0	1.449715	-3.399437	1.728361
58	1	0	-3.493518	-1.188955	-2.794927
59	1	0	-1.926594	-4.051049	-4.154394
60	1	0	0.666432	-4.436955	-2.426288
61	1	0	7.346889	1.731677	-2.096190
62	1	0	5.905092	4.581256	1.164846
63	1	0	-2.583183	0.345978	0.469400
64	1	0	-4.832999	1.441765	0.978587
65	1	0	-5.631290	2.137615	-0.422259
66	1	0	-4.766422	-0.280823	-0.671211
67	1	0	-0.448810	3.610619	-1.073964
68	1	0	-3.341700	6.238439	0.756347
69	1	0	-5.355678	5.272009	1.214165
70	1	0	-1.225025	6.853240	0.107792
71	1	0	-3.671508	1.416585	-2.610755
72	1	0	-0.968899	0.019483	3.461121
73	1	0	-3.217994	-4.002587	1.262210
74	1	0	-1.871469	-5.148605	1.046063
75	1	0	-2.990753	-4.191805	3.752524
76	1	0	-1.621859	-5.310654	3.551085
77	1	0	-3.249571	-5.793844	3.039121

Cartesian coordinates of the optimized geometry of (4‴*S*)-12E at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.928215	3.109487	0.485174
2	6	0	5.829041	2.754790	-0.526569
3	6	0	5.684823	1.520067	-1.162664
4	6	0	4.661590	0.620000	-0.818345
5	6	0	3.775985	1.024352	0.191071
6	6	0	3.893838	2.248945	0.851213
7	6	0	4.528082	-0.727792	-1.495846
8	6	0	3.644895	-1.663371	-0.662650
9	6	0	2.390727	-0.878095	-0.247920
10	8	0	2.749121	0.209895	0.616329
11	8	0	4.347555	-2.195729	0.459961
12	6	0	1.293059	-1.667007	0.490426
13	6	0	1.669658	-2.163363	1.895327
14	6	0	0.658707	-1.552176	2.841259
15	6	0	-0.573958	-1.026527	2.059566
16	6	0	-0.026103	-0.813650	0.618970
17	6	0	-0.855261	-1.330251	-0.532381
18	6	0	-0.225919	-2.472106	-1.016053
19	8	0	0.948323	-2.789240	-0.380675
20	6	0	-2.065138	-0.900842	-1.090868
21	6	0	-2.603546	-1.653623	-2.146395
22	6	0	-1.967336	-2.810699	-2.606285
23	6	0	-0.756659	-3.242025	-2.040380
24	8	0	-2.529163	-3.521573	-3.626528
25	8	0	-0.198154	-4.397179	-2.521282
26	8	0	0.765393	-1.400557	4.039162
27	8	0	6.532509	1.117443	-2.154611
28	8	0	5.012183	4.300039	1.147206
29	6	0	-2.731105	0.342418	-0.541599
30	8	0	-2.002395	1.489072	-1.068919
31	6	0	-2.412610	2.716226	-0.587963
32	6	0	-3.705539	2.899551	-0.071372
33	6	0	-4.705092	1.760385	-0.034154
34	6	0	-4.215851	0.558964	-0.859557
35	6	0	-1.487113	3.754748	-0.686955
36	6	0	-1.857557	5.026675	-0.246310
37	6	0	-3.125842	5.252816	0.294845
38	6	0	-4.030423	4.191794	0.377678
39	8	0	-5.255585	4.482662	0.909360
40	8	0	-0.927046	6.020555	-0.357583
41	8	0	-4.426991	0.768259	-2.255009
42	1	0	0.203873	0.252378	0.544551
43	8	0	-1.018003	0.194651	2.591866
44	6	0	-1.702876	-2.078915	2.117600
45	8	0	-1.223268	-3.303587	1.871311
46	6	0	-2.188053	-4.394574	1.791846
47	8	0	-2.861598	-1.816868	2.354416
48	6	0	-1.443117	-5.624888	1.317134
49	1	0	6.630088	3.429994	-0.815889
50	1	0	3.188987	2.524181	1.626318
51	1	0	4.100544	-0.617727	-2.500978
52	1	0	5.510759	-1.190801	-1.627492
53	1	0	3.336680	-2.526212	-1.256815
54	1	0	1.935756	-0.472414	-1.163408
55	1	0	4.773724	-1.457045	0.919219
56	1	0	2.682870	-1.896352	2.191412
57	1	0	1.588010	-3.253588	1.941158
58	1	0	-3.519868	-1.340673	-2.630474
59	1	0	-1.947206	-4.271052	-3.828285
60	1	0	0.678978	-4.518558	-2.129462
61	1	0	7.209985	1.793339	-2.297214
62	1	0	5.755122	4.813225	0.799862
63	1	0	-2.617976	0.351669	0.548768
64	1	0	-4.888313	1.429669	0.998030
65	1	0	-5.673312	2.069093	-0.448913
66	1	0	-4.789148	-0.331825	-0.588313
67	1	0	-0.499076	3.571487	-1.091702
68	1	0	-3.422727	6.233611	0.652637
69	1	0	-5.791606	3.680245	0.967354
70	1	0	-1.296389	6.845604	-0.012784
71	1	0	-3.678770	1.294062	-2.577572
72	1	0	-1.051935	0.088154	3.556854
73	1	0	-2.629096	-4.532445	2.782740
74	1	0	-2.980106	-4.097381	1.100270
75	1	0	-1.002462	-5.458713	0.330246
76	1	0	-2.139923	-6.465115	1.246498
77	1	0	-0.647620	-5.897438	2.016293

Cartesian coordinates of the optimized geometry of (4‴*S*)-12F at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.635991	-1.942676	-0.075083
2	6	0	-4.797723	-3.030851	0.792714
3	6	0	-3.693025	-3.817936	1.121242
4	6	0	-2.409528	-3.553118	0.607488
5	6	0	-2.301148	-2.472165	-0.272958
6	6	0	-3.387048	-1.674194	-0.640201
7	6	0	-1.198155	-4.367173	1.021005
8	6	0	0.051290	-4.001994	0.197406
9	6	0	0.045335	-2.478944	-0.001693
10	8	0	-1.080397	-2.146887	-0.832917
11	8	0	0.083283	-4.699528	-1.048253
12	6	0	1.280883	-1.801314	-0.625912
13	6	0	1.725643	-2.299803	-2.006747
14	6	0	1.717070	-1.092979	-2.927836
15	6	0	1.659398	0.221429	-2.084683
16	6	0	1.043033	-0.257940	-0.733938
17	6	0	1.654684	0.244827	0.546817
18	6	0	2.428176	-0.785621	1.068471
19	8	0	2.364660	-1.957946	0.352540
20	6	0	1.547771	1.468718	1.213884
21	6	0	2.287480	1.640680	2.392798
22	6	0	3.113441	0.617572	2.872730
23	6	0	3.186679	-0.625706	2.219228
24	8	0	3.831354	0.820947	4.015641
25	8	0	4.008354	-1.582264	2.757905
26	8	0	1.715268	-1.107650	-4.136744
27	8	0	-3.789717	-4.877048	1.978544
28	8	0	-5.730311	-1.172065	-0.330357
29	6	0	0.556913	2.474009	0.670394
30	8	0	-0.757792	1.919593	0.983111
31	6	0	-1.814759	2.586883	0.406055
32	6	0	-1.715038	3.944771	0.083613
33	6	0	-0.448428	4.728180	0.364252
34	6	0	0.567110	3.914635	1.191406
35	6	0	-2.970257	1.834848	0.187976
36	6	0	-4.060725	2.455612	-0.412132
37	6	0	-4.011596	3.807453	-0.767496
38	6	0	-2.843610	4.534657	-0.511166
39	8	0	-2.736871	5.858475	-0.827886
40	8	0	-5.172000	1.680808	-0.651079
41	8	0	0.269183	3.958189	2.586839
42	1	0	-0.024948	-0.047841	-0.813513
43	8	0	0.856828	1.197153	-2.698338
44	6	0	3.085691	0.780110	-1.961521
45	8	0	3.958912	-0.121563	-1.534040
46	6	0	5.339825	0.318812	-1.338373
47	8	0	3.342520	1.932108	-2.262049
48	6	0	6.101490	-0.840989	-0.732837
49	1	0	-5.772735	-3.226404	1.227981
50	1	0	-3.239177	-0.851108	-1.329616
51	1	0	-0.990998	-4.206212	2.086982
52	1	0	-1.388129	-5.439301	0.905224
53	1	0	0.956026	-4.304135	0.730723
54	1	0	-0.095164	-2.009015	0.982017
55	1	0	-0.703019	-4.431952	-1.547439
56	1	0	1.095365	-3.094981	-2.403209
57	1	0	2.746130	-2.692282	-1.949845
58	1	0	2.207230	2.555193	2.967087
59	1	0	4.302933	-0.000639	4.225063
60	1	0	3.856626	-2.427209	2.309998
61	1	0	-4.707883	-4.975237	2.267645
62	1	0	-5.453114	-0.291592	-0.645321
63	1	0	0.645637	2.504913	-0.422537
64	1	0	0.018821	5.036615	-0.580259
65	1	0	-0.676766	5.650274	0.908965
66	1	0	1.564307	4.349719	1.076882
67	1	0	-2.994830	0.786062	0.454408
68	1	0	-4.863300	4.287973	-1.241547
69	1	0	-3.569367	6.170891	-1.209221
70	1	0	-5.855104	2.202753	-1.095136
71	1	0	-0.419584	3.294096	2.745155
72	1	0	1.453514	1.933391	-2.925134
73	1	0	5.738883	0.617450	-2.311056
74	1	0	5.325231	1.194245	-0.685060
75	1	0	6.085053	-1.710184	-1.396015
76	1	0	5.679391	-1.127201	0.234217
77	1	0	7.143501	-0.545634	-0.580196

Cartesian coordinates of the optimized geometry of (4‴*S*)-12G at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.896724	3.118857	0.475774
2	6	0	5.788809	2.775483	-0.543524
3	6	0	5.654274	1.540049	-1.180151
4	6	0	4.647825	0.623709	-0.823234
5	6	0	3.765019	1.021036	0.195296
6	6	0	3.874260	2.245757	0.852021
7	6	0	4.519175	-0.733580	-1.488476
8	6	0	3.640535	-1.671448	-0.648375
9	6	0	2.386895	-0.887114	-0.233912
10	8	0	2.751636	0.195085	0.633029
11	8	0	4.348748	-2.198008	0.470808
12	6	0	1.288276	-1.678021	0.501113
13	6	0	1.661197	-2.179122	1.905162
14	6	0	0.645087	-1.574616	2.850461
15	6	0	-0.583581	-1.043217	2.066226
16	6	0	-0.029994	-0.823681	0.628901
17	6	0	-0.855068	-1.333664	-0.528273
18	6	0	-0.226788	-2.475537	-1.013083
19	8	0	0.944957	-2.797096	-0.374060
20	6	0	-2.060426	-0.897627	-1.091483
21	6	0	-2.596125	-1.645771	-2.151562
22	6	0	-1.962271	-2.804224	-2.611346
23	6	0	-0.755404	-3.241149	-2.041614
24	8	0	-2.522008	-3.510261	-3.636234
25	8	0	-0.198248	-4.396595	-2.523865
26	8	0	0.746474	-1.432669	4.049888
27	8	0	6.561438	1.268096	-2.164302
28	8	0	4.971511	4.309990	1.137413
29	6	0	-2.724684	0.347175	-0.542789
30	8	0	-1.969022	1.489251	-1.044220
31	6	0	-2.379217	2.718266	-0.568863
32	6	0	-3.680363	2.910765	-0.084598
33	6	0	-4.692802	1.786125	-0.066954
34	6	0	-4.201603	0.583336	-0.884706
35	6	0	-1.441044	3.750381	-0.640884
36	6	0	-1.810552	5.022195	-0.204613
37	6	0	-3.093356	5.257947	0.304473
38	6	0	-4.007999	4.203264	0.356880
39	8	0	-5.276947	4.374643	0.834576
40	8	0	-0.869949	6.009592	-0.287571
41	8	0	-4.385040	0.795441	-2.286029
42	1	0	0.200950	0.242532	0.560452
43	8	0	-1.027855	0.176377	2.601751
44	6	0	-1.713674	-2.094732	2.116342
45	8	0	-1.234977	-3.318377	1.862884
46	6	0	-2.200741	-4.408180	1.778464
47	8	0	-2.871983	-1.833080	2.355198
48	6	0	-1.457387	-5.636700	1.296706
49	1	0	6.581870	3.448315	-0.853534
50	1	0	3.172561	2.512699	1.632839
51	1	0	4.089729	-0.643310	-2.495443
52	1	0	5.498036	-1.216780	-1.600877
53	1	0	3.336761	-2.535721	-1.242105
54	1	0	1.932533	-0.477547	-1.147865
55	1	0	4.735631	-1.453919	0.955623
56	1	0	2.671796	-1.909951	2.208152
57	1	0	1.583296	-3.269780	1.946115
58	1	0	-3.507782	-1.326474	-2.640196
59	1	0	-1.942979	-4.262493	-3.836056
60	1	0	0.674185	-4.525181	-2.124035
61	1	0	6.359914	0.420016	-2.582155
62	1	0	5.705055	4.831282	0.782014
63	1	0	-2.631715	0.344990	0.549669
64	1	0	-4.895913	1.466516	0.964009
65	1	0	-5.649003	2.123557	-0.479604
66	1	0	-4.787062	-0.304385	-0.628410
67	1	0	-0.444774	3.560964	-1.021997
68	1	0	-3.376680	6.247539	0.654501
69	1	0	-5.406182	5.300511	1.083225
70	1	0	-1.241238	6.837940	0.046798
71	1	0	-3.631969	1.324295	-2.591179
72	1	0	-1.078568	0.062595	3.565062
73	1	0	-2.641017	-4.550857	2.769018
74	1	0	-2.993173	-4.106716	1.089200
75	1	0	-0.661319	-5.913499	1.993558
76	1	0	-1.017792	-5.466074	0.310105
77	1	0	-2.155030	-6.475943	1.222708

Cartesian coordinates of the optimized geometry of (4‴*S*)-12H at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.094798	2.847065	0.657842
2	6	0	6.041659	2.465607	-0.300767
3	6	0	5.902574	1.231702	-0.939702
4	6	0	4.839475	0.358855	-0.650412
5	6	0	3.909489	0.789559	0.306893
6	6	0	4.020447	2.014134	0.968181
7	6	0	4.710822	-0.988957	-1.329239
8	6	0	3.766929	-1.901170	-0.537300
9	6	0	2.508794	-1.087081	-0.195549
10	8	0	2.841697	0.002161	0.677790
11	8	0	4.403484	-2.438925	0.622155
12	6	0	1.353046	-1.836560	0.491772
13	6	0	1.641740	-2.303987	1.929596
14	6	0	0.732926	-1.473728	2.801673
15	6	0	-0.510919	-1.023331	1.986711
16	6	0	0.053445	-0.940706	0.536123
17	6	0	-0.768610	-1.508512	-0.594532
18	6	0	-0.136654	-2.668376	-1.029836
19	8	0	1.028998	-2.968249	-0.369668
20	6	0	-1.954901	-1.079809	-1.203258
21	6	0	-2.476021	-1.861584	-2.245856
22	6	0	-1.838561	-3.036361	-2.655887
23	6	0	-0.643091	-3.458298	-2.052170
24	8	0	-2.378843	-3.769997	-3.672159
25	8	0	-0.064738	-4.609123	-2.516414
26	8	0	0.906563	-1.110898	3.944499
27	8	0	6.793991	0.803463	-1.881259
28	8	0	5.171324	4.038053	1.319996
29	6	0	-2.607061	0.202358	-0.731464
30	8	0	-1.804988	1.302919	-1.254480
31	6	0	-2.197816	2.560738	-0.844611
32	6	0	-3.509531	2.806626	-0.416198
33	6	0	-4.551836	1.710091	-0.389688
34	6	0	-4.064241	0.461378	-1.137471
35	6	0	-1.230231	3.564670	-0.924742
36	6	0	-1.580354	4.862517	-0.554133
37	6	0	-2.873362	5.151955	-0.101757
38	6	0	-3.817284	4.124066	-0.038953
39	8	0	-5.096693	4.347230	0.386818
40	8	0	-0.611480	5.821630	-0.642855
41	8	0	-4.191298	0.618159	-2.551972
42	1	0	0.312524	0.111165	0.389574
43	8	0	-0.959573	0.232170	2.422873
44	6	0	-1.568070	-2.137408	2.127286
45	8	0	-2.792143	-1.661807	2.349411
46	6	0	-3.852575	-2.654235	2.490154
47	8	0	-1.287113	-3.319575	2.042765
48	6	0	-5.135388	-1.907938	2.790338
49	1	0	6.874029	3.119701	-0.546997
50	1	0	3.280989	2.309813	1.702432
51	1	0	4.337152	-0.874794	-2.355106
52	1	0	5.688652	-1.473457	-1.409006
53	1	0	3.472020	-2.761969	-1.141351
54	1	0	2.113909	-0.681791	-1.138803
55	1	0	4.827809	-1.706523	1.093239
56	1	0	2.685542	-2.224546	2.224111
57	1	0	1.326581	-3.348522	2.025966
58	1	0	-3.373258	-1.551668	-2.766166
59	1	0	-1.805144	-4.536471	-3.828428
60	1	0	0.757938	-4.775307	-2.033920
61	1	0	7.497161	1.459837	-1.985435
62	1	0	5.948141	4.528706	1.017075
63	1	0	-2.551747	0.248187	0.362356
64	1	0	-4.800665	1.440469	0.645720
65	1	0	-5.483107	2.053758	-0.851235
66	1	0	-4.683278	-0.399118	-0.866684
67	1	0	-0.226773	3.334143	-1.261804
68	1	0	-3.141784	6.162206	0.197064
69	1	0	-5.208540	5.285165	0.595647
70	1	0	-0.971641	6.671332	-0.352800
71	1	0	-3.407297	1.102776	-2.852804
72	1	0	-0.820964	0.257089	3.385495
73	1	0	-3.911883	-3.224611	1.559426
74	1	0	-3.574510	-3.340296	3.294235
75	1	0	-5.049025	-1.336848	3.718753
76	1	0	-5.953744	-2.625089	2.902345
77	1	0	-5.390436	-1.220714	1.978828

Cartesian coordinates of the optimized geometry of (4‴*S*)-12I at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.042190	2.925754	0.726722
2	6	0	5.958410	2.613277	-0.285180
3	6	0	5.795361	1.429230	-1.007381
4	6	0	4.738641	0.539050	-0.749237
5	6	0	3.839006	0.900869	0.264218
6	6	0	3.974462	2.074338	1.008359
7	6	0	4.585520	-0.757256	-1.517424
8	6	0	3.667548	-1.723044	-0.759644
9	6	0	2.420397	-0.936978	-0.324753
10	8	0	2.779624	0.090955	0.609974
11	8	0	4.337456	-2.334210	0.342570
12	6	0	1.289297	-1.740810	0.342963
13	6	0	1.623603	-2.322599	1.726317
14	6	0	0.656104	-1.676924	2.692993
15	6	0	-0.559615	-1.083154	1.932595
16	6	0	-0.011892	-0.860980	0.493584
17	6	0	-0.850899	-1.324591	-0.673202
18	6	0	-0.227352	-2.441924	-1.218172
19	8	0	0.941217	-2.804147	-0.595776
20	6	0	-2.048810	-0.847928	-1.219201
21	6	0	-2.584013	-1.532301	-2.322067
22	6	0	-1.950155	-2.661310	-2.848952
23	6	0	-0.746962	-3.135988	-2.301438
24	8	0	-2.504034	-3.299436	-3.920515
25	8	0	-0.176491	-4.242061	-2.871889
26	8	0	0.783172	-1.544788	3.891124
27	8	0	6.655886	1.068819	-2.004461
28	8	0	5.143285	4.065380	1.470732
29	6	0	-2.699455	0.378840	-0.617552
30	8	0	-1.980052	1.540061	-1.126466
31	6	0	-2.377528	2.752924	-0.600785
32	6	0	-3.658316	2.922744	-0.049916
33	6	0	-4.657716	1.783071	-0.020330
34	6	0	-4.190698	0.608097	-0.895168
35	6	0	-1.452889	3.793081	-0.690774
36	6	0	-1.811474	5.052422	-0.206400
37	6	0	-3.067403	5.264660	0.368104
38	6	0	-3.971608	4.202546	0.441108
39	8	0	-5.184602	4.480151	1.006666
40	8	0	-0.881840	6.047988	-0.309937
41	8	0	-4.434005	0.865054	-2.277520
42	1	0	0.244012	0.200648	0.441484
43	8	0	-0.943425	0.145018	2.495408
44	6	0	-1.735259	-2.082818	1.980962
45	8	0	-1.309122	-3.329366	1.737054
46	6	0	-2.309816	-4.392900	1.706061
47	8	0	-2.881072	-1.764118	2.211919
48	6	0	-2.564184	-4.942518	3.098238
49	1	0	6.786057	3.281697	-0.507843
50	1	0	3.258421	2.317553	1.783909
51	1	0	4.176466	-0.571453	-2.519081
52	1	0	5.559457	-1.233693	-1.664923
53	1	0	3.354747	-2.542422	-1.410417
54	1	0	1.994847	-0.469063	-1.224635
55	1	0	4.776330	-1.632615	0.845940
56	1	0	2.654581	-2.157230	2.033466
57	1	0	1.444817	-3.402483	1.721389
58	1	0	-3.494677	-1.184540	-2.792984
59	1	0	-1.928234	-4.042544	-4.159879
60	1	0	0.667195	-4.431038	-2.436129
61	1	0	7.355831	1.731872	-2.085423
62	1	0	5.911563	4.576052	1.179437
63	1	0	-2.563213	0.356284	0.469579
64	1	0	-4.813594	1.421278	1.005837
65	1	0	-5.636242	2.103787	-0.400249
66	1	0	-4.759717	-0.290308	-0.640796
67	1	0	-0.474365	3.620426	-1.122416
68	1	0	-3.355330	6.235635	0.758529
69	1	0	-5.723323	3.678483	1.047826
70	1	0	-1.241971	6.863316	0.066260
71	1	0	-3.695357	1.405664	-2.597621
72	1	0	-0.955523	0.022894	3.459240
73	1	0	-3.219359	-3.993978	1.253803
74	1	0	-1.875234	-5.144270	1.045536
75	1	0	-3.003018	-4.179308	3.745573
76	1	0	-1.636574	-5.302463	3.551731
77	1	0	-3.263545	-5.781855	3.033911

Cartesian coordinates of the optimized geometry of (4‴*S*)-12J at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.317633	2.400275	-0.182026
2	6	0	4.394743	3.411476	0.779893
3	6	0	3.223302	4.074822	1.161958
4	6	0	1.971038	3.745322	0.614700
5	6	0	1.954773	2.726038	-0.344218
6	6	0	3.103408	2.061392	-0.772400
7	6	0	0.693939	4.427559	1.069354
8	6	0	-0.535904	3.967093	0.259142
9	6	0	-0.360714	2.469007	-0.020562
10	8	0	0.762540	2.323646	-0.908767
11	8	0	-0.691980	4.712979	-0.947321
12	6	0	-1.524131	1.669184	-0.633102
13	6	0	-2.057343	2.136282	-1.992127
14	6	0	-1.968831	0.941081	-2.926795
15	6	0	-1.730529	-0.366598	-2.103126
16	6	0	-1.108702	0.167462	-0.776394
17	6	0	-1.593192	-0.415169	0.525257
18	6	0	-2.475646	0.504522	1.082577
19	8	0	-2.591362	1.677430	0.373921
20	6	0	-1.296720	-1.611154	1.186048
21	6	0	-1.964133	-1.875257	2.391397
22	6	0	-2.900771	-0.971723	2.905687
23	6	0	-3.163099	0.249151	2.259784
24	8	0	-3.540418	-1.268330	4.074191
25	8	0	-4.082773	1.090852	2.830261
26	8	0	-2.028439	0.964782	-4.133875
27	8	0	3.228730	5.066546	2.097768
28	8	0	5.417379	1.669352	-0.566502
29	6	0	-0.208302	-2.491334	0.608806
30	8	0	1.041186	-1.782177	0.860143
31	6	0	2.169558	-2.357183	0.310522
32	6	0	2.217322	-3.728097	0.026981
33	6	0	1.029227	-4.628082	0.308459
34	6	0	-0.041586	-3.913652	1.154566
35	6	0	3.250935	-1.499494	0.097755
36	6	0	4.428986	-2.021799	-0.443984
37	6	0	4.517948	-3.384644	-0.751085
38	6	0	3.422392	-4.215547	-0.515983
39	8	0	3.580093	-5.535419	-0.839085
40	8	0	5.522444	-1.252958	-0.703255
41	8	0	0.310170	-3.900872	2.536497
42	1	0	-0.028524	0.087151	-0.910975
43	8	0	-0.855418	-1.244161	-2.763115
44	6	0	-3.081084	-1.078993	-1.925356
45	8	0	-4.029640	-0.280255	-1.456093
46	6	0	-5.344009	-0.871131	-1.205433
47	8	0	-3.221825	-2.251275	-2.223983
48	6	0	-6.195580	0.188323	-0.538890
49	1	0	5.345386	3.670024	1.239005
50	1	0	3.037469	1.274798	-1.513565
51	1	0	0.526899	4.219325	2.133792
52	1	0	0.779232	5.515772	0.980812
53	1	0	-1.448896	4.137056	0.834739
54	1	0	-0.120172	1.972752	0.929884
55	1	0	0.085424	4.533806	-1.497557
56	1	0	-1.509520	2.984220	-2.402440
57	1	0	-3.104851	2.440720	-1.901351
58	1	0	-1.742679	-2.768596	2.961754
59	1	0	-4.110524	-0.518092	4.305117
60	1	0	-4.055388	1.949113	2.382705
61	1	0	4.131628	5.216946	2.411268
62	1	0	6.205529	1.982236	-0.099188
63	1	0	-0.337893	-2.553468	-0.478950
64	1	0	0.568520	-4.972167	-0.628528
65	1	0	1.332053	-5.525383	0.863384
66	1	0	-0.987991	-4.457032	1.080838
67	1	0	3.150513	-0.447486	0.339106
68	1	0	5.426287	-3.792657	-1.178962
69	1	0	2.761567	-6.019145	-0.664692
70	1	0	5.335013	-0.307460	-0.551648
71	1	0	0.916783	-3.155441	2.665411
72	1	0	-1.375521	-2.043426	-2.963633
73	1	0	-5.755606	-1.194466	-2.164943
74	1	0	-5.203435	-1.750729	-0.573205
75	1	0	-6.304841	1.066018	-1.181725
76	1	0	-5.760339	0.500759	0.414139
77	1	0	-7.191217	-0.221066	-0.345284

Cartesian coordinates of the optimized geometry of (4‴*S*)-12K at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.158520	2.698578	0.496780
2	6	0	6.073016	2.258427	-0.468033
3	6	0	5.879190	1.013444	-1.070077
4	6	0	4.792341	0.186530	-0.737475
5	6	0	3.896217	0.675358	0.224222
6	6	0	4.061960	1.912724	0.849456
7	6	0	4.605011	-1.174408	-1.375038
8	6	0	3.645778	-2.031303	-0.540394
9	6	0	2.422822	-1.165220	-0.199817
10	8	0	2.809299	-0.064150	0.635891
11	8	0	4.285467	-2.558245	0.622243
12	6	0	1.254135	-1.852674	0.529429
13	6	0	1.552859	-2.290397	1.974037
14	6	0	0.692137	-1.402219	2.838595
15	6	0	-0.551519	-0.929754	2.032026
16	6	0	-0.008833	-0.907311	0.571964
17	6	0	-0.867694	-1.467048	-0.534164
18	6	0	-0.289103	-2.661322	-0.949608
19	8	0	0.870706	-2.994025	-0.294590
20	6	0	-2.038737	-0.999560	-1.143155
21	6	0	-2.602248	-1.779468	-2.164796
22	6	0	-2.019999	-2.989868	-2.553585
23	6	0	-0.838827	-3.450674	-1.949830
24	8	0	-2.599071	-3.719649	-3.551066
25	8	0	-0.314183	-4.634505	-2.394725
26	8	0	0.899480	-1.015808	3.967726
27	8	0	6.737526	0.528856	-2.015096
28	8	0	5.289791	3.903755	1.123784
29	6	0	-2.635119	0.315602	-0.687410
30	8	0	-1.743397	1.369081	-1.158163
31	6	0	-2.076645	2.644714	-0.750004
32	6	0	-3.391476	2.968687	-0.389167
33	6	0	-4.499963	1.939742	-0.433873
34	6	0	-4.050917	0.666168	-1.164030
35	6	0	-1.044184	3.584871	-0.761578
36	6	0	-1.330794	4.897500	-0.388293
37	6	0	-2.625887	5.263875	-0.002541
38	6	0	-3.635584	4.298353	-0.008188
39	8	0	-4.920068	4.597429	0.350602
40	8	0	-0.298499	5.792211	-0.407053
41	8	0	-4.092966	0.833525	-2.581959
42	1	0	0.287733	0.129681	0.395174
43	8	0	-0.945199	0.354201	2.435968
44	6	0	-1.638992	-2.004095	2.237014
45	8	0	-2.814587	-1.483841	2.591443
46	6	0	-3.899766	-2.424574	2.857861
47	8	0	-1.408793	-3.192968	2.106532
48	6	0	-4.661467	-2.757915	1.587640
49	1	0	6.922442	2.876573	-0.747270
50	1	0	3.347309	2.253626	1.588665
51	1	0	4.215672	-1.076125	-2.396727
52	1	0	5.564182	-1.694244	-1.458906
53	1	0	3.310781	-2.897947	-1.114383
54	1	0	2.024639	-0.773106	-1.147256
55	1	0	4.739856	-1.827416	1.066961
56	1	0	2.604288	-2.242074	2.247482
57	1	0	1.201632	-3.319424	2.105566
58	1	0	-3.486006	-1.440803	-2.690129
59	1	0	-2.059343	-4.512505	-3.696312
60	1	0	0.507310	-4.823293	-1.918543
61	1	0	7.461568	1.156503	-2.148555
62	1	0	6.077939	4.356876	0.792946
63	1	0	-2.630568	0.349059	0.408859
64	1	0	-4.824813	1.680450	0.582822
65	1	0	-5.379778	2.343959	-0.944767
66	1	0	-4.736047	-0.154244	-0.930302
67	1	0	-0.040127	3.294710	-1.046901
68	1	0	-2.845502	6.285271	0.297912
69	1	0	-4.985689	5.538426	0.565445
70	1	0	-0.616335	6.658189	-0.115862
71	1	0	-3.258991	1.255609	-2.839555
72	1	0	-0.817007	0.395704	3.399099
73	1	0	-3.475765	-3.317321	3.320617
74	1	0	-4.528305	-1.902678	3.580999
75	1	0	-4.018561	-3.267471	0.866028
76	1	0	-5.065964	-1.853193	1.125525
77	1	0	-5.498008	-3.420311	1.831275

Cartesian coordinates of the optimized geometry of (4‴*S*)-12L at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.286532	2.448292	-0.179559
2	6	0	4.352563	3.452409	0.786258
3	6	0	3.175927	4.104353	1.171466
4	6	0	1.926205	3.768543	0.619306
5	6	0	1.921282	2.751817	-0.346430
6	6	0	3.075075	2.101086	-0.775254
7	6	0	0.634883	4.431184	1.071634
8	6	0	-0.588226	3.958989	0.253338
9	6	0	-0.391105	2.464622	-0.028235
10	8	0	0.733759	2.341624	-0.916531
11	8	0	-0.746020	4.706817	-0.948943
12	6	0	-1.544318	1.650360	-0.641138
13	6	0	-2.082853	2.108349	-2.001058
14	6	0	-1.984016	0.911035	-2.932420
15	6	0	-1.726127	-0.391138	-2.106434
16	6	0	-1.110179	0.153597	-0.780989
17	6	0	-1.587428	-0.431582	0.522463
18	6	0	-2.481597	0.478231	1.077212
19	8	0	-2.611725	1.648144	0.365087
20	6	0	-1.276297	-1.622243	1.186332
21	6	0	-1.940803	-1.891182	2.392085
22	6	0	-2.888840	-0.998196	2.903906
23	6	0	-3.166216	0.217675	2.254840
24	8	0	-3.524900	-1.299698	4.073193
25	8	0	-4.096392	1.049587	2.823015
26	8	0	-2.049054	0.931041	-4.139224
27	8	0	3.306983	5.071948	2.123685
28	8	0	5.393022	1.729406	-0.567169
29	6	0	-0.177776	-2.491659	0.611572
30	8	0	1.061711	-1.760688	0.853922
31	6	0	2.197457	-2.325713	0.309806
32	6	0	2.261237	-3.695670	0.036880
33	6	0	1.090091	-4.612554	0.321533
34	6	0	0.010337	-3.910092	1.162022
35	6	0	3.269867	-1.455173	0.090858
36	6	0	4.452143	-1.966352	-0.447571
37	6	0	4.556985	-3.332865	-0.744536
38	6	0	3.470977	-4.173718	-0.499963
39	8	0	3.522558	-5.513520	-0.769576
40	8	0	5.537557	-1.188832	-0.714775
41	8	0	0.357936	-3.885056	2.547221
42	1	0	-0.029106	0.085463	-0.915512
43	8	0	-0.839893	-1.256771	-2.767071
44	6	0	-3.065545	-1.123182	-1.923736
45	8	0	-4.026027	-0.336253	-1.458836
46	6	0	-5.329733	-0.947060	-1.199904
47	8	0	-3.187728	-2.299568	-2.213970
48	6	0	-6.197321	0.103170	-0.539498
49	1	0	5.290136	3.727443	1.258309
50	1	0	3.016871	1.318022	-1.520748
51	1	0	0.452982	4.211636	2.132728
52	1	0	0.688575	5.523229	0.976469
53	1	0	-1.503162	4.117906	0.828447
54	1	0	-0.142988	1.969629	0.920736
55	1	0	0.022518	4.517638	-1.508594
56	1	0	-1.543217	2.959120	-2.416346
57	1	0	-3.132816	2.404108	-1.910285
58	1	0	-1.707082	-2.780103	2.964402
59	1	0	-4.105441	-0.556704	4.301448
60	1	0	-4.080306	1.906516	2.372434
61	1	0	2.445910	5.463117	2.325119
62	1	0	6.176331	2.046834	-0.094552
63	1	0	-0.309675	-2.561294	-0.475548
64	1	0	0.644419	-4.967179	-0.617695
65	1	0	1.421349	-5.505870	0.860852
66	1	0	-0.930480	-4.464178	1.092115
67	1	0	3.157763	-0.402817	0.325205
68	1	0	5.477791	-3.718906	-1.170962
69	1	0	4.400421	-5.738165	-1.108608
70	1	0	5.341000	-0.244566	-0.565798
71	1	0	0.965378	-3.139589	2.670427
72	1	0	-1.346150	-2.067373	-2.957355
73	1	0	-5.738272	-1.285055	-2.155652
74	1	0	-5.172585	-1.818961	-0.560954
75	1	0	-6.323236	0.973670	-1.189036
76	1	0	-5.764968	0.430468	0.409858
77	1	0	-7.185338	-0.321494	-0.339855

Cartesian coordinates of the optimized geometry of (4‴*S*)-12M at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.651470	-1.907630	-0.072308
2	6	0	-4.820702	-2.997231	0.792346
3	6	0	-3.721706	-3.793550	1.117628
4	6	0	-2.436745	-3.537171	0.603245
5	6	0	-2.320965	-2.454425	-0.274020
6	6	0	-3.400956	-1.646895	-0.637665
7	6	0	-1.231390	-4.362002	1.012936
8	6	0	0.019984	-4.003917	0.189186
9	6	0	0.025516	-2.480175	-0.004973
10	8	0	-1.098188	-2.136834	-0.834207
11	8	0	0.045072	-4.697450	-1.058837
12	6	0	1.266086	-1.810249	-0.627604
13	6	0	1.708672	-2.309683	-2.008805
14	6	0	1.709107	-1.101480	-2.928131
15	6	0	1.660538	0.212041	-2.082856
16	6	0	1.039448	-0.265061	-0.733635
17	6	0	1.653411	0.231412	0.548398
18	6	0	2.418823	-0.805325	1.069524
19	8	0	2.347841	-1.975911	0.351746
20	6	0	1.555347	1.455228	1.216723
21	6	0	2.294887	1.620652	2.396690
22	6	0	3.112497	0.590750	2.876334
23	6	0	3.177090	-0.652335	2.221403
24	8	0	3.830646	0.787491	4.020050
25	8	0	3.990923	-1.615317	2.759977
26	8	0	1.707875	-1.114128	-4.137021
27	8	0	-3.825482	-4.854275	1.972115
28	8	0	-5.740030	-1.128083	-0.324379
29	6	0	0.572407	2.467698	0.672732
30	8	0	-0.746986	1.929380	0.990127
31	6	0	-1.798243	2.602223	0.408344
32	6	0	-1.687881	3.960124	0.078620
33	6	0	-0.410315	4.730261	0.360574
34	6	0	0.597371	3.907775	1.193053
35	6	0	-2.957733	1.859263	0.193100
36	6	0	-4.044438	2.486549	-0.411407
37	6	0	-3.985091	3.833096	-0.774069
38	6	0	-2.812140	4.553779	-0.523480
39	8	0	-2.820478	5.867236	-0.897029
40	8	0	-5.160828	1.717964	-0.645708
41	8	0	0.295173	3.958453	2.584920
42	1	0	-0.027000	-0.047459	-0.814079
43	8	0	0.865267	1.195027	-2.694567
44	6	0	3.090869	0.760044	-1.958129
45	8	0	3.956948	-0.148540	-1.530887
46	6	0	5.341265	0.280937	-1.334612
47	8	0	3.356545	1.910247	-2.257848
48	6	0	6.093439	-0.884841	-0.728700
49	1	0	-5.796835	-3.186789	1.227762
50	1	0	-3.247443	-0.822842	-1.324699
51	1	0	-1.021893	-4.206231	2.079225
52	1	0	-1.429815	-5.432231	0.893839
53	1	0	0.922937	-4.314844	0.720475
54	1	0	-0.110690	-2.012345	0.980346
55	1	0	-0.739459	-4.421680	-1.556363
56	1	0	1.073342	-3.100043	-2.406861
57	1	0	2.726415	-2.709192	-1.951635
58	1	0	2.221940	2.535266	2.971822
59	1	0	4.296017	-0.037715	4.229192
60	1	0	3.833362	-2.458921	2.311518
61	1	0	-4.743766	-4.945432	2.263096
62	1	0	-5.456487	-0.249022	-0.637883
63	1	0	0.659694	2.496012	-0.420329
64	1	0	0.073015	5.029229	-0.580268
65	1	0	-0.616045	5.651186	0.921177
66	1	0	1.597118	4.335867	1.077525
67	1	0	-2.989932	0.811948	0.464478
68	1	0	-4.822961	4.332114	-1.249948
69	1	0	-1.967000	6.275438	-0.697481
70	1	0	-5.838589	2.243445	-1.093958
71	1	0	-0.393472	3.294543	2.745667
72	1	0	1.468244	1.924899	-2.925056
73	1	0	5.743020	0.576303	-2.307172
74	1	0	5.333273	1.156508	-0.681371
75	1	0	6.070697	-1.753792	-1.392000
76	1	0	5.668466	-1.167864	0.238026
77	1	0	7.137611	-0.597623	-0.575314

Cartesian coordinates of the optimized geometry of (4‴*S*)-12N at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.823265	1.008276	-0.296217
2	6	0	-5.626052	0.285084	0.590505
3	6	0	-5.253320	-1.018886	0.935398
4	6	0	-4.090077	-1.618520	0.421893
5	6	0	-3.329319	-0.849620	-0.465726
6	6	0	-3.680474	0.442475	-0.854612
7	6	0	-3.652696	-3.009427	0.842920
8	6	0	-2.393864	-3.484400	0.085594
9	6	0	-1.485370	-2.261447	-0.096009
10	8	0	-2.158864	-1.356718	-0.991338
11	8	0	-2.719954	-4.088581	-1.165586
12	6	0	-0.055300	-2.437545	-0.636637
13	6	0	0.094750	-3.096053	-2.016885
14	6	0	0.734192	-2.044596	-2.895167
15	6	0	1.460734	-0.985167	-2.020637
16	6	0	0.647509	-1.031802	-0.694728
17	6	0	1.391851	-1.000641	0.613605
18	6	0	1.382575	-2.291525	1.131014
19	8	0	0.674042	-3.199078	0.378298
20	6	0	1.986556	0.048843	1.321468
21	6	0	2.623907	-0.257841	2.532314
22	6	0	2.656893	-1.571765	3.012788
23	6	0	2.014117	-2.615061	2.323941
24	8	0	3.289639	-1.833396	4.193580
25	8	0	2.046766	-3.863271	2.886178
26	8	0	0.668497	-1.935412	-4.099870
27	8	0	-5.988833	-1.773709	1.800398
28	8	0	-5.096925	2.313152	-0.633709
29	6	0	1.819249	1.453954	0.783207
30	8	0	0.411019	1.779804	0.988130
31	6	0	0.000883	2.990102	0.467828
32	6	0	0.911494	4.030940	0.262094
33	6	0	2.380887	3.870444	0.591057
34	6	0	2.646213	2.588429	1.398875
35	6	0	-1.367311	3.112085	0.204444
36	6	0	-1.848564	4.317967	-0.308391
37	6	0	-0.969294	5.386067	-0.537925
38	6	0	0.387757	5.231135	-0.253118
39	8	0	1.286907	6.240921	-0.459141
40	8	0	-3.160641	4.518659	-0.613153
41	8	0	2.333654	2.766219	2.781214
42	1	0	-0.099124	-0.241128	-0.784030
43	8	0	1.377570	0.285188	-2.612655
44	6	0	2.907632	-1.471786	-1.813447
45	8	0	3.789291	-0.474496	-1.823431
46	6	0	5.182895	-0.843354	-1.600923
47	8	0	3.185015	-2.646551	-1.648464
48	6	0	6.001128	0.429942	-1.647436
49	1	0	-6.517978	0.731525	1.021982
50	1	0	-3.051763	0.999327	-1.538007
51	1	0	-3.452569	-3.018192	1.921832
52	1	0	-4.452108	-3.738836	0.675071
53	1	0	-1.877513	-4.254924	0.663090
54	1	0	-1.379339	-1.771212	0.881907
55	1	0	-3.122071	-3.401698	-1.718593
56	1	0	-0.838776	-3.468286	-2.436068
57	1	0	0.792779	-3.936065	-1.937666
58	1	0	3.068447	0.523420	3.135799
59	1	0	3.195874	-2.780314	4.382388
60	1	0	1.544016	-4.480172	2.335006
61	1	0	-6.761636	-1.272807	2.097413
62	1	0	-5.897689	2.612988	-0.179502
63	1	0	2.004087	1.447799	-0.298186
64	1	0	2.978139	3.848789	-0.330532
65	1	0	2.742218	4.725658	1.171312
66	1	0	3.710751	2.338721	1.355010
67	1	0	-2.022232	2.267888	0.387385
68	1	0	-1.352744	6.317303	-0.943664
69	1	0	0.822437	7.018864	-0.798228
70	1	0	-3.677375	3.697749	-0.508129
71	1	0	1.375957	2.644220	2.869688
72	1	0	1.456024	0.149969	-3.572724
73	1	0	5.253224	-1.346505	-0.633030
74	1	0	5.477034	-1.554103	-2.377612
75	1	0	5.906156	0.922609	-2.618969
76	1	0	7.055787	0.189288	-1.485306
77	1	0	5.684604	1.128402	-0.867769

Cartesian coordinates of the optimized geometry of (4‴*S*)-12O at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.903145	3.123923	0.487061
2	6	0	5.797149	2.782423	-0.531187
3	6	0	5.664200	1.547921	-1.169952
4	6	0	4.657421	0.630680	-0.816215
5	6	0	3.772640	1.026203	0.201299
6	6	0	3.880318	2.249884	0.860154
7	6	0	4.530581	-0.725710	-1.483632
8	6	0	3.650556	-1.665041	-0.646648
9	6	0	2.395891	-0.881526	-0.233600
10	8	0	2.758578	0.199274	0.635810
11	8	0	4.356667	-2.192911	0.473243
12	6	0	1.295913	-1.673721	0.497960
13	6	0	1.666164	-2.176766	1.902099
14	6	0	0.650891	-1.569972	2.846715
15	6	0	-0.577157	-1.038239	2.061908
16	6	0	-0.022800	-0.819592	0.624676
17	6	0	-0.847457	-1.330519	-0.532388
18	6	0	-0.217410	-2.470966	-1.018344
19	8	0	0.954592	-2.791474	-0.379646
20	6	0	-2.054748	-0.897604	-1.093710
21	6	0	-2.590036	-1.645954	-2.153941
22	6	0	-1.953537	-2.802101	-2.615717
23	6	0	-0.745063	-3.236648	-2.047340
24	8	0	-2.512669	-3.508681	-3.640292
25	8	0	-0.185945	-4.390165	-2.531128
26	8	0	0.752238	-1.426394	4.045927
27	8	0	6.573157	1.277874	-2.152959
28	8	0	4.976268	4.314035	1.150649
29	6	0	-2.720801	0.344951	-0.542926
30	8	0	-1.991452	1.492004	-1.068306
31	6	0	-2.401647	2.718747	-0.586055
32	6	0	-3.694757	2.901712	-0.069805
33	6	0	-4.694573	1.762719	-0.034331
34	6	0	-4.205387	0.562291	-0.861243
35	6	0	-1.475889	3.757147	-0.683557
36	6	0	-1.846264	5.028711	-0.241764
37	6	0	-3.114709	5.254472	0.299161
38	6	0	-4.019545	4.193549	0.380522
39	8	0	-5.244869	4.484146	0.911939
40	8	0	-0.915548	6.022481	-0.351746
41	8	0	-4.416000	0.773584	-2.256475
42	1	0	0.208549	0.246567	0.555992
43	8	0	-1.021029	0.181730	2.596904
44	6	0	-1.708332	-2.088669	2.110546
45	8	0	-1.229966	-3.313009	1.860362
46	6	0	-2.196307	-4.402229	1.774136
47	8	0	-2.867289	-1.825350	2.344624
48	6	0	-1.451872	-5.632111	1.297606
49	1	0	6.590517	3.456006	-0.838776
50	1	0	3.177133	2.515441	1.640104
51	1	0	4.103229	-0.634233	-2.491379
52	1	0	5.509829	-1.208451	-1.594618
53	1	0	3.348246	-2.528569	-1.242220
54	1	0	1.943402	-0.470686	-1.147931
55	1	0	4.743358	-1.449467	0.959214
56	1	0	2.677404	-1.911267	2.206093
57	1	0	1.584426	-3.267198	1.942093
58	1	0	-3.504545	-1.330431	-2.639779
59	1	0	-1.932511	-4.259806	-3.841081
60	1	0	0.686054	-4.518921	-2.130364
61	1	0	6.372770	0.430381	-2.572541
62	1	0	5.710219	4.836212	0.797399
63	1	0	-2.608299	0.352583	0.547514
64	1	0	-4.878145	1.430673	0.997364
65	1	0	-5.662604	2.072215	-0.448925
66	1	0	-4.778997	-0.328751	-0.591528
67	1	0	-0.487718	3.574152	-1.088091
68	1	0	-3.411538	6.234937	0.657893
69	1	0	-5.780919	3.681711	0.969429
70	1	0	-1.284796	6.847335	-0.006370
71	1	0	-3.668591	1.301377	-2.577668
72	1	0	-1.066732	0.069971	3.560756
73	1	0	-2.640600	-4.542669	2.763202
74	1	0	-2.985705	-4.101366	1.081126
75	1	0	-0.658969	-5.908290	1.998281
76	1	0	-1.007972	-5.463409	0.312592
77	1	0	-2.149806	-6.470966	1.222043

Cartesian coordinates of the optimized geometry of (4‴*S*)-12P at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.104604	2.819543	0.657991
2	6	0	6.049554	2.432452	-0.300244
3	6	0	5.903939	1.199004	-0.938580
4	6	0	4.836081	0.332053	-0.649075
5	6	0	3.908243	0.768324	0.307772
6	6	0	4.025657	1.992606	0.968481
7	6	0	4.700411	-1.015449	-1.327132
8	6	0	3.751523	-1.922159	-0.534806
9	6	0	2.497668	-1.101107	-0.193908
10	8	0	2.836085	-0.013144	0.678818
11	8	0	4.384872	-2.462437	0.625204
12	6	0	1.337732	-1.843914	0.493636
13	6	0	1.623743	-2.312901	1.931486
14	6	0	0.717004	-1.479949	2.803317
15	6	0	-0.523938	-1.023793	1.987208
16	6	0	0.043527	-0.940605	0.537908
17	6	0	-0.780240	-1.501547	-0.594716
18	6	0	-0.155862	-2.665611	-1.029678
19	8	0	1.006658	-2.973665	-0.368016
20	6	0	-1.962379	-1.064032	-1.204955
21	6	0	-2.488009	-1.841221	-2.248662
22	6	0	-1.858469	-3.020483	-2.658214
23	6	0	-0.666738	-3.451274	-2.053165
24	8	0	-2.402736	-3.749601	-3.675355
25	8	0	-0.096414	-4.605874	-2.517349
26	8	0	0.890527	-1.118868	3.946681
27	8	0	6.793271	0.765479	-1.879680
28	8	0	5.187509	4.010372	1.319607
29	6	0	-2.603288	0.223873	-0.733872
30	8	0	-1.793497	1.317290	-1.257009
31	6	0	-2.171770	2.578381	-0.842766
32	6	0	-3.482714	2.839376	-0.412589
33	6	0	-4.534850	1.748508	-0.394330
34	6	0	-4.056071	0.495281	-1.145436
35	6	0	-1.193679	3.569382	-0.920230
36	6	0	-1.528568	4.872082	-0.545957
37	6	0	-2.814672	5.175648	-0.091748
38	6	0	-3.772021	4.160647	-0.028687
39	8	0	-5.011438	4.525359	0.417608
40	8	0	-0.547084	5.818049	-0.633455
41	8	0	-4.177732	0.659546	-2.557148
42	1	0	0.309083	0.110060	0.394270
43	8	0	-0.969713	0.232213	2.424710
44	6	0	-1.585047	-2.134686	2.123465
45	8	0	-2.808729	-1.655361	2.340138
46	6	0	-3.872380	-2.644924	2.476979
47	8	0	-1.307446	-3.317679	2.040007
48	6	0	-5.154069	-1.895347	2.773711
49	1	0	6.885487	3.081921	-0.546641
50	1	0	3.287639	2.292672	1.702401
51	1	0	4.327544	-0.899935	-2.353137
52	1	0	5.675665	-1.505193	-1.406417
53	1	0	3.452194	-2.781799	-1.138344
54	1	0	2.105161	-0.694356	-1.137528
55	1	0	4.813453	-1.732050	1.095568
56	1	0	2.667587	-2.236432	2.226666
57	1	0	1.305728	-3.356582	2.027479
58	1	0	-3.382201	-1.525381	-2.770645
59	1	0	-1.834294	-4.519988	-3.831693
60	1	0	0.724985	-4.778155	-2.034780
61	1	0	7.500096	1.417913	-1.983837
62	1	0	5.967067	4.496661	1.016674
63	1	0	-2.549959	0.269431	0.360072
64	1	0	-4.792701	1.467410	0.636835
65	1	0	-5.462186	2.083286	-0.876794
66	1	0	-4.686239	-0.357338	-0.876659
67	1	0	-0.193342	3.326836	-1.258043
68	1	0	-3.085242	6.181522	0.213395
69	1	0	-5.590638	3.752329	0.457381
70	1	0	-0.896832	6.670571	-0.338657
71	1	0	-3.382833	1.127351	-2.856596
72	1	0	-0.830083	0.256224	3.387243
73	1	0	-3.930421	-3.214591	1.545740
74	1	0	-3.598752	-3.332243	3.281474
75	1	0	-5.974639	-2.610379	2.882956
76	1	0	-5.404959	-1.207183	1.961662
77	1	0	-5.068948	-1.324934	3.702655

Cartesian coordinates of the optimized geometry of (4‴*S*)-12Q at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.924200	3.060804	0.479080
2	6	0	5.813635	2.710141	-0.540182
3	6	0	5.668412	1.478560	-1.177147
4	6	0	4.651274	0.569499	-0.822509
5	6	0	3.772405	0.972578	0.193933
6	6	0	3.893367	2.197126	0.853800
7	6	0	4.510623	-0.785944	-1.489171
8	6	0	3.621633	-1.716141	-0.651060
9	6	0	2.375066	-0.919863	-0.237983
10	8	0	2.749152	0.158658	0.630040
11	8	0	4.323083	-2.250218	0.468719
12	6	0	1.266396	-1.697780	0.495426
13	6	0	1.632222	-2.206388	1.898679
14	6	0	0.629344	-1.582881	2.845703
15	6	0	-0.592689	-1.032855	2.063709
16	6	0	-0.039104	-0.824196	0.624848
17	6	0	-0.873686	-1.323333	-0.530065
18	6	0	-0.262176	-2.473421	-1.016689
19	8	0	0.907138	-2.810338	-0.381399
20	6	0	-2.074325	-0.870795	-1.090140
21	6	0	-2.623681	-1.611321	-2.148513
22	6	0	-2.007220	-2.778665	-2.609589
23	6	0	-0.804555	-3.231920	-2.043442
24	8	0	-2.579934	-3.477240	-3.632030
25	8	0	-0.265372	-4.394940	-2.527074
26	8	0	0.736520	-1.439769	4.044420
27	8	0	6.572399	1.196449	-2.161443
28	8	0	5.107177	4.277110	1.070074
29	6	0	-2.716389	0.384918	-0.540847
30	8	0	-1.951694	1.515005	-1.053505
31	6	0	-2.338891	2.750176	-0.574991
32	6	0	-3.630580	2.966041	-0.074589
33	6	0	-4.659291	1.852825	-0.052309
34	6	0	-4.191274	0.640627	-0.874595
35	6	0	-1.384689	3.766718	-0.660574
36	6	0	-1.728372	5.046849	-0.222186
37	6	0	-2.997388	5.304350	0.303148
38	6	0	-3.927892	4.267921	0.373026
39	8	0	-5.152729	4.585910	0.889914
40	8	0	-0.852610	6.094248	-0.270177
41	8	0	-4.382225	0.856791	-2.271816
42	1	0	0.207532	0.238391	0.554562
43	8	0	-1.015458	0.194990	2.598064
44	6	0	-1.740182	-2.064849	2.117050
45	8	0	-1.282786	-3.296374	1.863435
46	6	0	-2.266979	-4.369900	1.780947
47	8	0	-2.893441	-1.782811	2.357427
48	6	0	-1.546292	-5.609789	1.293954
49	1	0	6.606410	3.386561	-0.836758
50	1	0	3.185237	2.454255	1.634462
51	1	0	4.084157	-0.690749	-2.496907
52	1	0	5.484994	-1.278405	-1.600095
53	1	0	3.310052	-2.576889	-1.245936
54	1	0	1.926628	-0.504994	-1.152464
55	1	0	4.721945	-1.510821	0.951007
56	1	0	2.648786	-1.958092	2.199494
57	1	0	1.532046	-3.295281	1.938997
58	1	0	-3.532545	-1.280814	-2.634945
59	1	0	-2.012587	-4.238026	-3.833071
60	1	0	0.605364	-4.537510	-2.128232
61	1	0	6.363310	0.349404	-2.577576
62	1	0	4.433398	4.409300	1.751813
63	1	0	-2.615548	0.386071	0.550844
64	1	0	-4.864231	1.525474	0.976832
65	1	0	-5.613822	2.187245	-0.478580
66	1	0	-4.790047	-0.235644	-0.611134
67	1	0	-0.399653	3.542583	-1.056673
68	1	0	-3.258220	6.296101	0.653326
69	1	0	-5.708499	3.796406	0.938110
70	1	0	-0.015841	5.795677	-0.653100
71	1	0	-3.619622	1.366750	-2.585805
72	1	0	-1.069603	0.082803	3.561371
73	1	0	-2.705408	-4.506972	2.773105
74	1	0	-3.057048	-4.053766	1.095566
75	1	0	-0.752303	-5.901456	1.987103
76	1	0	-1.107832	-5.444930	0.305856
77	1	0	-2.258333	-6.436974	1.221305

Cartesian coordinates of the optimized geometry of (4‴*S*)-12R at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.852533	1.300476	-0.167414
2	6	0	-5.717479	0.532843	0.623797
3	6	0	-5.397456	-0.796956	0.901942
4	6	0	-4.224218	-1.399949	0.410438
5	6	0	-3.404444	-0.602199	-0.393537
6	6	0	-3.700367	0.725538	-0.709115
7	6	0	-3.843477	-2.823593	0.770073
8	6	0	-2.610131	-3.308384	-0.016425
9	6	0	-1.628118	-2.130148	-0.105422
10	8	0	-2.236808	-1.116880	-0.925472
11	8	0	-2.970160	-3.795299	-1.309805
12	6	0	-0.210880	-2.368246	-0.662483
13	6	0	-0.109574	-2.980573	-2.069421
14	6	0	0.568452	-1.928702	-2.915888
15	6	0	1.373326	-0.953926	-2.013308
16	6	0	0.583775	-1.011139	-0.672750
17	6	0	1.356841	-1.089099	0.616220
18	6	0	1.261149	-2.393532	1.086124
19	8	0	0.472968	-3.217019	0.316404
20	6	0	2.048179	-0.114197	1.342288
21	6	0	2.686715	-0.507479	2.526312
22	6	0	2.628882	-1.837247	2.960263
23	6	0	1.894308	-2.804667	2.251400
24	8	0	3.264806	-2.188701	4.115722
25	8	0	1.848501	-4.071642	2.769035
26	8	0	0.483080	-1.760341	-4.112719
27	8	0	-6.193559	-1.582825	1.685643
28	8	0	-5.178737	2.607107	-0.373439
29	6	0	1.959228	1.312597	0.848867
30	8	0	0.581182	1.717237	1.114727
31	6	0	0.220941	2.930457	0.573977
32	6	0	1.179136	3.921524	0.335461
33	6	0	2.640361	3.697852	0.670047
34	6	0	2.865091	2.389274	1.454347
35	6	0	-1.137947	3.104240	0.306945
36	6	0	-1.553686	4.304964	-0.258579
37	6	0	-0.636787	5.325401	-0.531673
38	6	0	0.714567	5.122412	-0.228118
39	8	0	1.656300	6.082050	-0.465672
40	8	0	-2.892701	4.432109	-0.547237
41	8	0	2.608324	2.555824	2.848623
42	1	0	-0.109835	-0.169693	-0.708814
43	8	0	1.354346	0.343615	-2.549563
44	6	0	2.792837	-1.533197	-1.859585
45	8	0	3.733914	-0.591538	-1.868905
46	6	0	5.107345	-1.051104	-1.695481
47	8	0	3.002140	-2.726605	-1.733299
48	6	0	6.000788	0.171176	-1.723951
49	1	0	-6.608929	0.991294	1.040474
50	1	0	-3.024327	1.290217	-1.340602
51	1	0	-3.637938	-2.890628	1.846346
52	1	0	-4.671418	-3.512685	0.573682
53	1	0	-2.139808	-4.149420	0.498956
54	1	0	-1.491532	-1.725864	0.907529
55	1	0	-3.343543	-3.048731	-1.802394
56	1	0	-1.064546	-3.294243	-2.487594
57	1	0	0.551194	-3.853220	-2.030363
58	1	0	3.202406	0.217733	3.143442
59	1	0	3.099577	-3.131090	4.276125
60	1	0	1.284226	-4.628570	2.213470
61	1	0	-6.966986	-1.076073	1.970736
62	1	0	-4.386685	3.111751	-0.636420
63	1	0	2.102661	1.323272	-0.238468
64	1	0	3.236489	3.673737	-0.251753
65	1	0	3.031680	4.528430	1.266752
66	1	0	3.913918	2.089106	1.369920
67	1	0	-1.839079	2.305512	0.511639
68	1	0	-0.962716	6.261486	-0.977726
69	1	0	1.233413	6.868550	-0.838038
70	1	0	-3.065553	5.287463	-0.964966
71	1	0	1.648684	2.481725	2.966564
72	1	0	1.400293	0.244746	-3.516202
73	1	0	5.170954	-1.589232	-0.746133
74	1	0	5.338153	-1.752221	-2.501793
75	1	0	5.748321	0.860387	-0.913311
76	1	0	5.910671	0.701357	-2.675984
77	1	0	7.042552	-0.138333	-1.599538

Cartesian coordinates of the optimized geometry of (4‴*R*)-12A at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.495845	-4.149043	-0.663441
2	6	0	-4.656304	-3.810489	-1.369554
3	6	0	-5.044794	-2.473155	-1.434383
4	6	0	-4.305972	-1.449913	-0.811510
5	6	0	-3.145572	-1.833421	-0.129327
6	6	0	-2.729261	-3.165581	-0.039394
7	6	0	-4.753022	-0.004533	-0.860501
8	6	0	-4.027050	0.830207	0.202149
9	6	0	-2.536797	0.463507	0.158914
10	8	0	-2.361879	-0.913618	0.534098
11	8	0	-4.583460	0.644596	1.502691
12	6	0	-1.612720	1.283581	1.075731
13	6	0	-1.810784	1.108249	2.574308
14	6	0	-0.487603	1.511933	3.180799
15	6	0	0.661161	1.326235	2.122423
16	6	0	-0.094022	1.051059	0.770006
17	6	0	0.161317	2.085706	-0.300115
18	6	0	-0.865595	3.023525	-0.191196
19	8	0	-1.824204	2.694899	0.741435
20	6	0	1.156759	2.267950	-1.263346
21	6	0	1.100355	3.429715	-2.054017
22	6	0	0.078537	4.369365	-1.908972
23	6	0	-0.945373	4.166546	-0.969552
24	8	0	0.063854	5.478344	-2.704087
25	8	0	-1.942748	5.103122	-0.896146
26	8	0	-0.290988	1.947920	4.291642
27	8	0	-6.168642	-2.079682	-2.103362
28	8	0	-3.159552	-5.471786	-0.628888
29	6	0	2.213035	1.248238	-1.617508
30	8	0	2.720140	0.609685	-0.427291
31	6	0	3.670799	-0.367388	-0.636609
32	6	0	3.803207	-1.016544	-1.871470
33	6	0	2.917039	-0.673808	-3.048758
34	6	0	1.714606	0.159274	-2.596136
35	6	0	4.472548	-0.687604	0.465731
36	6	0	5.435662	-1.686336	0.327655
37	6	0	5.609244	-2.353069	-0.890811
38	6	0	4.795817	-2.009874	-1.969144
39	8	0	4.913384	-2.622283	-3.184906
40	8	0	6.257085	-2.055011	1.354816
41	8	0	0.694179	-0.645908	-2.008151
42	1	0	0.075895	0.029747	0.438264
43	8	0	1.458931	2.479454	2.105320
44	6	0	1.516359	0.153167	2.602947
45	8	0	0.891546	-1.017670	2.537563
46	6	0	1.617783	-2.179938	3.048921
47	8	0	2.634927	0.330587	3.055277
48	6	0	0.718053	-3.385727	2.886456
49	1	0	-5.235897	-4.589314	-1.854823
50	1	0	-1.823008	-3.407337	0.505941
51	1	0	-4.564481	0.424547	-1.853378
52	1	0	-5.831739	0.069733	-0.692069
53	1	0	-4.134952	1.894785	-0.015311
54	1	0	-2.180901	0.594415	-0.872283
55	1	0	-4.501564	-0.294015	1.726384
56	1	0	-1.973398	0.045865	2.793674
57	1	0	-2.651259	1.671087	2.978943
58	1	0	1.856572	3.617433	-2.809724
59	1	0	-0.711401	6.009676	-2.463891
60	1	0	-2.584701	4.835684	-0.222623
61	1	0	-6.615655	-2.856463	-2.467889
62	1	0	-2.344718	-5.583314	-0.119483
63	1	0	3.047505	1.769660	-2.105998
64	1	0	3.482680	-0.116799	-3.807099
65	1	0	2.557727	-1.583192	-3.541117
66	1	0	1.247532	0.648075	-3.455252
67	1	0	4.328890	-0.158519	1.400819
68	1	0	6.369924	-3.121979	-0.981208
69	1	0	5.607553	-3.294763	-3.140274
70	1	0	6.048935	-1.524156	2.136487
71	1	0	1.115392	-1.208098	-1.342266
72	1	0	2.292322	2.225273	2.541231
73	1	0	2.545423	-2.274366	2.479431
74	1	0	1.869924	-1.986564	4.094551
75	1	0	0.481583	-3.558395	1.832869
76	1	0	-0.214689	-3.258988	3.442538
77	1	0	1.230513	-4.271890	3.271721

Cartesian coordinates of the optimized geometry of (4‴*R*)-12B at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.371486	-4.207990	-0.625642
2	6	0	-4.537561	-3.903848	-1.338057
3	6	0	-4.958403	-2.577041	-1.415841
4	6	0	-4.246763	-1.530599	-0.799935
5	6	0	-3.079768	-1.880020	-0.110760
6	6	0	-2.631339	-3.200774	-0.007648
7	6	0	-4.727911	-0.096786	-0.863590
8	6	0	-4.025151	0.765343	0.192956
9	6	0	-2.526745	0.433519	0.157936
10	8	0	-2.320944	-0.935733	0.547100
11	8	0	-4.581231	0.579692	1.493622
12	6	0	-1.624116	1.282419	1.069702
13	6	0	-1.823134	1.119258	2.569525
14	6	0	-0.510337	1.558366	3.174319
15	6	0	0.645063	1.383123	2.121484
16	6	0	-0.100632	1.076986	0.770509
17	6	0	0.136394	2.104966	-0.310116
18	6	0	-0.907021	3.025362	-0.210973
19	8	0	-1.862496	2.686123	0.721195
20	6	0	1.128490	2.294310	-1.275032
21	6	0	1.054970	3.448730	-2.074865
22	6	0	0.018468	4.373326	-1.937388
23	6	0	-1.004275	4.160585	-0.998690
24	8	0	-0.012972	5.476085	-2.740734
25	8	0	-2.017661	5.080752	-0.935576
26	8	0	-0.326356	2.012705	4.279975
27	8	0	-6.089461	-2.217636	-2.091824
28	8	0	-3.003031	-5.521765	-0.578681
29	6	0	2.191710	1.281192	-1.627027
30	8	0	2.691961	0.638256	-0.436788
31	6	0	3.634433	-0.348166	-0.639779
32	6	0	3.768825	-0.996833	-1.877041
33	6	0	2.896967	-0.639902	-3.060633
34	6	0	1.696117	0.197867	-2.613681
35	6	0	4.422561	-0.679206	0.466315
36	6	0	5.373943	-1.690269	0.335232
37	6	0	5.549013	-2.357297	-0.883085
38	6	0	4.747893	-2.000962	-1.969443
39	8	0	4.868542	-2.613434	-3.184725
40	8	0	6.123169	-1.987437	1.438179
41	8	0	0.666369	-0.603475	-2.036852
42	1	0	0.091363	0.055459	0.451943
43	8	0	1.420379	2.551349	2.091793
44	6	0	1.522263	0.234162	2.620665
45	8	0	0.923382	-0.950753	2.566126
46	6	0	1.669671	-2.089546	3.101433
47	8	0	2.633558	0.442155	3.077485
48	6	0	0.809764	-3.321523	2.920411
49	1	0	-5.096723	-4.700524	-1.818235
50	1	0	-1.721689	-3.415569	0.543388
51	1	0	-4.546751	0.327162	-1.860047
52	1	0	-5.808581	-0.046694	-0.698777
53	1	0	-4.157501	1.824870	-0.035615
54	1	0	-2.169993	0.562359	-0.873178
55	1	0	-4.472387	-0.353156	1.729615
56	1	0	-1.964037	0.056305	2.800767
57	1	0	-2.676176	1.669128	2.965634
58	1	0	1.807965	3.641647	-2.832491
59	1	0	-0.797563	5.996029	-2.505999
60	1	0	-2.657154	4.807679	-0.262001
61	1	0	-6.515255	-3.008756	-2.450951
62	1	0	-2.186191	-5.608549	-0.067673
63	1	0	3.027654	1.806301	-2.109164
64	1	0	3.473509	-0.080649	-3.809090
65	1	0	2.536755	-1.543255	-3.563217
66	1	0	1.238586	0.692829	-3.474384
67	1	0	4.291971	-0.158716	1.406130
68	1	0	6.295381	-3.141078	-0.984400
69	1	0	5.553111	-3.295385	-3.137000
70	1	0	6.758006	-2.683971	1.219805
71	1	0	1.078883	-1.171051	-1.370094
72	1	0	2.254757	2.320042	2.538698
73	1	0	2.614895	-2.159036	2.558216
74	1	0	1.887435	-1.884865	4.152702
75	1	0	0.607526	-3.505470	1.861540
76	1	0	-0.141431	-3.219745	3.449817
77	1	0	1.336573	-4.190915	3.324135

Cartesian coordinates of the optimized geometry of (4‴*R*)-12C at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.399091	-4.175209	-0.641398
2	6	0	-4.564880	-3.860231	-1.349896
3	6	0	-4.980306	-2.528509	-1.417249
4	6	0	-4.263199	-1.492440	-0.795244
5	6	0	-3.095673	-1.854419	-0.109270
6	6	0	-2.654071	-3.175557	-0.016966
7	6	0	-4.736095	-0.055359	-0.849156
8	6	0	-4.021292	0.799367	0.205554
9	6	0	-2.526199	0.453927	0.163433
10	8	0	-2.333649	-0.916257	0.554710
11	8	0	-4.572434	0.615922	1.508664
12	6	0	-1.610951	1.295760	1.068838
13	6	0	-1.806353	1.141586	2.570155
14	6	0	-0.488696	1.577055	3.166699
15	6	0	0.662610	1.372727	2.114857
16	6	0	-0.090608	1.072791	0.765466
17	6	0	0.155367	2.096284	-0.317361
18	6	0	-0.878863	3.027185	-0.219292
19	8	0	-1.835627	2.700792	0.716074
20	6	0	1.147646	2.273326	-1.284666
21	6	0	1.083213	3.425639	-2.088345
22	6	0	0.055494	4.360218	-1.952500
23	6	0	-0.967031	4.160541	-1.010801
24	8	0	0.032772	5.460328	-2.759737
25	8	0	-1.971309	5.090637	-0.948357
26	8	0	-0.298151	2.047704	4.264297
27	8	0	-6.110781	-2.159966	-2.089124
28	8	0	-2.937626	-5.455804	-0.535960
29	6	0	2.203916	1.251649	-1.633128
30	8	0	2.707138	0.616597	-0.439730
31	6	0	3.646505	-0.372705	-0.641121
32	6	0	3.775466	-1.030372	-1.871775
33	6	0	2.898021	-0.683001	-3.054076
34	6	0	1.701244	0.162213	-2.609470
35	6	0	4.440574	-0.696591	0.465727
36	6	0	5.391800	-1.707797	0.336743
37	6	0	5.561432	-2.383612	-0.877229
38	6	0	4.755921	-2.036557	-1.960247
39	8	0	4.870174	-2.657336	-3.172098
40	8	0	6.205009	-2.080475	1.369046
41	8	0	0.670556	-0.631143	-2.023512
42	1	0	0.088605	0.048959	0.446768
43	8	0	1.462971	2.523039	2.079586
44	6	0	1.514532	0.205864	2.616444
45	8	0	0.882371	-0.961988	2.582596
46	6	0	1.605449	-2.118036	3.112490
47	8	0	2.638415	0.386798	3.054344
48	6	0	0.688976	-3.316938	3.001243
49	1	0	-5.140993	-4.640017	-1.841279
50	1	0	-1.747680	-3.414644	0.525561
51	1	0	-4.558758	0.371363	-1.845155
52	1	0	-5.815377	0.000921	-0.677196
53	1	0	-4.146359	1.860255	-0.020838
54	1	0	-2.173217	0.577480	-0.869659
55	1	0	-4.454440	-0.314729	1.749062
56	1	0	-1.951350	0.080489	2.807137
57	1	0	-2.654990	1.698285	2.966047
58	1	0	1.836904	3.609113	-2.847626
59	1	0	-0.746625	5.988263	-2.525544
60	1	0	-2.613383	4.824388	-0.274494
61	1	0	-6.543623	-2.945838	-2.451137
62	1	0	-3.527331	-6.052758	-1.017446
63	1	0	3.040280	1.769258	-2.122619
64	1	0	3.472004	-0.133196	-3.811433
65	1	0	2.532838	-1.590532	-3.545501
66	1	0	1.242716	0.652341	-3.472459
67	1	0	4.300226	-0.160735	1.397437
68	1	0	6.312646	-3.162563	-0.960557
69	1	0	5.554599	-3.339234	-3.120480
70	1	0	6.000581	-1.542395	2.146754
71	1	0	1.083879	-1.201362	-1.359514
72	1	0	2.303186	2.268482	2.502009
73	1	0	2.520399	-2.239047	2.527639
74	1	0	1.880373	-1.898447	4.147123
75	1	0	0.426961	-3.513919	1.958110
76	1	0	-0.229730	-3.164923	3.574058
77	1	0	1.199904	-4.198854	3.398092

Cartesian coordinates of the optimized geometry of (4‴*R*)-12D at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.953633	-3.533194	-0.971276
2	6	0	-4.984577	-3.029667	-1.773776
3	6	0	-5.170487	-1.647674	-1.852609
4	6	0	-4.353251	-0.744917	-1.150820
5	6	0	-3.326686	-1.295178	-0.370881
6	6	0	-3.115413	-2.671097	-0.265189
7	6	0	-4.579842	0.749999	-1.219434
8	6	0	-3.845351	1.467302	-0.080193
9	6	0	-2.424924	0.889805	0.009223
10	8	0	-2.483536	-0.497923	0.374804
11	8	0	-4.542245	1.359943	1.159802
12	6	0	-1.483250	1.573600	1.016948
13	6	0	-1.859963	1.447369	2.488338
14	6	0	-0.555600	1.525096	3.250292
15	6	0	0.641257	1.144518	2.307521
16	6	0	0.005519	1.092906	0.873879
17	6	0	0.566820	2.109878	-0.088591
18	6	0	-0.332857	3.167345	-0.140445
19	8	0	-1.451707	2.989881	0.641965
20	6	0	1.750415	2.153038	-0.831202
21	6	0	1.980211	3.280767	-1.632960
22	6	0	1.067052	4.339493	-1.668534
23	6	0	-0.117785	4.297991	-0.915338
24	8	0	1.326441	5.418204	-2.464517
25	8	0	-0.971015	5.365618	-1.006380
26	8	0	-0.400211	1.856065	4.403082
27	8	0	-6.160257	-1.095692	-2.614576
28	8	0	-3.717023	-4.871942	-0.848478
29	6	0	2.739383	1.016434	-0.699496
30	8	0	2.072367	-0.183876	-1.185027
31	6	0	2.785025	-1.354553	-1.026133
32	6	0	4.183311	-1.340195	-0.945106
33	6	0	4.965955	-0.047363	-1.023898
34	6	0	4.075102	1.133615	-1.441139
35	6	0	2.036528	-2.532938	-0.989067
36	6	0	2.709687	-3.747134	-0.854742
37	6	0	4.105704	-3.782139	-0.755017
38	6	0	4.822018	-2.583131	-0.802370
39	8	0	6.185249	-2.555272	-0.716568
40	8	0	1.948827	-4.881121	-0.814039
41	8	0	3.872882	1.173637	-2.853440
42	1	0	0.035293	0.074529	0.486829
43	8	0	1.653774	2.112535	2.425326
44	6	0	1.217845	-0.199268	2.767730
45	8	0	0.380827	-1.217883	2.610860
46	6	0	0.854910	-2.527591	3.062046
47	8	0	2.334123	-0.270232	3.252858
48	6	0	-0.148959	-3.564148	2.607448
49	1	0	-5.632761	-3.703405	-2.328469
50	1	0	-2.314227	-3.057487	0.352123
51	1	0	-4.237174	1.149478	-2.183129
52	1	0	-5.647476	0.980511	-1.152351
53	1	0	-3.778508	2.536864	-0.288840
54	1	0	-1.959469	0.975712	-0.983129
55	1	0	-4.642357	0.418163	1.361848
56	1	0	-2.287474	0.453181	2.666924
57	1	0	-2.585748	2.187987	2.823434
58	1	0	2.860073	3.346044	-2.260315
59	1	0	0.589738	6.042785	-2.374653
60	1	0	-1.758630	5.195278	-0.469905
61	1	0	-6.680689	-1.797489	-3.030039
62	1	0	-4.347747	-5.363490	-1.392827
63	1	0	2.954710	0.870172	0.367595
64	1	0	5.431199	0.174747	-0.054116
65	1	0	5.785429	-0.135721	-1.744503
66	1	0	4.567688	2.073025	-1.173763
67	1	0	0.955901	-2.501215	-1.061472
68	1	0	4.628327	-4.728489	-0.641919
69	1	0	6.524615	-3.458860	-0.650361
70	1	0	2.522972	-5.652728	-0.709469
71	1	0	3.149151	0.559637	-3.051075
72	1	0	2.343583	1.700902	2.977489
73	1	0	0.948639	-2.489232	4.150470
74	1	0	1.845047	-2.694996	2.633276
75	1	0	-0.188364	-3.618222	1.516237
76	1	0	-1.148139	-3.342073	2.991766
77	1	0	0.153447	-4.544970	2.985718

Cartesian coordinates of the optimized geometry of (4‴*R*)-12E at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.930208	-3.888972	-0.568285
2	6	0	-5.020882	-3.504312	-1.357686
3	6	0	-5.295994	-2.147105	-1.520295
4	6	0	-4.509539	-1.148428	-0.915783
5	6	0	-3.420778	-1.580186	-0.150461
6	6	0	-3.118567	-2.932311	0.039910
7	6	0	-4.834072	0.322468	-1.067286
8	6	0	-4.099196	1.159070	-0.011343
9	6	0	-2.643106	0.675106	0.050777
10	8	0	-2.597022	-0.687123	0.498716
11	8	0	-4.735427	1.097203	1.263557
12	6	0	-1.702895	1.466025	0.976307
13	6	0	-2.009391	1.405769	2.472776
14	6	0	-0.674439	1.640136	3.130412
15	6	0	0.465662	1.100382	2.217024
16	6	0	-0.193003	1.049731	0.790756
17	6	0	0.306263	2.094928	-0.175404
18	6	0	-0.660252	3.090030	-0.248774
19	8	0	-1.768179	2.859835	0.533552
20	6	0	1.482735	2.197850	-0.925820
21	6	0	1.636603	3.322324	-1.749873
22	6	0	0.656613	4.318717	-1.805418
23	6	0	-0.521788	4.215143	-1.049133
24	8	0	0.844543	5.394662	-2.624307
25	8	0	-1.444978	5.220505	-1.160365
26	8	0	-0.431432	2.219591	4.166705
27	8	0	-6.347785	-1.708517	-2.272763
28	8	0	-3.704979	-5.229082	-0.437982
29	6	0	2.540569	1.124180	-0.792416
30	8	0	1.969984	-0.104865	-1.333552
31	6	0	2.765320	-1.225146	-1.211021
32	6	0	4.154021	-1.117040	-1.079048
33	6	0	4.844543	0.229119	-1.072614
34	6	0	3.886577	1.354871	-1.488924
35	6	0	2.106269	-2.458259	-1.267024
36	6	0	2.864824	-3.625674	-1.181941
37	6	0	4.255428	-3.565699	-1.031667
38	6	0	4.879072	-2.319046	-0.981976
39	8	0	6.232899	-2.194323	-0.844193
40	8	0	2.302264	-4.869616	-1.228127
41	8	0	3.729509	1.416181	-2.906977
42	1	0	-0.130674	0.039515	0.385337
43	8	0	1.562104	1.972863	2.275696
44	6	0	0.796261	-0.332010	2.672427
45	8	0	2.101986	-0.532194	2.842523
46	6	0	2.501893	-1.876939	3.241863
47	8	0	-0.066672	-1.175843	2.839062
48	6	0	4.013515	-1.892086	3.328668
49	1	0	-5.636726	-4.263696	-1.829087
50	1	0	-2.265099	-3.207492	0.650735
51	1	0	-4.561572	0.678132	-2.069650
52	1	0	-5.910346	0.490576	-0.963059
53	1	0	-4.107631	2.213857	-0.293603
54	1	0	-2.223673	0.731386	-0.964366
55	1	0	-4.775496	0.167372	1.531162
56	1	0	-2.323868	0.387352	2.728884
57	1	0	-2.778606	2.105279	2.796538
58	1	0	2.509125	3.428404	-2.381695
59	1	0	0.065035	5.967586	-2.552984
60	1	0	-2.229285	4.997249	-0.638508
61	1	0	-6.836370	-2.468630	-2.618539
62	1	0	-2.935286	-5.371360	0.130806
63	1	0	2.733898	0.958657	0.274834
64	1	0	5.249970	0.447359	-0.075617
65	1	0	5.698132	0.226176	-1.758075
66	1	0	4.300913	2.319786	-1.182333
67	1	0	1.026422	-2.485030	-1.372602
68	1	0	4.828119	-4.484993	-0.959376
69	1	0	6.636208	-3.073245	-0.815912
70	1	0	1.345239	-4.784187	-1.340955
71	1	0	3.047036	0.769409	-3.142756
72	1	0	1.632587	2.262337	3.201298
73	1	0	2.123391	-2.581616	2.496847
74	1	0	2.027863	-2.104485	4.200382
75	1	0	4.349096	-2.888317	3.631202
76	1	0	4.372365	-1.169584	4.066832
77	1	0	4.462370	-1.657814	2.359534

Cartesian coordinates of the optimized geometry of (4‴*R*)-12F at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.519268	-4.134616	-0.676598
2	6	0	-4.677229	-3.789017	-1.383439
3	6	0	-5.058813	-2.449619	-1.446506
4	6	0	-4.315417	-1.431156	-0.821167
5	6	0	-3.157570	-1.821623	-0.138583
6	6	0	-2.748164	-3.156037	-0.050425
7	6	0	-4.755582	0.016419	-0.867768
8	6	0	-4.027597	0.844945	0.198282
9	6	0	-2.538824	0.471908	0.155733
10	8	0	-2.369427	-0.906908	0.526708
11	8	0	-4.586578	0.658162	1.497452
12	6	0	-1.612405	1.285715	1.075736
13	6	0	-1.814716	1.109935	2.573672
14	6	0	-0.490987	1.506846	3.183534
15	6	0	0.659425	1.315482	2.127942
16	6	0	-0.094221	1.045164	0.773535
17	6	0	0.169747	2.079304	-0.295122
18	6	0	-0.852277	3.022760	-0.187364
19	8	0	-1.815144	2.698370	0.742067
20	6	0	1.169694	2.259532	-1.254093
21	6	0	1.122308	3.423327	-2.042289
22	6	0	0.104944	4.367941	-1.898602
23	6	0	-0.923193	4.168112	-0.963146
24	8	0	0.099016	5.478750	-2.690881
25	8	0	-1.915408	5.109824	-0.890550
26	8	0	-0.294785	1.941791	4.294794
27	8	0	-6.179824	-2.049120	-2.116013
28	8	0	-3.189910	-5.459096	-0.643652
29	6	0	2.223800	1.237080	-1.607113
30	8	0	2.717009	0.583458	-0.420320
31	6	0	3.675584	-0.386612	-0.631458
32	6	0	3.818710	-1.027974	-1.872087
33	6	0	2.931167	-0.675016	-3.048536
34	6	0	1.725498	0.157070	-2.594258
35	6	0	4.470525	-0.709434	0.472104
36	6	0	5.441081	-1.703454	0.333730
37	6	0	5.627055	-2.359004	-0.885980
38	6	0	4.821003	-2.014003	-1.969368
39	8	0	5.049485	-2.689845	-3.134891
40	8	0	6.255823	-2.071950	1.366006
41	8	0	0.703945	-0.651267	-2.018080
42	1	0	0.069727	0.022328	0.443523
43	8	0	1.463461	2.464200	2.112743
44	6	0	1.507331	0.137294	2.609102
45	8	0	0.875662	-1.029755	2.543059
46	6	0	1.595066	-2.196553	3.054171
47	8	0	2.626787	0.308140	3.061685
48	6	0	0.687037	-3.396401	2.894286
49	1	0	-5.260339	-4.564181	-1.870362
50	1	0	-1.843713	-3.403359	0.495365
51	1	0	-4.563165	0.447055	-1.859226
52	1	0	-5.834242	0.095333	-0.701164
53	1	0	-4.130395	1.910619	-0.016305
54	1	0	-2.181549	0.604741	-0.874826
55	1	0	-4.514097	-0.282286	1.716626
56	1	0	-1.982884	0.048113	2.791538
57	1	0	-2.653478	1.676305	2.976880
58	1	0	1.882530	3.609188	-2.794408
59	1	0	-0.673338	6.014572	-2.451242
60	1	0	-2.559247	4.846326	-0.217250
61	1	0	-6.630906	-2.822859	-2.481991
62	1	0	-2.376921	-5.575917	-0.132469
63	1	0	3.064663	1.757221	-2.085654
64	1	0	3.490246	-0.109194	-3.806333
65	1	0	2.544119	-1.575122	-3.543728
66	1	0	1.264856	0.649285	-3.454374
67	1	0	4.317635	-0.186464	1.409198
68	1	0	6.388739	-3.122200	-0.993088
69	1	0	4.464446	-2.362201	-3.831144
70	1	0	6.037842	-1.546612	2.148674
71	1	0	1.112131	-1.185686	-1.321782
72	1	0	2.294688	2.205487	2.550167
73	1	0	2.521040	-2.297532	2.483078
74	1	0	1.850325	-2.003906	4.099148
75	1	0	0.447509	-3.568351	1.841287
76	1	0	-0.243782	-3.263019	3.452019
77	1	0	1.194384	-4.285606	3.279283

Cartesian coordinates of the optimized geometry of (4‴*R*)-12G at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.330690	-4.212195	-0.618070
2	6	0	-4.498419	-3.917072	-1.331924
3	6	0	-4.930757	-2.591306	-1.409801
4	6	0	-4.228869	-1.541707	-0.793159
5	6	0	-3.058469	-1.883910	-0.101988
6	6	0	-2.600064	-3.198573	0.000806
7	6	0	-4.720352	-0.111337	-0.857305
8	6	0	-4.020961	0.758613	0.195341
9	6	0	-2.521133	0.434073	0.159710
10	8	0	-2.310143	-0.931740	0.557410
11	8	0	-4.573914	0.574354	1.497559
12	6	0	-1.620322	1.291732	1.064807
13	6	0	-1.818308	1.140857	2.566124
14	6	0	-0.507950	1.595339	3.164788
15	6	0	0.648673	1.404001	2.116623
16	6	0	-0.096569	1.086980	0.766835
17	6	0	0.139180	2.108761	-0.319819
18	6	0	-0.905641	3.028199	-0.226646
19	8	0	-1.861632	2.692570	0.706286
20	6	0	1.131317	2.293745	-1.285559
21	6	0	1.057162	3.443884	-2.091477
22	6	0	0.019729	4.368207	-1.959327
23	6	0	-1.003627	4.159085	-1.020486
24	8	0	-0.012316	5.466880	-2.768301
25	8	0	-2.018258	5.078351	-0.963159
26	8	0	-0.326818	2.071142	4.261807
27	8	0	-6.064091	-2.242375	-2.087346
28	8	0	-2.853325	-5.486039	-0.501729
29	6	0	2.193576	1.278204	-1.633805
30	8	0	2.691021	0.636940	-0.441721
31	6	0	3.626132	-0.357292	-0.640151
32	6	0	3.759257	-1.009871	-1.875504
33	6	0	2.893584	-0.648968	-3.062339
34	6	0	1.695619	0.194858	-2.619466
35	6	0	4.408114	-0.692354	0.469103
36	6	0	5.351632	-1.711372	0.343266
37	6	0	5.525236	-2.382515	-0.872987
38	6	0	4.730276	-2.022254	-1.962532
39	8	0	4.849737	-2.638516	-3.176063
40	8	0	6.095085	-2.012027	1.449214
41	8	0	0.660842	-0.600629	-2.043839
42	1	0	0.097387	0.063799	0.454797
43	8	0	1.431301	2.566513	2.077393
44	6	0	1.518131	0.253856	2.627067
45	8	0	0.907467	-0.925496	2.592968
46	6	0	1.647096	-2.065594	3.135018
47	8	0	2.635039	0.457353	3.072256
48	6	0	0.758937	-3.284183	3.008138
49	1	0	-5.063390	-4.707352	-1.819421
50	1	0	-1.692278	-3.421889	0.547761
51	1	0	-4.544735	0.312078	-1.855021
52	1	0	-5.800932	-0.068418	-0.689774
53	1	0	-4.160031	1.816480	-0.037029
54	1	0	-2.166266	0.558164	-0.872651
55	1	0	-4.442567	-0.352908	1.744040
56	1	0	-1.950984	0.079050	2.807157
57	1	0	-2.674873	1.688687	2.957330
58	1	0	1.810259	3.633367	-2.849878
59	1	0	-0.797542	5.987204	-2.536566
60	1	0	-2.658067	4.807902	-0.288834
61	1	0	-6.484877	-3.036388	-2.445825
62	1	0	-3.435708	-6.094613	-0.977546
63	1	0	3.031075	1.800624	-2.116275
64	1	0	3.475312	-0.092736	-3.809051
65	1	0	2.530626	-1.550740	-3.565751
66	1	0	1.242511	0.690717	-3.482023
67	1	0	4.278149	-0.169361	1.407589
68	1	0	6.265444	-3.172639	-0.970169
69	1	0	5.527148	-3.327254	-3.123920
70	1	0	6.722781	-2.716313	1.235138
71	1	0	1.069437	-1.173418	-1.379116
72	1	0	2.270959	2.328764	2.510885
73	1	0	2.574749	-2.166039	2.566717
74	1	0	1.899014	-1.840268	4.174303
75	1	0	0.519656	-3.487105	1.960620
76	1	0	-0.172988	-3.152208	3.564386
77	1	0	1.281649	-4.154780	3.414567

Cartesian coordinates of the optimized geometry of (4‴*R*)-12H at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.964676	-3.536043	-0.978803
2	6	0	-4.993291	-3.029120	-1.781751
3	6	0	-5.174634	-1.649160	-1.860669
4	6	0	-4.353999	-0.746727	-1.158057
5	6	0	-3.329726	-1.298078	-0.379626
6	6	0	-3.122659	-2.677227	-0.273286
7	6	0	-4.578435	0.748503	-1.224774
8	6	0	-3.846082	1.461538	-0.081667
9	6	0	-2.425384	0.884618	0.007637
10	8	0	-2.482205	-0.505558	0.365433
11	8	0	-4.545036	1.349157	1.156702
12	6	0	-1.486549	1.564276	1.020900
13	6	0	-1.864663	1.426560	2.490855
14	6	0	-0.561472	1.495568	3.255872
15	6	0	0.638256	1.132496	2.309874
16	6	0	0.003398	1.088354	0.875759
17	6	0	0.562504	2.112338	-0.080400
18	6	0	-0.339632	3.167972	-0.125981
19	8	0	-1.458211	2.982968	0.655124
20	6	0	1.746172	2.162586	-0.822351
21	6	0	1.973639	3.295542	-1.617327
22	6	0	1.057996	4.352336	-1.646753
23	6	0	-0.126915	4.303725	-0.894023
24	8	0	1.314966	5.436253	-2.436361
25	8	0	-0.982364	5.370060	-0.978976
26	8	0	-0.409136	1.808611	4.414084
27	8	0	-6.162330	-1.093014	-2.622370
28	8	0	-3.831147	-4.893774	-0.933552
29	6	0	2.737561	1.027446	-0.696576
30	8	0	2.070602	-0.172613	-1.182991
31	6	0	2.785128	-1.342657	-1.029017
32	6	0	4.183637	-1.326900	-0.953636
33	6	0	4.964363	-0.032899	-1.032446
34	6	0	4.070538	1.148474	-1.442441
35	6	0	2.038043	-2.521923	-0.990763
36	6	0	2.712992	-3.735574	-0.861242
37	6	0	4.109424	-3.769328	-0.767619
38	6	0	4.824298	-2.569428	-0.815977
39	8	0	6.187756	-2.540206	-0.735910
40	8	0	1.953261	-4.870509	-0.818671
41	8	0	3.863211	1.193497	-2.853785
42	1	0	0.036246	0.072475	0.482478
43	8	0	1.642417	2.108316	2.436287
44	6	0	1.226221	-0.210229	2.757906
45	8	0	0.396182	-1.233929	2.595379
46	6	0	0.881823	-2.543107	3.034996
47	8	0	2.344242	-0.277097	3.239420
48	6	0	-0.121824	-3.582462	2.586170
49	1	0	-5.633123	-3.713511	-2.329648
50	1	0	-2.317180	-3.050886	0.349564
51	1	0	-4.233064	1.149732	-2.186722
52	1	0	-5.645997	0.979856	-1.159710
53	1	0	-3.778727	2.531916	-0.285883
54	1	0	-1.958287	0.976149	-0.983397
55	1	0	-4.655844	0.406569	1.349170
56	1	0	-2.294700	0.432000	2.660992
57	1	0	-2.589511	2.165735	2.831224
58	1	0	2.853315	3.366553	-2.244323
59	1	0	0.576567	6.058368	-2.343337
60	1	0	-1.770200	5.194661	-0.444458
61	1	0	-6.683132	-1.794294	-3.038423
62	1	0	-3.093215	-5.125924	-0.352571
63	1	0	2.956510	0.878577	0.369470
64	1	0	5.433606	0.186894	-0.064071
65	1	0	5.780797	-0.118312	-1.756839
66	1	0	4.563107	2.087435	-1.173477
67	1	0	0.957165	-2.491003	-1.059414
68	1	0	4.633565	-4.715267	-0.658272
69	1	0	6.528583	-3.443490	-0.673086
70	1	0	2.528957	-5.641869	-0.720896
71	1	0	3.140125	0.578739	-3.051376
72	1	0	2.335885	1.698080	2.984847
73	1	0	0.987253	-2.510037	4.122477
74	1	0	1.867918	-2.703558	2.594375
75	1	0	-0.171602	-3.631914	1.495086
76	1	0	-1.117913	-3.366342	2.981833
77	1	0	0.188908	-4.563458	2.957170

Cartesian coordinates of the optimized geometry of (4‴*R*)-12I at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402093	-4.190513	-0.643065
2	6	0	-4.564442	-3.877095	-1.357584
3	6	0	-4.976977	-2.547523	-1.432424
4	6	0	-4.260432	-1.507303	-0.811631
5	6	0	-3.097245	-1.865906	-0.120747
6	6	0	-2.657173	-3.189656	-0.020423
7	6	0	-4.732961	-0.070455	-0.872017
8	6	0	-4.027069	0.784448	0.188301
9	6	0	-2.530666	0.443228	0.155094
10	8	0	-2.334034	-0.928022	0.541382
11	8	0	-4.586654	0.598791	1.487360
12	6	0	-1.624279	1.284629	1.070003
13	6	0	-1.827697	1.121024	2.569179
14	6	0	-0.513556	1.551326	3.177442
15	6	0	0.643314	1.368646	2.127505
16	6	0	-0.101409	1.069157	0.774296
17	6	0	0.145844	2.096943	-0.304406
18	6	0	-0.891820	3.024187	-0.206516
19	8	0	-1.852146	2.690101	0.722213
20	6	0	1.143370	2.284065	-1.264241
21	6	0	1.080258	3.441104	-2.061120
22	6	0	0.048841	4.371538	-1.925344
23	6	0	-0.978830	4.162289	-0.991254
24	8	0	0.027569	5.476626	-2.725424
25	8	0	-1.986220	5.088681	-0.929039
26	8	0	-0.329260	2.004358	4.283514
27	8	0	-6.104046	-2.178985	-2.110096
28	8	0	-3.041927	-5.506638	-0.599123
29	6	0	2.204789	1.268289	-1.614554
30	8	0	2.689861	0.609291	-0.427884
31	6	0	3.642206	-0.368511	-0.632943
32	6	0	3.788410	-1.008694	-1.876321
33	6	0	2.916121	-0.640896	-3.059377
34	6	0	1.710963	0.194471	-2.611013
35	6	0	4.424155	-0.701111	0.474234
36	6	0	5.384736	-1.705829	0.342093
37	6	0	5.572590	-2.361458	-0.877205
38	6	0	4.778247	-2.004530	-1.968176
39	8	0	5.010574	-2.682574	-3.131376
40	8	0	6.128284	-2.003316	1.448449
41	8	0	0.680618	-0.611438	-2.047350
42	1	0	0.083112	0.045856	0.456965
43	8	0	1.427138	2.531065	2.100397
44	6	0	1.511174	0.212508	2.626766
45	8	0	0.903183	-0.967604	2.570776
46	6	0	1.640866	-2.112888	3.104543
47	8	0	2.623877	0.411612	3.084037
48	6	0	0.766366	-3.335945	2.933487
49	1	0	-5.127206	-4.668985	-1.841468
50	1	0	-1.750201	-3.411683	0.532158
51	1	0	-4.547458	0.355314	-1.866899
52	1	0	-5.813621	-0.014412	-0.709074
53	1	0	-4.152296	1.845399	-0.037654
54	1	0	-2.171613	0.572361	-0.875264
55	1	0	-4.486969	-0.335957	1.719847
56	1	0	-1.975639	0.058666	2.798733
57	1	0	-2.678294	1.675619	2.963913
58	1	0	1.838073	3.632098	-2.814391
59	1	0	-0.753638	6.001918	-2.491230
60	1	0	-2.627967	4.820225	-0.255729
61	1	0	-6.534713	-2.966355	-2.471638
62	1	0	-2.227899	-5.600372	-0.084866
63	1	0	3.047597	1.792520	-2.085286
64	1	0	3.486786	-0.071991	-3.806105
65	1	0	2.528780	-1.534084	-3.566666
66	1	0	1.260015	0.693046	-3.472578
67	1	0	4.283332	-0.187488	1.416354
68	1	0	6.321187	-3.138383	-0.995584
69	1	0	4.431596	-2.352516	-3.831637
70	1	0	6.768996	-2.694219	1.228910
71	1	0	1.079435	-1.148358	-1.347539
72	1	0	2.259269	2.293235	2.548122
73	1	0	2.581340	-2.194155	2.554682
74	1	0	1.868438	-1.907287	4.153497
75	1	0	0.554407	-3.520885	1.876710
76	1	0	-0.179710	-3.222187	3.469552
77	1	0	1.286729	-4.209766	3.335980

Cartesian coordinates of the optimized geometry of (4‴*R*)-12J at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.459848	-4.178265	-0.753226
2	6	0	-4.632441	-3.842597	-1.440507
3	6	0	-5.041543	-2.510231	-1.474127
4	6	0	-4.311842	-1.488907	-0.837649
5	6	0	-3.139481	-1.869373	-0.174724
6	6	0	-2.701707	-3.196369	-0.116357
7	6	0	-4.779057	-0.049038	-0.854401
8	6	0	-4.050144	0.778212	0.212581
9	6	0	-2.556746	0.429218	0.146809
10	8	0	-2.363673	-0.951270	0.499993
11	8	0	-4.588916	0.566137	1.516486
12	6	0	-1.628353	1.243127	1.064060
13	6	0	-1.812347	1.054526	2.563187
14	6	0	-0.485748	1.464879	3.157665
15	6	0	0.655393	1.259044	2.096024
16	6	0	-0.112000	1.016123	0.741602
17	6	0	0.138332	2.073353	-0.307043
18	6	0	-0.890590	3.006308	-0.178076
19	8	0	-1.847655	2.657449	0.748371
20	6	0	1.131533	2.277244	-1.268757
21	6	0	1.071473	3.455350	-2.034543
22	6	0	0.048322	4.390065	-1.868217
23	6	0	-0.973793	4.165426	-0.932063
24	8	0	0.030961	5.515624	-2.639586
25	8	0	-1.973138	5.097934	-0.837190
26	8	0	-0.282315	1.917627	4.260336
27	8	0	-6.177783	-2.120646	-2.124137
28	8	0	-3.103395	-5.496168	-0.749923
29	6	0	2.188162	1.267540	-1.650028
30	8	0	2.698874	0.598163	-0.478632
31	6	0	3.654242	-0.368019	-0.717439
32	6	0	3.784437	-0.983686	-1.969675
33	6	0	2.891182	-0.614487	-3.133560
34	6	0	1.688280	0.203254	-2.654676
35	6	0	4.462292	-0.712789	0.372408
36	6	0	5.429559	-1.702452	0.204042
37	6	0	5.601452	-2.336062	-1.032236
38	6	0	4.781596	-1.968905	-2.097817
39	8	0	4.897012	-2.548226	-3.330115
40	8	0	6.256558	-2.094213	1.218316
41	8	0	0.672724	-0.619400	-2.082800
42	1	0	0.053014	0.002600	0.384693
43	8	0	1.489928	2.384197	2.091854
44	6	0	1.470999	0.048371	2.554112
45	8	0	0.785153	-1.090053	2.502271
46	6	0	1.453471	-2.307470	2.964369
47	8	0	2.612810	0.173116	2.963111
48	6	0	1.319550	-2.465124	4.467833
49	1	0	-5.205532	-4.619634	-1.936263
50	1	0	-1.784843	-3.434757	0.412864
51	1	0	-4.610262	0.399685	-1.842153
52	1	0	-5.856272	0.007538	-0.670059
53	1	0	-4.173086	1.844657	0.012615
54	1	0	-2.214224	0.578769	-0.886475
55	1	0	-4.483907	-0.372879	1.728629
56	1	0	-1.964085	-0.010483	2.776459
57	1	0	-2.652600	1.609303	2.978978
58	1	0	1.825733	3.660334	-2.787728
59	1	0	-0.744409	6.040965	-2.386907
60	1	0	-2.611728	4.816055	-0.166363
61	1	0	-6.616307	-2.896948	-2.499848
62	1	0	-2.282019	-5.605918	-0.250688
63	1	0	3.021051	1.801902	-2.127002
64	1	0	3.451335	-0.036698	-3.880371
65	1	0	2.532217	-1.512333	-3.646915
66	1	0	1.215976	0.712279	-3.499005
67	1	0	4.317434	-0.211624	1.322447
68	1	0	6.365743	-3.098318	-1.145717
69	1	0	5.594756	-3.218033	-3.306550
70	1	0	6.048725	-1.584724	2.014185
71	1	0	1.097372	-1.188928	-1.425312
72	1	0	2.340390	2.081139	2.457521
73	1	0	2.496380	-2.264985	2.646616
74	1	0	0.941853	-3.104940	2.424331
75	1	0	1.835868	-1.659102	4.994819
76	1	0	1.768270	-3.416056	4.771041
77	1	0	0.268168	-2.470619	4.767868

Cartesian coordinates of the optimized geometry of (4‴*R*)-12K at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.899671	-3.904389	-0.574317
2	6	0	-4.996909	-3.524802	-1.357439
3	6	0	-5.285130	-2.166900	-1.511495
4	6	0	-4.506647	-1.167340	-0.903552
5	6	0	-3.410616	-1.595581	-0.142606
6	6	0	-3.095230	-2.943582	0.037501
7	6	0	-4.843186	0.301578	-1.048496
8	6	0	-4.108707	1.141440	0.004958
9	6	0	-2.649946	0.664935	0.060706
10	8	0	-2.596127	-0.696023	0.510691
11	8	0	-4.739382	1.074772	1.282463
12	6	0	-1.709886	1.462774	0.980179
13	6	0	-2.011401	1.407754	2.477893
14	6	0	-0.675628	1.653454	3.129416
15	6	0	0.463788	1.113524	2.215982
16	6	0	-0.198791	1.052449	0.791673
17	6	0	0.292858	2.095442	-0.180711
18	6	0	-0.678399	3.085808	-0.255660
19	8	0	-1.782382	2.854717	0.531961
20	6	0	1.466548	2.200234	-0.935168
21	6	0	1.612188	3.321056	-1.765717
22	6	0	0.627134	4.312309	-1.823499
23	6	0	-0.548049	4.207249	-1.062494
24	8	0	0.807025	5.384754	-2.648921
25	8	0	-1.476359	5.207823	-1.175396
26	8	0	-0.431970	2.242037	4.160514
27	8	0	-6.343046	-1.734408	-2.259013
28	8	0	-3.564532	-5.213590	-0.381668
29	6	0	2.530952	1.133328	-0.798467
30	8	0	1.966489	-0.102364	-1.329788
31	6	0	2.767328	-1.218298	-1.200006
32	6	0	4.157817	-1.099170	-1.073406
33	6	0	4.839520	0.251593	-1.079346
34	6	0	3.873025	1.367840	-1.501151
35	6	0	2.116912	-2.453738	-1.244302
36	6	0	2.882547	-3.616130	-1.152509
37	6	0	4.273420	-3.546360	-1.006808
38	6	0	4.890509	-2.293336	-0.969126
39	8	0	6.244097	-2.160199	-0.836377
40	8	0	2.217692	-4.808278	-1.200811
41	8	0	3.710710	1.416989	-2.919111
42	1	0	-0.132852	0.040708	0.390504
43	8	0	1.557077	1.990584	2.267417
44	6	0	0.800865	-0.315434	2.677088
45	8	0	2.109303	-0.516012	2.825271
46	6	0	2.514338	-1.859242	3.224426
47	8	0	-0.059891	-1.156936	2.864566
48	6	0	4.026966	-1.873679	3.292413
49	1	0	-5.617930	-4.275653	-1.839346
50	1	0	-2.240241	-3.230263	0.637738
51	1	0	-4.578597	0.661637	-2.051448
52	1	0	-5.920091	0.461652	-0.938124
53	1	0	-4.124627	2.196410	-0.276339
54	1	0	-2.235362	0.721826	-0.956390
55	1	0	-4.762418	0.145545	1.554182
56	1	0	-2.318339	0.388507	2.739763
57	1	0	-2.783837	2.104027	2.800915
58	1	0	2.482121	3.428000	-2.400963
59	1	0	0.024051	5.953156	-2.579424
60	1	0	-2.259754	4.980841	-0.653765
61	1	0	-6.825993	-2.495894	-2.609378
62	1	0	-4.185531	-5.780632	-0.859935
63	1	0	2.728814	0.976391	0.269257
64	1	0	5.245912	0.480282	-0.085061
65	1	0	5.691397	0.249173	-1.766957
66	1	0	4.282253	2.337701	-1.203355
67	1	0	1.039439	-2.504874	-1.346030
68	1	0	4.866813	-4.453749	-0.926446
69	1	0	6.654313	-3.035676	-0.804316
70	1	0	2.851585	-5.534551	-1.119644
71	1	0	3.030099	0.765300	-3.146749
72	1	0	1.623968	2.290292	3.190093
73	1	0	2.126593	-2.566464	2.486654
74	1	0	2.052487	-2.083494	4.189624
75	1	0	4.394757	-1.148395	4.023452
76	1	0	4.463548	-1.642756	2.316884
77	1	0	4.366629	-2.868691	3.594486

Cartesian coordinates of the optimized geometry of (4‴*R*)-12L at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.976796	-3.516461	-0.972510
2	6	0	-5.006384	-3.006913	-1.772964
3	6	0	-5.185158	-1.623906	-1.850386
4	6	0	-4.362117	-0.726032	-1.149112
5	6	0	-3.337165	-1.282278	-0.371291
6	6	0	-3.132876	-2.659339	-0.267132
7	6	0	-4.581062	0.770060	-1.216272
8	6	0	-3.841289	1.482546	-0.077484
9	6	0	-2.423665	0.897645	0.009471
10	8	0	-2.488673	-0.490006	0.373813
11	8	0	-4.536952	1.377678	1.163385
12	6	0	-1.477537	1.576058	1.016611
13	6	0	-1.853499	1.451953	2.488378
14	6	0	-0.548011	1.526290	3.248627
15	6	0	0.645626	1.135420	2.305864
16	6	0	0.009000	1.088142	0.872462
17	6	0	0.574760	2.103566	-0.089232
18	6	0	-0.320316	3.164950	-0.140643
19	8	0	-1.439485	2.992290	0.641918
20	6	0	1.758792	2.143016	-0.831256
21	6	0	1.993455	3.269997	-1.632669
22	6	0	1.084457	4.332263	-1.668200
23	6	0	-0.100493	4.295130	-0.914970
24	8	0	1.348502	5.410168	-2.463424
25	8	0	-0.949010	5.366300	-1.005160
26	8	0	-0.389203	1.861595	4.399654
27	8	0	-6.173156	-1.066017	-2.610349
28	8	0	-3.747008	-4.856483	-0.851051
29	6	0	2.743711	1.003388	-0.698161
30	8	0	2.080468	-0.193788	-1.193694
31	6	0	2.789109	-1.366944	-1.031720
32	6	0	4.189348	-1.357483	-0.939163
33	6	0	4.970591	-0.060442	-1.008044
34	6	0	4.082205	1.122208	-1.433437
35	6	0	2.037982	-2.541473	-1.004092
36	6	0	2.707180	-3.759781	-0.868222
37	6	0	4.099421	-3.800194	-0.757506
38	6	0	4.821971	-2.604790	-0.793278
39	8	0	6.179427	-2.716256	-0.685078
40	8	0	1.940772	-4.890077	-0.837187
41	8	0	3.890717	1.158053	-2.844959
42	1	0	0.033283	0.069910	0.484483
43	8	0	1.666378	2.094957	2.421997
44	6	0	1.211186	-0.212526	2.768210
45	8	0	0.367313	-1.225079	2.609651
46	6	0	0.829312	-2.537918	3.064851
47	8	0	2.325510	-0.290863	3.256728
48	6	0	-0.172811	-3.569139	2.594585
49	1	0	-5.658929	-3.676812	-2.327214
50	1	0	-2.332608	-3.050496	0.348340
51	1	0	-4.237679	1.168525	-2.180129
52	1	0	-5.647380	1.006093	-1.147481
53	1	0	-3.769251	2.551933	-0.285304
54	1	0	-1.959053	0.982294	-0.983405
55	1	0	-4.641908	0.436254	1.364633
56	1	0	-2.283848	0.459134	2.667823
57	1	0	-2.576697	2.195041	2.823493
58	1	0	2.874114	3.333040	-2.259181
59	1	0	0.614389	6.037822	-2.373637
60	1	0	-1.737331	5.199215	-0.468676
61	1	0	-6.697904	-1.764641	-3.025723
62	1	0	-4.381340	-5.344400	-1.394463
63	1	0	2.953296	0.853130	0.369402
64	1	0	5.423825	0.172233	-0.033894
65	1	0	5.790637	-0.127781	-1.734447
66	1	0	4.576443	2.059393	-1.162609
67	1	0	0.958072	-2.505355	-1.084404
68	1	0	4.631784	-4.739156	-0.643850
69	1	0	6.588649	-1.840566	-0.705202
70	1	0	2.512042	-5.663270	-0.727678
71	1	0	3.159835	0.553420	-3.046002
72	1	0	2.350209	1.680236	2.979260
73	1	0	0.907834	-2.501582	4.154560
74	1	0	1.824622	-2.709098	2.649955
75	1	0	-0.197871	-3.620492	1.502800
76	1	0	-1.176072	-3.343799	2.966168
77	1	0	0.120488	-4.552075	2.974517

Cartesian coordinates of the optimized geometry of (4‴*R*)-12M at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.818072	-3.562946	-1.032613
2	6	0	-4.832798	-3.098619	-1.878172
3	6	0	-5.050125	-1.723213	-1.988492
4	6	0	-4.280507	-0.788321	-1.275191
5	6	0	-3.270488	-1.300237	-0.449493
6	6	0	-3.027233	-2.668085	-0.312519
7	6	0	-4.536924	0.699990	-1.382667
8	6	0	-3.838060	1.464567	-0.250343
9	6	0	-2.415206	0.905044	-0.107608
10	8	0	-2.476863	-0.467373	0.311236
11	8	0	-4.562554	1.388982	0.976022
12	6	0	-1.494729	1.629690	0.888574
13	6	0	-1.914647	1.611512	2.354487
14	6	0	-0.624685	1.755941	3.131146
15	6	0	0.563704	1.183765	2.283429
16	6	0	-0.011497	1.110740	0.819493
17	6	0	0.615013	2.087265	-0.145611
18	6	0	-0.263723	3.154468	-0.284534
19	8	0	-1.426616	3.022661	0.438300
20	6	0	1.829340	2.080352	-0.839609
21	6	0	2.117459	3.174840	-1.668361
22	6	0	1.228368	4.248278	-1.783021
23	6	0	0.007589	4.251788	-1.089170
24	8	0	1.546010	5.294185	-2.601172
25	8	0	-0.823835	5.326327	-1.261522
26	8	0	-0.474663	2.252511	4.223200
27	8	0	-6.025741	-1.210151	-2.794286
28	8	0	-3.550700	-4.893068	-0.881260
29	6	0	2.773843	0.913937	-0.653555
30	8	0	2.125744	-0.251704	-1.242847
31	6	0	2.800319	-1.444341	-1.081752
32	6	0	4.181885	-1.471064	-0.863085
33	6	0	4.995352	-0.196973	-0.796564
34	6	0	4.178079	1.018361	-1.259724
35	6	0	2.028726	-2.606755	-1.187613
36	6	0	2.662918	-3.842246	-1.060652
37	6	0	4.040890	-3.917237	-0.825852
38	6	0	4.779211	-2.737891	-0.730460
39	8	0	6.127553	-2.747672	-0.508478
40	8	0	1.986102	-5.025966	-1.144595
41	8	0	4.119401	1.100949	-2.684099
42	1	0	0.010002	0.082892	0.456702
43	8	0	1.692039	2.007849	2.403070
44	6	0	0.922788	-0.201644	2.835752
45	8	0	-0.087522	-1.061828	2.769427
46	6	0	0.134194	-2.411797	3.291973
47	8	0	2.028432	-0.430733	3.294461
48	6	0	-0.119807	-2.463157	4.787223
49	1	0	-5.444550	-3.797582	-2.442718
50	1	0	-2.236029	-3.022794	0.336709
51	1	0	-4.186174	1.081559	-2.350702
52	1	0	-5.610121	0.909797	-1.339680
53	1	0	-3.779565	2.527550	-0.493381
54	1	0	-1.928419	0.954020	-1.092340
55	1	0	-4.624628	0.454988	1.224413
56	1	0	-2.339457	0.630801	2.597703
57	1	0	-2.648716	2.374572	2.610633
58	1	0	3.026249	3.198281	-2.256168
59	1	0	0.817489	5.933822	-2.568845
60	1	0	-1.643200	5.182438	-0.766386
61	1	0	-6.513866	-1.932240	-3.214259
62	1	0	-4.150031	-5.409395	-1.438171
63	1	0	2.881974	0.726384	0.422379
64	1	0	5.354671	-0.024884	0.226913
65	1	0	5.887076	-0.276780	-1.426502
66	1	0	4.661668	1.937861	-0.917096
67	1	0	0.960032	-2.527667	-1.359880
68	1	0	4.515730	-4.887689	-0.722126
69	1	0	6.439150	-3.662399	-0.459468
70	1	0	1.049050	-4.848728	-1.307182
71	1	0	3.399733	0.518117	-2.970669
72	1	0	2.332548	1.502271	2.936178
73	1	0	1.151614	-2.712784	3.037695
74	1	0	-0.576686	-3.024714	2.737171
75	1	0	-1.131027	-2.121140	5.023480
76	1	0	0.600787	-1.846382	5.329752
77	1	0	-0.016658	-3.496003	5.133683

Cartesian coordinates of the optimized geometry of (4‴*R*)-12N at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.401885	-4.193566	-0.722039
2	6	0	-4.579024	-3.874918	-1.409984
3	6	0	-5.005829	-2.545580	-1.447903
4	6	0	-4.289293	-1.515368	-0.815733
5	6	0	-3.110973	-1.880982	-0.150718
6	6	0	-2.656978	-3.199671	-0.088177
7	6	0	-4.772595	-0.080757	-0.838730
8	6	0	-4.048348	0.762715	0.219039
9	6	0	-2.552417	0.425865	0.152743
10	8	0	-2.348922	-0.948899	0.521184
11	8	0	-4.581466	0.557144	1.526335
12	6	0	-1.627262	1.256089	1.058378
13	6	0	-1.807745	1.086268	2.560222
14	6	0	-0.482347	1.512778	3.145979
15	6	0	0.658128	1.292570	2.086724
16	6	0	-0.110570	1.031740	0.736008
17	6	0	0.133598	2.078085	-0.324894
18	6	0	-0.899036	3.008188	-0.205255
19	8	0	-1.853890	2.665467	0.725741
20	6	0	1.123602	2.273969	-1.291500
21	6	0	1.058103	3.442976	-2.070605
22	6	0	0.032084	4.376010	-1.912716
23	6	0	-0.987750	4.158259	-0.972422
24	8	0	0.009233	5.492764	-2.696735
25	8	0	-1.990540	5.088102	-0.886978
26	8	0	-0.279694	1.986160	4.240098
27	8	0	-6.147312	-2.174060	-2.099171
28	8	0	-2.929190	-5.472202	-0.646908
29	6	0	2.179998	1.261259	-1.665460
30	8	0	2.691918	0.602280	-0.488991
31	6	0	3.640926	-0.371962	-0.719105
32	6	0	3.767141	-1.000544	-1.965304
33	6	0	2.876175	-0.636920	-3.132581
34	6	0	1.676654	0.189768	-2.660877
35	6	0	4.447081	-0.711387	0.373855
36	6	0	5.407893	-1.708862	0.215054
37	6	0	5.575582	-2.355483	-1.015025
38	6	0	4.757782	-1.993477	-2.083899
39	8	0	4.869312	-2.585694	-3.310435
40	8	0	6.232492	-2.096029	1.233067
41	8	0	0.657072	-0.623531	-2.082966
42	1	0	0.058109	0.015041	0.390114
43	8	0	1.494424	2.416057	2.067718
44	6	0	1.472544	0.086461	2.559668
45	8	0	0.784562	-1.050950	2.525139
46	6	0	1.451422	-2.264205	3.000365
47	8	0	2.616027	0.214856	2.963181
48	6	0	1.323099	-2.401775	4.506262
49	1	0	-5.155129	-4.650078	-1.908678
50	1	0	-1.740591	-3.440053	0.437165
51	1	0	-4.613156	0.363182	-1.830227
52	1	0	-5.849560	-0.034716	-0.649911
53	1	0	-4.182091	1.826110	0.009737
54	1	0	-2.213440	0.566572	-0.882961
55	1	0	-4.450439	-0.375120	1.753453
56	1	0	-1.952263	0.023322	2.788140
57	1	0	-2.650423	1.641735	2.970126
58	1	0	1.809881	3.641607	-2.827966
59	1	0	-0.768085	6.017582	-2.449020
60	1	0	-2.628098	4.810781	-0.213288
61	1	0	-6.577414	-2.956567	-2.471558
62	1	0	-3.520449	-6.064311	-1.132461
63	1	0	3.012316	1.791189	-2.148524
64	1	0	3.439063	-0.067623	-3.883857
65	1	0	2.513612	-1.537373	-3.638778
66	1	0	1.207167	0.693958	-3.509729
67	1	0	4.305440	-0.200354	1.319106
68	1	0	6.334676	-3.123943	-1.121291
69	1	0	5.561215	-3.261232	-3.279352
70	1	0	6.027381	-1.578066	2.024147
71	1	0	1.079419	-1.196589	-1.427066
72	1	0	2.346652	2.114470	2.430575
73	1	0	0.935304	-3.067009	2.472734
74	1	0	2.493118	-2.228638	2.677851
75	1	0	0.272891	-2.401068	4.810421
76	1	0	1.843279	-1.590070	5.020590
77	1	0	1.770835	-3.349726	4.820058

Cartesian coordinates of the optimized geometry of (4‴*R*)-12O at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.275334	-4.224820	-0.577202
2	6	0	-4.456193	-3.940084	-1.273459
3	6	0	-4.906603	-2.619502	-1.336839
4	6	0	-4.210295	-1.565005	-0.722456
5	6	0	-3.026881	-1.896742	-0.048502
6	6	0	-2.549482	-3.205760	0.038633
7	6	0	-4.720995	-0.140768	-0.771218
8	6	0	-4.006129	0.739314	0.262947
9	6	0	-2.505577	0.423429	0.200296
10	8	0	-2.284307	-0.937988	0.608139
11	8	0	-4.530851	0.556948	1.577247
12	6	0	-1.590910	1.294711	1.077692
13	6	0	-1.756864	1.162922	2.584435
14	6	0	-0.442497	1.652832	3.145416
15	6	0	0.695858	1.444778	2.081203
16	6	0	-0.072458	1.097584	0.750399
17	6	0	0.129532	2.107727	-0.353223
18	6	0	-0.918983	3.020736	-0.250395
19	8	0	-1.849740	2.691827	0.710342
20	6	0	1.088134	2.273985	-1.354992
21	6	0	0.984845	3.406021	-2.182446
22	6	0	-0.052856	4.328742	-2.037766
23	6	0	-1.046732	4.134304	-1.064822
24	8	0	-0.115539	5.409761	-2.869151
25	8	0	-2.066660	5.047432	-0.998582
26	8	0	-0.248334	2.164042	4.224221
27	8	0	-6.053174	-2.280948	-1.997341
28	8	0	-2.779807	-5.493065	-0.476599
29	6	0	2.143219	1.249378	-1.706946
30	8	0	2.708377	0.685284	-0.509721
31	6	0	3.609372	-0.338202	-0.687940
32	6	0	3.694269	-1.056268	-1.887008
33	6	0	2.784968	-0.756013	-3.053761
34	6	0	1.613442	0.132106	-2.624790
35	6	0	4.428956	-0.626605	0.410951
36	6	0	5.356937	-1.661637	0.306386
37	6	0	5.482480	-2.396275	-0.877890
38	6	0	4.652368	-2.083533	-1.953454
39	8	0	4.720901	-2.765746	-3.137233
40	8	0	6.190144	-2.000858	1.336085
41	8	0	0.628256	-0.592359	-1.892365
42	1	0	0.131539	0.075536	0.438659
43	8	0	1.477400	2.606457	2.008016
44	6	0	1.574331	0.304298	2.597693
45	8	0	0.956823	-0.871404	2.614351
46	6	0	1.709747	-2.003884	3.152679
47	8	0	2.705938	0.512405	3.002930
48	6	0	0.806500	-3.216727	3.097579
49	1	0	-5.017699	-4.734302	-1.758529
50	1	0	-1.631071	-3.420379	0.571085
51	1	0	-4.577394	0.285099	-1.773068
52	1	0	-5.797366	-0.111399	-0.575512
53	1	0	-4.158152	1.794879	0.028256
54	1	0	-2.170827	0.536471	-0.839980
55	1	0	-4.355746	-0.359205	1.837996
56	1	0	-1.862467	0.102488	2.844131
57	1	0	-2.615518	1.700733	2.984795
58	1	0	1.712344	3.581353	-2.968722
59	1	0	-0.896586	5.930645	-2.625029
60	1	0	-2.686588	4.784574	-0.302991
61	1	0	-6.468881	-3.078217	-2.354524
62	1	0	-3.361524	-6.106144	-0.947456
63	1	0	2.947302	1.754740	-2.259546
64	1	0	3.338194	-0.255425	-3.859945
65	1	0	2.400524	-1.685118	-3.490592
66	1	0	1.166315	0.608120	-3.508143
67	1	0	4.324519	-0.045375	1.319783
68	1	0	6.216108	-3.193479	-0.945033
69	1	0	5.389751	-3.461122	-3.067011
70	1	0	6.011533	-1.424120	2.092043
71	1	0	0.273711	-1.278898	-2.473094
72	1	0	2.335527	2.367289	2.402575
73	1	0	2.010545	-1.754709	4.173413
74	1	0	2.609213	-2.128131	2.545052
75	1	0	0.517462	-3.442453	2.067546
76	1	0	-0.097402	-3.062024	3.692867
77	1	0	1.340232	-4.081996	3.501091

Cartesian coordinates of the optimized geometry of (4‴*R*)-12P at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.681743	-4.072840	-0.655565
2	6	0	-4.831657	-3.699649	-1.361313
3	6	0	-5.159596	-2.344614	-1.452467
4	6	0	-4.370516	-1.345337	-0.860978
5	6	0	-3.221181	-1.763916	-0.177487
6	6	0	-2.867064	-3.110441	-0.061114
7	6	0	-4.756477	0.113900	-0.927022
8	6	0	-4.015617	0.925435	0.142961
9	6	0	-2.541953	0.516034	0.119065
10	8	0	-2.380653	-0.871516	0.441408
11	8	0	-4.519931	0.666428	1.451566
12	6	0	-1.610715	1.286527	1.074314
13	6	0	-1.833708	1.060907	2.561995
14	6	0	-0.499795	1.355501	3.205095
15	6	0	0.652247	1.211373	2.142755
16	6	0	-0.095602	1.019787	0.776005
17	6	0	0.203942	2.085922	-0.251263
18	6	0	-0.800534	3.045621	-0.124340
19	8	0	-1.780361	2.712582	0.783411
20	6	0	1.218646	2.277139	-1.192765
21	6	0	1.201661	3.466032	-1.944198
22	6	0	0.200330	4.424861	-1.782712
23	6	0	-0.840812	4.215995	-0.864336
24	8	0	0.224232	5.559735	-2.540483
25	8	0	-1.816684	5.173437	-0.771049
26	8	0	-0.295154	1.688641	4.350141
27	8	0	-6.273222	-1.917150	-2.120823
28	8	0	-3.302963	-5.379271	-0.524609
29	6	0	2.263781	1.250706	-1.560983
30	8	0	2.757408	0.583054	-0.380606
31	6	0	3.711913	-0.386876	-0.606641
32	6	0	3.849838	-1.008964	-1.854755
33	6	0	2.966330	-0.643837	-3.027488
34	6	0	1.764701	0.185270	-2.564289
35	6	0	4.512053	-0.727215	0.490744
36	6	0	5.478945	-1.719568	0.334065
37	6	0	5.657948	-2.359689	-0.897808
38	6	0	4.846177	-1.996527	-1.970901
39	8	0	4.969203	-2.582130	-3.199352
40	8	0	6.299438	-2.106554	1.355207
41	8	0	0.737594	-0.627548	-1.999237
42	1	0	0.043443	0.007277	0.405597
43	8	0	1.458175	2.360288	2.189272
44	6	0	1.495922	0.009559	2.568338
45	8	0	0.876502	-1.154549	2.405748
46	6	0	1.588641	-2.348550	2.860044
47	8	0	2.598358	0.157746	3.068329
48	6	0	0.708938	-3.543578	2.562924
49	1	0	-5.462330	-4.451159	-1.829621
50	1	0	-1.972363	-3.396883	0.478155
51	1	0	-4.535184	0.535792	-1.916680
52	1	0	-5.837517	0.228482	-0.788576
53	1	0	-4.074075	1.995100	-0.093099
54	1	0	-2.173899	0.684555	-0.902688
55	1	0	-5.442352	0.954811	1.472104
56	1	0	-2.072903	0.004473	2.732768
57	1	0	-2.643874	1.657392	2.980285
58	1	0	1.974294	3.661031	-2.681237
59	1	0	-0.540056	6.102960	-2.292016
60	1	0	-2.470539	4.899873	-0.111571
61	1	0	-6.761280	-2.681075	-2.458355
62	1	0	-3.938452	-5.946334	-0.983236
63	1	0	3.107144	1.772896	-2.032905
64	1	0	3.535486	-0.075994	-3.775104
65	1	0	2.605356	-1.543715	-3.535900
66	1	0	1.304578	0.693497	-3.415873
67	1	0	4.363960	-0.219053	1.436663
68	1	0	6.421576	-3.123889	-1.002145
69	1	0	5.664942	-3.253697	-3.167375
70	1	0	6.085554	-1.594892	2.148078
71	1	0	1.150590	-1.196098	-1.333555
72	1	0	2.265619	2.089919	2.662544
73	1	0	2.542915	-2.393282	2.329963
74	1	0	1.789593	-2.235252	3.928379
75	1	0	0.521826	-3.635740	1.489452
76	1	0	-0.249473	-3.466373	3.083422
77	1	0	1.211654	-4.453959	2.901857

Cartesian coordinates of the optimized geometry of (4‴*R*)-12Q at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.608283	-4.111940	-0.633414
2	6	0	-4.762266	-3.759589	-1.343224
3	6	0	-5.109876	-2.410029	-1.442671
4	6	0	-4.336615	-1.395923	-0.855548
5	6	0	-3.182876	-1.793886	-0.167089
6	6	0	-2.809223	-3.134385	-0.042601
7	6	0	-4.742493	0.057452	-0.932003
8	6	0	-4.015479	0.886326	0.134278
9	6	0	-2.536370	0.497061	0.117025
10	8	0	-2.357037	-0.886093	0.448924
11	8	0	-4.520054	0.629341	1.443166
12	6	0	-1.617843	1.286186	1.069273
13	6	0	-1.841393	1.070374	2.558254
14	6	0	-0.514255	1.395814	3.200833
15	6	0	0.642836	1.254210	2.143863
16	6	0	-0.098990	1.036294	0.777186
17	6	0	0.188332	2.095760	-0.260127
18	6	0	-0.826273	3.045744	-0.141357
19	8	0	-1.803801	2.708190	0.767362
20	6	0	1.200676	2.288891	-1.203405
21	6	0	1.173056	3.472058	-1.963500
22	6	0	0.162908	4.422708	-1.808645
23	6	0	-0.877362	4.210160	-0.889941
24	8	0	0.176415	5.552588	-2.574210
25	8	0	-1.862828	5.158630	-0.805017
26	8	0	-0.318629	1.749205	4.341362
27	8	0	-6.228403	-2.002975	-2.115621
28	8	0	-3.210325	-5.411880	-0.494770
29	6	0	2.249296	1.265002	-1.568450
30	8	0	2.740680	0.597893	-0.387226
31	6	0	3.691682	-0.376923	-0.608755
32	6	0	3.828605	-1.001268	-1.858279
33	6	0	2.950384	-0.631413	-3.033423
34	6	0	1.749932	0.199771	-2.572059
35	6	0	4.486219	-0.720167	0.488917
36	6	0	5.447738	-1.718616	0.336157
37	6	0	5.625227	-2.361682	-0.894676
38	6	0	4.817071	-1.993864	-1.971956
39	8	0	4.939954	-2.582518	-3.198842
40	8	0	6.205102	-2.027029	1.430403
41	8	0	0.720799	-0.610884	-2.007630
42	1	0	0.055316	0.021807	0.418632
43	8	0	1.435042	2.412887	2.179043
44	6	0	1.500431	0.068471	2.586972
45	8	0	0.894997	-1.105277	2.441011
46	6	0	1.621003	-2.283464	2.914618
47	8	0	2.600475	0.237529	3.085104
48	6	0	0.759491	-3.494101	2.627424
49	1	0	-5.380957	-4.522902	-1.808415
50	1	0	-1.911425	-3.404488	0.499948
51	1	0	-4.524544	0.475618	-1.923984
52	1	0	-5.825321	0.158317	-0.796801
53	1	0	-4.087793	1.953492	-0.109259
54	1	0	-2.167535	0.663642	-0.904732
55	1	0	-5.446013	0.906460	1.459386
56	1	0	-2.061495	0.011291	2.738030
57	1	0	-2.663241	1.655949	2.969010
58	1	0	1.943492	3.668483	-2.702468
59	1	0	-0.593312	6.089990	-2.329901
60	1	0	-2.514973	4.883353	-0.144571
61	1	0	-6.705002	-2.776075	-2.448621
62	1	0	-3.835670	-5.990683	-0.952653
63	1	0	3.092735	1.787820	-2.039649
64	1	0	3.523399	-0.062944	-3.777649
65	1	0	2.588945	-1.529189	-3.545137
66	1	0	1.291636	0.708444	-3.424347
67	1	0	4.351816	-0.219561	1.438921
68	1	0	6.379177	-3.135874	-1.012342
69	1	0	5.630402	-3.259364	-3.165646
70	1	0	6.847026	-2.711958	1.196636
71	1	0	1.131707	-1.178662	-1.340011
72	1	0	2.248409	2.154607	2.649215
73	1	0	2.579246	-2.321714	2.391392
74	1	0	1.813565	-2.153743	3.982629
75	1	0	0.580612	-3.602411	1.554021
76	1	0	-0.203327	-3.423560	3.140714
77	1	0	1.272298	-4.393183	2.981121

Cartesian coordinates of the optimized geometry of (4‴*R*)-12R at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.329407	-4.178534	-0.703638
2	6	0	-4.533160	-3.873801	-1.350638
3	6	0	-4.981202	-2.551211	-1.365249
4	6	0	-4.260359	-1.514064	-0.749094
5	6	0	-3.055663	-1.865708	-0.124974
6	6	0	-2.579407	-3.177144	-0.087803
7	6	0	-4.767701	-0.087705	-0.745871
8	6	0	-4.028409	0.755488	0.301071
9	6	0	-2.527761	0.446344	0.184918
10	8	0	-2.284181	-0.925874	0.527916
11	8	0	-4.520351	0.523006	1.619094
12	6	0	-1.590839	1.291651	1.063373
13	6	0	-1.766823	1.158821	2.569217
14	6	0	-0.451247	1.631936	3.138780
15	6	0	0.692606	1.398602	2.086388
16	6	0	-0.069978	1.072402	0.745608
17	6	0	0.162673	2.091405	-0.348227
18	6	0	-0.877241	3.018370	-0.245245
19	8	0	-1.825488	2.691765	0.696465
20	6	0	1.165056	2.290321	-1.305468
21	6	0	1.090602	3.445806	-2.103633
22	6	0	0.053825	4.369734	-1.966445
23	6	0	-0.970532	4.156076	-1.029006
24	8	0	0.025063	5.473794	-2.765415
25	8	0	-1.977932	5.080937	-0.961318
26	8	0	-0.257382	2.146331	4.215806
27	8	0	-6.148258	-2.192643	-1.977012
28	8	0	-2.834829	-5.449658	-0.652430
29	6	0	2.240765	1.283266	-1.650601
30	8	0	2.712400	0.634135	-0.458469
31	6	0	3.610360	-0.393191	-0.639255
32	6	0	3.741678	-1.057874	-1.863288
33	6	0	2.904630	-0.684451	-3.062107
34	6	0	1.749597	0.236521	-2.678866
35	6	0	4.375419	-0.740378	0.481529
36	6	0	5.291813	-1.785402	0.374017
37	6	0	5.460198	-2.471076	-0.833918
38	6	0	4.686893	-2.096924	-1.931989
39	8	0	4.802075	-2.724919	-3.141653
40	8	0	6.072538	-2.181168	1.424592
41	8	0	0.700151	-0.568353	-2.146175
42	1	0	0.122358	0.045240	0.440476
43	8	0	1.502087	2.539563	2.021421
44	6	0	1.534273	0.235507	2.614855
45	8	0	0.894077	-0.927513	2.603294
46	6	0	1.608349	-2.079119	3.155180
47	8	0	2.657220	0.419822	3.053901
48	6	0	0.675954	-3.268628	3.084317
49	1	0	-5.113312	-4.654370	-1.836000
50	1	0	-1.642109	-3.407058	0.403647
51	1	0	-4.643817	0.368694	-1.736804
52	1	0	-5.839418	-0.061453	-0.526422
53	1	0	-4.186032	1.819075	0.109872
54	1	0	-2.236504	0.610412	-0.862943
55	1	0	-4.385986	-0.414053	1.823719
56	1	0	-1.887975	0.099344	2.825686
57	1	0	-2.621934	1.705373	2.964589
58	1	0	1.847933	3.643016	-2.855595
59	1	0	-0.755959	5.997880	-2.527458
60	1	0	-2.611731	4.817653	-0.278443
61	1	0	-6.578341	-2.978871	-2.341523
62	1	0	-3.432568	-6.048649	-1.121337
63	1	0	3.084664	1.816578	-2.110745
64	1	0	3.521339	-0.183915	-3.819517
65	1	0	2.495391	-1.578546	-3.542827
66	1	0	1.402788	0.778747	-3.568605
67	1	0	4.242293	-0.195088	1.408502
68	1	0	6.184002	-3.277052	-0.902066
69	1	0	5.460417	-3.430602	-3.074552
70	1	0	5.870683	-1.631529	2.194821
71	1	0	-0.067580	0.006867	-2.021213
72	1	0	2.345685	2.284452	2.436842
73	1	0	2.514468	-2.225981	2.562684
74	1	0	1.897404	-1.836606	4.180779
75	1	0	0.398681	-3.487401	2.049669
76	1	0	-0.233562	-3.091473	3.664588
77	1	0	1.181425	-4.146715	3.496418

Cartesian coordinates of the optimized geometry of (4‴*R*)-12S at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.218887	-4.256281	-0.561340
2	6	0	-4.399858	-3.987507	-1.263781
3	6	0	-4.863873	-2.672059	-1.335833
4	6	0	-4.181036	-1.607097	-0.724352
5	6	0	-2.996652	-1.922911	-0.044532
6	6	0	-2.505973	-3.226410	0.051553
7	6	0	-4.706634	-0.188660	-0.781752
8	6	0	-4.005864	0.703575	0.251703
9	6	0	-2.501649	0.404327	0.196594
10	8	0	-2.266571	-0.953234	0.609879
11	8	0	-4.534146	0.521183	1.564561
12	6	0	-1.600326	1.287771	1.075623
13	6	0	-1.768927	1.155679	2.582046
14	6	0	-0.461812	1.661717	3.145699
15	6	0	0.681726	1.465566	2.084694
16	6	0	-0.078917	1.107510	0.752764
17	6	0	0.114605	2.118928	-0.351122
18	6	0	-0.943699	3.020844	-0.251163
19	8	0	-1.874062	2.681530	0.706368
20	6	0	1.073914	2.294871	-1.350281
21	6	0	0.961879	3.426380	-2.177379
22	6	0	-0.085175	4.338771	-2.034877
23	6	0	-1.080314	4.133427	-1.065401
24	8	0	-0.156222	5.419829	-2.865629
25	8	0	-2.110122	5.035720	-1.002239
26	8	0	-0.276529	2.176686	4.224311
27	8	0	-6.011409	-2.349040	-2.002458
28	8	0	-2.710730	-5.518802	-0.451595
29	6	0	2.136204	1.278003	-1.703137
30	8	0	2.695378	0.705769	-0.507380
31	6	0	3.594319	-0.320042	-0.684436
32	6	0	3.686805	-1.028724	-1.890991
33	6	0	2.789047	-0.714639	-3.062948
34	6	0	1.613725	0.167567	-2.633517
35	6	0	4.400228	-0.621863	0.418208
36	6	0	5.322819	-1.661968	0.314773
37	6	0	5.456944	-2.386326	-0.875178
38	6	0	4.638473	-2.058883	-1.958218
39	8	0	4.716387	-2.731509	-3.146797
40	8	0	6.088290	-1.929127	1.416016
41	8	0	0.625788	-0.564700	-1.912579
42	1	0	0.137579	0.087310	0.443402
43	8	0	1.449144	2.636740	2.010203
44	6	0	1.573331	0.338348	2.607901
45	8	0	0.975203	-0.847499	2.617585
46	6	0	1.740886	-1.966489	3.166555
47	8	0	2.696711	0.565268	3.025174
48	6	0	0.866845	-3.198903	3.081485
49	1	0	-4.951034	-4.790052	-1.747021
50	1	0	-1.587595	-3.428403	0.589013
51	1	0	-4.563152	0.234355	-1.784836
52	1	0	-5.784107	-0.170064	-0.590914
53	1	0	-4.168730	1.756355	0.011816
54	1	0	-2.163386	0.517751	-0.842486
55	1	0	-4.350168	-0.391792	1.830261
56	1	0	-1.862621	0.094350	2.842748
57	1	0	-2.634874	1.683871	2.979507
58	1	0	1.689591	3.609141	-2.961776
59	1	0	-0.942543	5.933245	-2.622624
60	1	0	-2.727406	4.768062	-0.306144
61	1	0	-6.417681	-3.152538	-2.356527
62	1	0	-3.285438	-6.140922	-0.919176
63	1	0	2.941550	1.790776	-2.247073
64	1	0	3.349278	-0.203463	-3.857603
65	1	0	2.409488	-1.638495	-3.514897
66	1	0	1.170863	0.650263	-3.515380
67	1	0	4.302475	-0.057598	1.336350
68	1	0	6.182299	-3.191933	-0.957313
69	1	0	5.380214	-3.431649	-3.077214
70	1	0	6.691873	-2.658862	1.218779
71	1	0	0.278230	-1.249205	-2.499913
72	1	0	2.303796	2.412837	2.421205
73	1	0	2.657936	-2.065867	2.581262
74	1	0	2.010535	-1.717597	4.196080
75	1	0	0.609232	-3.424630	2.043075
76	1	0	-0.055317	-3.068317	3.654175
77	1	0	1.409317	-4.054602	3.493709

Cartesian coordinates of the optimized geometry of (4‴*R*)-12T at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.441383	-4.152585	-0.661509
2	6	0	-4.605557	-3.826258	-1.367540
3	6	0	-5.010868	-2.491162	-1.429600
4	6	0	-4.285090	-1.462847	-0.804716
5	6	0	-3.119726	-1.836198	-0.121141
6	6	0	-2.688095	-3.160966	-0.034163
7	6	0	-4.747067	-0.021995	-0.853131
8	6	0	-4.025806	0.822904	0.205039
9	6	0	-2.533171	0.466786	0.160734
10	8	0	-2.349706	-0.906319	0.545317
11	8	0	-4.578012	0.637848	1.507378
12	6	0	-1.611664	1.298226	1.069444
13	6	0	-1.810985	1.141912	2.570021
14	6	0	-0.490394	1.562601	3.170642
15	6	0	0.660885	1.352595	2.120017
16	6	0	-0.092514	1.062659	0.768571
17	6	0	0.165216	2.086512	-0.311333
18	6	0	-0.861745	3.025687	-0.213531
19	8	0	-1.823427	2.705549	0.718626
20	6	0	1.163345	2.260841	-1.273247
21	6	0	1.110647	3.416254	-2.073278
22	6	0	0.089196	4.357780	-1.938577
23	6	0	-0.938176	4.162522	-1.001278
24	8	0	0.077982	5.460600	-2.741972
25	8	0	-1.934981	5.100227	-0.938783
26	8	0	-0.297422	2.026575	4.270627
27	8	0	-6.139149	-2.111317	-2.098804
28	8	0	-2.989430	-5.436937	-0.561507
29	6	0	2.217892	1.236447	-1.619629
30	8	0	2.708126	0.587858	-0.429144
31	6	0	3.658531	-0.391708	-0.632401
32	6	0	3.799599	-1.041959	-1.868620
33	6	0	2.919798	-0.686818	-3.050035
34	6	0	1.717564	0.154032	-2.603378
35	6	0	4.447614	-0.714848	0.475281
36	6	0	5.409637	-1.718263	0.345845
37	6	0	5.592931	-2.383327	-0.869075
38	6	0	4.792841	-2.038000	-1.956768
39	8	0	5.018502	-2.723277	-3.117322
40	8	0	6.218188	-2.087396	1.382805
41	8	0	0.689135	-0.645668	-2.027640
42	1	0	0.076993	0.037229	0.449674
43	8	0	1.469616	2.497137	2.088875
44	6	0	1.503751	0.177804	2.618813
45	8	0	0.864076	-0.985712	2.577793
46	6	0	1.578936	-2.149125	3.103142
47	8	0	2.627513	0.349555	3.060551
48	6	0	0.655720	-3.341919	2.982849
49	1	0	-5.188039	-4.600063	-1.860923
50	1	0	-1.783049	-3.409075	0.506565
51	1	0	-4.566443	0.407343	-1.847408
52	1	0	-5.825878	0.041844	-0.680939
53	1	0	-4.143002	1.885681	-0.016674
54	1	0	-2.180155	0.593026	-0.872125
55	1	0	-4.472052	-0.295827	1.741551
56	1	0	-1.966775	0.081588	2.803627
57	1	0	-2.655027	1.705473	2.965991
58	1	0	1.869404	3.597421	-2.828028
59	1	0	-0.697265	5.994730	-2.507972
60	1	0	-2.579285	4.839252	-0.264962
61	1	0	-6.578897	-2.892369	-2.462901
62	1	0	-3.584110	-6.027552	-1.044676
63	1	0	3.060063	1.753317	-2.099575
64	1	0	3.485943	-0.126958	-3.806971
65	1	0	2.528771	-1.585578	-3.544545
66	1	0	1.263016	0.645402	-3.467247
67	1	0	4.296679	-0.185014	1.408802
68	1	0	6.347480	-3.154525	-0.969088
69	1	0	4.433271	-2.399896	-3.815403
70	1	0	6.002114	-1.555602	2.161632
71	1	0	1.092097	-1.184633	-1.331793
72	1	0	2.305478	2.236801	2.516443
73	1	0	2.494695	-2.272169	2.519963
74	1	0	1.852465	-1.936836	4.139647
75	1	0	0.395196	-3.531579	1.937989
76	1	0	-0.263497	-3.187729	3.554256
77	1	0	1.160557	-4.228970	3.376013

Cartesian coordinates of the optimized geometry of (4‴*R*)-12U at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.416988	-4.186248	-0.656418
2	6	0	-4.572303	-3.867960	-1.374968
3	6	0	-4.985178	-2.538179	-1.445526
4	6	0	-4.274316	-1.500992	-0.809599
5	6	0	-3.112192	-1.866108	-0.115285
6	6	0	-2.673890	-3.188530	-0.022537
7	6	0	-4.740777	-0.058865	-0.853241
8	6	0	-4.026237	0.788392	0.210960
9	6	0	-2.533201	0.437827	0.168482
10	8	0	-2.351676	-0.933266	0.559025
11	8	0	-4.581838	0.596451	1.508595
12	6	0	-1.618154	1.276884	1.077279
13	6	0	-1.810902	1.113559	2.577994
14	6	0	-0.492627	1.546833	3.175338
15	6	0	0.656902	1.355051	2.119291
16	6	0	-0.097758	1.059888	0.769863
17	6	0	0.142984	2.089835	-0.308097
18	6	0	-0.894066	3.016763	-0.203652
19	8	0	-1.848095	2.682343	0.732116
20	6	0	1.134023	2.276099	-1.274995
21	6	0	1.064227	3.432426	-2.072357
22	6	0	0.033321	4.362605	-1.930371
23	6	0	-0.987339	4.154295	-0.988469
24	8	0	0.005995	5.466885	-2.731496
25	8	0	-1.994740	5.080431	-0.919833
26	8	0	-0.301135	2.007481	4.276892
27	8	0	-6.123882	-2.294177	-2.159388
28	8	0	-3.054563	-5.501767	-0.617068
29	6	0	2.195984	1.261992	-1.627843
30	8	0	2.705585	0.627500	-0.436812
31	6	0	3.654987	-0.351296	-0.643309
32	6	0	3.787315	-1.004040	-1.876235
33	6	0	2.902893	-0.662719	-3.055167
34	6	0	1.699839	0.170669	-2.605231
35	6	0	4.455538	-0.669731	0.460424
36	6	0	5.417106	-1.670413	0.325841
37	6	0	5.590433	-2.340885	-0.890595
38	6	0	4.778365	-1.999289	-1.970449
39	8	0	4.895868	-2.615128	-3.184442
40	8	0	6.237107	-2.037586	1.354669
41	8	0	0.678555	-0.633426	-2.017083
42	1	0	0.084307	0.038309	0.445331
43	8	0	1.450384	2.510253	2.089022
44	6	0	1.516635	0.190087	2.612010
45	8	0	0.892923	-0.982175	2.567554
46	6	0	1.623816	-2.136498	3.090545
47	8	0	2.638225	0.375523	3.053481
48	6	0	0.722268	-3.344258	2.955533
49	1	0	-5.141847	-4.642907	-1.874070
50	1	0	-1.769359	-3.414011	0.532536
51	1	0	-4.560695	0.383599	-1.842699
52	1	0	-5.818363	0.017234	-0.659823
53	1	0	-4.150789	1.849762	-0.011694
54	1	0	-2.177992	0.560659	-0.863803
55	1	0	-4.434438	-0.327333	1.759611
56	1	0	-1.953994	0.051065	2.809939
57	1	0	-2.659231	1.667528	2.978558
58	1	0	1.816679	3.623196	-2.831040
59	1	0	-0.773023	5.992798	-2.491528
60	1	0	-2.629194	4.814655	-0.238632
61	1	0	-6.310191	-1.345843	-2.177672
62	1	0	-2.243099	-5.596842	-0.099085
63	1	0	3.027923	1.786384	-2.117534
64	1	0	3.469458	-0.106310	-3.813257
65	1	0	2.544524	-1.572656	-3.547174
66	1	0	1.233881	0.658179	-3.465699
67	1	0	4.312381	-0.137641	1.393874
68	1	0	6.349861	-3.111340	-0.978307
69	1	0	5.588563	-3.288959	-3.137322
70	1	0	6.029556	-1.503901	2.134571
71	1	0	1.100048	-1.200748	-1.355738
72	1	0	2.290626	2.260062	2.514024
73	1	0	1.885660	-1.926569	4.130566
74	1	0	2.545994	-2.240182	2.513850
75	1	0	0.475486	-3.532869	1.907078
76	1	0	-0.204941	-3.208616	3.518701
77	1	0	1.238263	-4.224608	3.349283

Cartesian coordinates of the optimized geometry of (4‴*R*)-12V at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.275093	-4.204027	-0.712917
2	6	0	-4.488492	-3.913686	-1.348004
3	6	0	-4.955792	-2.600346	-1.350659
4	6	0	-4.245593	-1.553892	-0.732779
5	6	0	-3.032597	-1.889400	-0.120693
6	6	0	-2.535363	-3.195887	-0.095761
7	6	0	-4.774815	-0.135624	-0.718206
8	6	0	-4.037846	0.714540	0.324736
9	6	0	-2.533994	0.426615	0.194436
10	8	0	-2.268499	-0.943257	0.531372
11	8	0	-4.514976	0.471342	1.646224
12	6	0	-1.600893	1.284262	1.064633
13	6	0	-1.769472	1.162084	2.572051
14	6	0	-0.457712	1.658058	3.131337
15	6	0	0.684827	1.427183	2.077054
16	6	0	-0.079583	1.076457	0.742824
17	6	0	0.138120	2.085955	-0.362645
18	6	0	-0.908765	3.005394	-0.262290
19	8	0	-1.848548	2.679873	0.688425
20	6	0	1.133099	2.283601	-1.327649
21	6	0	1.044237	3.430423	-2.136798
22	6	0	0.000588	4.346992	-2.002593
23	6	0	-1.016423	4.134233	-1.056897
24	8	0	-0.042285	5.442578	-2.812444
25	8	0	-2.031047	5.051312	-0.992443
26	8	0	-0.266326	2.186452	4.201965
27	8	0	-6.132520	-2.254177	-1.951107
28	8	0	-2.860913	-5.504245	-0.739777
29	6	0	2.215142	1.282158	-1.669148
30	8	0	2.700540	0.650287	-0.473170
31	6	0	3.605100	-0.372170	-0.648600
32	6	0	3.734913	-1.048213	-1.866601
33	6	0	2.888251	-0.693569	-3.064362
34	6	0	1.726781	0.219709	-2.682626
35	6	0	4.378437	-0.702595	0.471607
36	6	0	5.301998	-1.741884	0.369653
37	6	0	5.469239	-2.438315	-0.832285
38	6	0	4.687578	-2.080774	-1.929964
39	8	0	4.801099	-2.720043	-3.133831
40	8	0	6.090840	-2.121793	1.419997
41	8	0	0.689343	-0.590066	-2.133635
42	1	0	0.122153	0.047904	0.448633
43	8	0	1.480078	2.576935	1.995734
44	6	0	1.542898	0.280779	2.615045
45	8	0	0.912579	-0.887788	2.631519
46	6	0	1.642865	-2.022345	3.197781
47	8	0	2.669490	0.481819	3.036858
48	6	0	0.716348	-3.218294	3.171843
49	1	0	-5.046850	-4.710179	-1.829530
50	1	0	-1.586845	-3.398727	0.390096
51	1	0	-4.668837	0.326361	-1.708607
52	1	0	-5.844422	-0.126984	-0.487297
53	1	0	-4.211676	1.776488	0.138332
54	1	0	-2.254604	0.596478	-0.855704
55	1	0	-4.375544	-0.466601	1.843286
56	1	0	-1.875695	0.103478	2.838572
57	1	0	-2.630024	1.700795	2.966306
58	1	0	1.795259	3.626350	-2.895368
59	1	0	-0.826923	5.961859	-2.575865
60	1	0	-2.661583	4.786648	-0.307075
61	1	0	-6.551468	-3.044784	-2.319298
62	1	0	-2.014062	-5.581417	-0.278397
63	1	0	3.051146	1.817800	-2.140818
64	1	0	3.496043	-0.193820	-3.829457
65	1	0	2.485071	-1.595746	-3.534974
66	1	0	1.367959	0.748865	-3.575407
67	1	0	4.246273	-0.148641	1.393582
68	1	0	6.198659	-3.239566	-0.896305
69	1	0	5.466509	-3.418765	-3.063693
70	1	0	5.889957	-1.565264	2.185493
71	1	0	-0.083571	-0.021534	-2.010201
72	1	0	2.334062	2.332227	2.395968
73	1	0	2.539493	-2.178273	2.593244
74	1	0	1.948319	-1.754287	4.212147
75	1	0	0.422340	-3.463874	2.147897
76	1	0	-0.183990	-3.031950	3.763443
77	1	0	1.234088	-4.083205	3.596380

Cartesian coordinates of the optimized geometry of (4‴*R*)-12W at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.029518	4.030753	-1.005215
2	6	0	3.135525	3.993345	-1.864881
3	6	0	3.903453	2.830283	-1.946435
4	6	0	3.601146	1.681621	-1.190625
5	6	0	2.501699	1.773117	-0.332829
6	6	0	1.723527	2.926136	-0.206972
7	6	0	4.395051	0.396923	-1.329558
8	6	0	3.974050	-0.664967	-0.294730
9	6	0	2.451211	-0.581991	-0.128835
10	8	0	2.135774	0.696064	0.450906
11	8	0	4.641586	-0.493005	0.953672
12	6	0	1.753430	-1.642858	0.737969
13	6	0	2.247226	-1.830259	2.169630
14	6	0	1.037522	-2.353552	2.910686
15	6	0	-0.265698	-1.848331	2.225365
16	6	0	0.205966	-1.379602	0.804694
17	6	0	-0.296620	-2.222966	-0.336568
18	6	0	0.720079	-3.101540	-0.685872
19	8	0	1.884135	-2.922892	0.030390
20	6	0	-1.509789	-2.221666	-1.028613
21	6	0	-1.683069	-3.162656	-2.052629
22	6	0	-0.668056	-4.074941	-2.362803
23	6	0	0.568082	-4.045571	-1.691964
24	8	0	-0.868881	-4.979524	-3.365274
25	8	0	1.526395	-4.939978	-2.087922
26	8	0	1.007854	-3.108180	3.858391
27	8	0	4.980388	2.732461	-2.780646
28	8	0	1.277745	5.166917	-0.991104
29	6	0	-2.501970	-1.134491	-0.686328
30	8	0	-1.913655	0.091825	-1.214964
31	6	0	-2.564884	1.251769	-0.863449
32	6	0	-3.930146	1.244331	-0.548015
33	6	0	-4.734677	-0.042118	-0.601988
34	6	0	-3.933996	-1.207590	-1.224268
35	6	0	-1.791053	2.410825	-0.868739
36	6	0	-2.392988	3.612592	-0.504498
37	6	0	-3.745390	3.661418	-0.161602
38	6	0	-4.497642	2.481243	-0.190935
39	8	0	-5.815612	2.598421	0.145884
40	8	0	-1.592711	4.730954	-0.484111
41	8	0	-3.955145	-1.160954	-2.648436
42	1	0	0.007726	-0.317380	0.670258
43	8	0	-1.201501	-2.890614	2.149881
44	6	0	-0.849066	-0.669862	3.028868
45	8	0	0.088123	0.257999	3.261939
46	6	0	-0.327027	1.450617	3.991660
47	8	0	-2.002068	-0.604316	3.396535
48	6	0	0.906458	2.300916	4.212064
49	1	0	3.361495	4.856872	-2.482981
50	1	0	0.883014	2.934488	0.477052
51	1	0	4.263169	-0.010136	-2.340567
52	1	0	5.467705	0.584525	-1.214463
53	1	0	4.253424	-1.661390	-0.646110
54	1	0	1.990262	-0.639302	-1.124894
55	1	0	4.355088	0.358136	1.317165
56	1	0	2.508860	-0.857670	2.599390
57	1	0	3.111642	-2.488115	2.256939
58	1	0	-2.591417	-3.178052	-2.642138
59	1	0	-0.058713	-5.503655	-3.465115
60	1	0	2.348676	-4.767580	-1.607048
61	1	0	5.103626	3.570192	-3.248662
62	1	0	0.394670	4.978864	-0.622307
63	1	0	-2.558566	-1.037972	0.405671
64	1	0	-5.058183	-0.336814	0.406299
65	1	0	-5.642780	0.083532	-1.205218
66	1	0	-4.396559	-2.156585	-0.938815
67	1	0	-0.742344	2.361259	-1.131062
68	1	0	-4.226724	4.589586	0.129081
69	1	0	-6.244001	1.731893	0.119572
70	1	0	-2.105420	5.502259	-0.203986
71	1	0	-3.265445	-0.535560	-2.919972
72	1	0	-1.237521	-3.295128	3.032034
73	1	0	-0.787055	1.135194	4.931452
74	1	0	-1.084067	1.966512	3.394831
75	1	0	1.648660	1.766810	4.811807
76	1	0	0.626797	3.214138	4.745240
77	1	0	1.363336	2.584096	3.259917

Cartesian coordinates of the optimized geometry of (4‴*R*)-12X at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.326548	-4.231538	-0.628622
2	6	0	-4.486506	-3.939266	-1.350781
3	6	0	-4.924228	-2.617897	-1.429688
4	6	0	-4.234044	-1.563825	-0.798892
5	6	0	-3.066446	-1.902996	-0.100829
6	6	0	-2.603468	-3.216337	0.000566
7	6	0	-4.727563	-0.131136	-0.851840
8	6	0	-4.029584	0.736761	0.206862
9	6	0	-2.530463	0.413150	0.168662
10	8	0	-2.324744	-0.951936	0.568900
11	8	0	-4.583196	0.544363	1.505282
12	6	0	-1.631226	1.273717	1.073022
13	6	0	-1.824531	1.119140	2.574588
14	6	0	-0.513949	1.576809	3.170904
15	6	0	0.640070	1.396356	2.117839
16	6	0	-0.107335	1.077286	0.770217
17	6	0	0.119461	2.101769	-0.315886
18	6	0	-0.930275	3.015057	-0.218990
19	8	0	-1.881613	2.672948	0.716827
20	6	0	1.108584	2.294067	-1.283274
21	6	0	1.025393	3.444521	-2.087765
22	6	0	-0.017208	4.362530	-1.952150
23	6	0	-1.037034	4.146388	-1.010994
24	8	0	-0.057532	5.461769	-2.759731
25	8	0	-2.056987	5.059406	-0.950513
26	8	0	-0.331615	2.047477	4.269803
27	8	0	-6.066219	-2.399197	-2.146540
28	8	0	-2.939245	-5.539698	-0.580876
29	6	0	2.178121	1.286861	-1.632973
30	8	0	2.683611	0.650934	-0.441343
31	6	0	3.631300	-0.330979	-0.642273
32	6	0	3.768318	-0.982436	-1.877776
33	6	0	2.893212	-0.634261	-3.061557
34	6	0	1.687894	0.197454	-2.615666
35	6	0	4.421985	-0.654616	0.464177
36	6	0	5.378970	-1.660642	0.335166
37	6	0	5.557023	-2.329926	-0.881479
38	6	0	4.753055	-1.981204	-1.968173
39	8	0	4.876286	-2.596257	-3.181855
40	8	0	6.130629	-1.950575	1.438363
41	8	0	0.663778	-0.608166	-2.034648
42	1	0	0.091450	0.055631	0.455982
43	8	0	1.412989	2.565340	2.077855
44	6	0	1.520449	0.252466	2.623650
45	8	0	0.922373	-0.933253	2.582125
46	6	0	1.672994	-2.067216	3.122033
47	8	0	2.633911	0.465494	3.072695
48	6	0	0.812014	-3.300832	2.958444
49	1	0	-5.040579	-4.727624	-1.846287
50	1	0	-1.696010	-3.421478	0.558753
51	1	0	-4.555842	0.308071	-1.844223
52	1	0	-5.806437	-0.074508	-0.659070
53	1	0	-4.173253	1.794025	-0.023856
54	1	0	-2.175831	0.535040	-0.863913
55	1	0	-4.413939	-0.372999	1.765912
56	1	0	-1.952433	0.056567	2.814964
57	1	0	-2.681632	1.663751	2.969310
58	1	0	1.775786	3.639762	-2.847361
59	1	0	-0.843297	5.979225	-2.523411
60	1	0	-2.687456	4.791401	-0.266518
61	1	0	-6.269675	-1.454487	-2.170821
62	1	0	-2.126467	-5.615958	-0.061792
63	1	0	3.010078	1.815798	-2.117819
64	1	0	3.465504	-0.073602	-3.812210
65	1	0	2.538062	-1.541255	-3.561182
66	1	0	1.226222	0.687004	-3.477262
67	1	0	4.289024	-0.132410	1.402685
68	1	0	6.307851	-3.109631	-0.981256
69	1	0	5.564535	-3.274393	-3.132713
70	1	0	6.768976	-2.644389	1.221550
71	1	0	1.081457	-1.175212	-1.370658
72	1	0	2.252428	2.336544	2.516540
73	1	0	2.614092	-2.141170	2.572257
74	1	0	1.898618	-1.853034	4.169725
75	1	0	0.601830	-3.494179	1.902811
76	1	0	-0.135140	-3.194508	3.494142
77	1	0	1.342072	-4.166520	3.365842

Cartesian coordinates of the optimized geometry of (4‴*R*)-12Y at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.939980	-3.869391	-0.592314
2	6	0	-5.033669	-3.475254	-1.372851
3	6	0	-5.305912	-2.116020	-1.522907
4	6	0	-4.513570	-1.124435	-0.914373
5	6	0	-3.422027	-1.565453	-0.158380
6	6	0	-3.122568	-2.919905	0.019375
7	6	0	-4.834788	0.348576	-1.051897
8	6	0	-4.092379	1.174215	0.007436
9	6	0	-2.637211	0.685954	0.057749
10	8	0	-2.592217	-0.680103	0.493552
11	8	0	-4.722205	1.103042	1.284989
12	6	0	-1.689702	1.466411	0.984753
13	6	0	-1.989420	1.397839	2.482261
14	6	0	-0.650186	1.623194	3.134301
15	6	0	0.482196	1.079536	2.213599
16	6	0	-0.182295	1.044832	0.789570
17	6	0	0.317954	2.096386	-0.169234
18	6	0	-0.644806	3.095825	-0.231590
19	8	0	-1.751194	2.863647	0.551914
20	6	0	1.492232	2.201200	-0.922820
21	6	0	1.648575	3.331761	-1.737876
22	6	0	0.672429	4.332546	-1.781910
23	6	0	-0.503989	4.227216	-1.022768
24	8	0	0.862315	5.414527	-2.592046
25	8	0	-1.423140	5.237214	-1.122545
26	8	0	-0.398495	2.198142	4.171002
27	8	0	-6.360339	-1.668423	-2.266311
28	8	0	-3.717885	-5.211129	-0.474096
29	6	0	2.544995	1.121502	-0.801184
30	8	0	1.966746	-0.101594	-1.344669
31	6	0	2.753080	-1.228254	-1.219810
32	6	0	4.145644	-1.131625	-1.093468
33	6	0	4.841496	0.214729	-1.099806
34	6	0	3.884748	1.347452	-1.509765
35	6	0	2.083669	-2.453585	-1.266438
36	6	0	2.832278	-3.629162	-1.176652
37	6	0	4.221077	-3.581613	-1.029260
38	6	0	4.858785	-2.341815	-0.987514
39	8	0	6.218255	-2.362943	-0.848181
40	8	0	2.254350	-4.866113	-1.214847
41	8	0	3.717933	1.407097	-2.924281
42	1	0	-0.126417	0.038065	0.374831
43	8	0	1.587275	1.940685	2.274746
44	6	0	0.800407	-0.358896	2.659537
45	8	0	2.103958	-0.570610	2.832351
46	6	0	2.490982	-1.920627	3.227021
47	8	0	-0.069632	-1.196777	2.818793
48	6	0	4.001758	-1.948092	3.324257
49	1	0	-5.654006	-4.229093	-1.847243
50	1	0	-2.266765	-3.202311	0.623572
51	1	0	-4.566160	0.712004	-2.052526
52	1	0	-5.910079	0.518696	-0.940987
53	1	0	-4.099528	2.231405	-0.265785
54	1	0	-2.223103	0.750001	-0.959136
55	1	0	-4.766214	0.170808	1.543443
56	1	0	-2.306256	0.379017	2.733723
57	1	0	-2.754380	2.098288	2.813961
58	1	0	2.519345	3.440622	-2.371695
59	1	0	0.085378	5.990049	-2.513687
60	1	0	-2.206521	5.013524	-0.599453
61	1	0	-6.852873	-2.424348	-2.615661
62	1	0	-2.945496	-5.360400	0.089249
63	1	0	2.745862	0.950979	0.263871
64	1	0	5.257614	0.445174	-0.108894
65	1	0	5.679105	0.225193	-1.809155
66	1	0	4.310317	2.307838	-1.205510
67	1	0	1.003281	-2.469938	-1.367952
68	1	0	4.798607	-4.495028	-0.949970
69	1	0	6.563299	-1.460711	-0.810887
70	1	0	1.298069	-4.769841	-1.325153
71	1	0	3.022936	0.771183	-3.153765
72	1	0	1.660537	2.226852	3.201211
73	1	0	2.112346	-2.618299	2.475548
74	1	0	2.008645	-2.149703	4.181002
75	1	0	4.361198	-1.231878	4.068263
76	1	0	4.459263	-1.713402	2.359309
77	1	0	4.327361	-2.948350	3.624261

Cartesian coordinates of the optimized geometry of (4‴*R*)-12Z at the B3LYP/6-31G(d,p) level in acetone (PCM).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.366654	-4.195945	-0.638749
2	6	0	-4.524828	-3.890608	-1.358244
3	6	0	-4.952000	-2.563033	-1.431218
4	6	0	-4.252745	-1.519889	-0.797362
5	6	0	-3.086006	-1.873999	-0.100781
6	6	0	-2.634746	-3.189326	-0.005955
7	6	0	-4.732310	-0.082141	-0.845161
8	6	0	-4.022842	0.776735	0.213388
9	6	0	-2.527568	0.436405	0.171284
10	8	0	-2.337525	-0.930238	0.572553
11	8	0	-4.575151	0.587735	1.512881
12	6	0	-1.616113	1.287449	1.072255
13	6	0	-1.807565	1.138217	2.574635
14	6	0	-0.491574	1.586735	3.165792
15	6	0	0.658890	1.382038	2.113525
16	6	0	-0.095213	1.072796	0.766247
17	6	0	0.142151	2.094801	-0.319905
18	6	0	-0.897529	3.019561	-0.222701
19	8	0	-1.851188	2.689140	0.714842
20	6	0	1.131945	2.275581	-1.289063
21	6	0	1.059531	3.425780	-2.094987
22	6	0	0.026725	4.354803	-1.959393
23	6	0	-0.993566	4.150903	-1.016110
24	8	0	-0.003267	5.453209	-2.768539
25	8	0	-2.003425	5.074975	-0.954707
26	8	0	-0.302670	2.066473	4.259590
27	8	0	-6.092807	-2.334636	-2.146634
28	8	0	-2.894162	-5.471829	-0.528075
29	6	0	2.192862	1.258739	-1.637316
30	8	0	2.700828	0.628248	-0.443672
31	6	0	3.643304	-0.358238	-0.644656
32	6	0	3.772858	-1.017660	-1.874300
33	6	0	2.892624	-0.675531	-3.056041
34	6	0	1.693199	0.165517	-2.611004
35	6	0	4.439939	-0.677461	0.461685
36	6	0	5.394379	-1.685710	0.333232
37	6	0	5.564740	-2.363057	-0.879781
38	6	0	4.756660	-2.020626	-1.962338
39	8	0	4.871460	-2.643022	-3.173271
40	8	0	6.210136	-2.053904	1.365108
41	8	0	0.666659	-0.630867	-2.021727
42	1	0	0.090185	0.049197	0.450112
43	8	0	1.455350	2.534517	2.072180
44	6	0	1.515530	0.219809	2.618451
45	8	0	0.885760	-0.949578	2.593526
46	6	0	1.613875	-2.101413	3.125936
47	8	0	2.640881	0.405805	3.050153
48	6	0	0.700512	-3.303390	3.022726
49	1	0	-5.098762	-4.661469	-1.862441
50	1	0	-1.731372	-3.420435	0.544933
51	1	0	-4.558433	0.357710	-1.836917
52	1	0	-5.810109	-0.014805	-0.649659
53	1	0	-4.156069	1.835799	-0.015380
54	1	0	-2.174279	0.553663	-0.862330
55	1	0	-4.407197	-0.329627	1.774489
56	1	0	-1.943183	0.077282	2.817770
57	1	0	-2.659123	1.691105	2.969776
58	1	0	1.811053	3.612177	-2.855688
59	1	0	-0.783653	5.978818	-2.532403
60	1	0	-2.637966	4.812007	-0.272507
61	1	0	-6.291873	-1.388802	-2.164741
62	1	0	-3.475551	-6.073462	-1.014003
63	1	0	3.025843	1.779531	-2.129194
64	1	0	3.463394	-0.124467	-3.814896
65	1	0	2.530486	-1.585216	-3.545726
66	1	0	1.231312	0.652388	-3.474060
67	1	0	4.299072	-0.140363	1.392590
68	1	0	6.318443	-3.139640	-0.962728
69	1	0	5.558049	-3.322716	-3.121338
70	1	0	6.004606	-1.515546	2.142327
71	1	0	1.084197	-1.202509	-1.361591
72	1	0	2.300057	2.282295	2.487109
73	1	0	2.527281	-2.222232	2.538655
74	1	0	1.891445	-1.876621	4.158747
75	1	0	0.436119	-3.505890	1.981259
76	1	0	-0.216949	-3.151448	3.597550
77	1	0	1.215147	-4.182004	3.422086