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Organic molecules visualizable by crystal data in introductory chemistry

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Abstract— *Generating checklists could provide new insights into the teaching strategies. Thus, the crystal structures' data of organic compounds learned in secondary chemical education were collected from the Cambridge Crystallographic Data Centre (CCDC) database. It has revealed that almost all the crystal data of these organic molecules are available, contrarily to an anticipation that liquid or gaseous ones at room temperature have few data. This index data would be fundamental for further studies hereafter.*

Keywords— ***ICT teaching material, Molecular geometry, Structural chemistry, X-ray crystallography.***

I. INTRODUCTION

As far, studies regarding the data of crystal structures of organic compounds as ICT teaching materials in secondary chemical education have been reported [1-9]. However, they have not been able to cover whole organic molecules of chemistry in secondary education. On the other hand, for second-year undergraduate and upper-division undergraduate, teaching materials of three-dimensional structural chemistry using the CCDC (Cambridge Crystallographic Data Centre) databases are available [10-14] whose contents seems to be slight difficult for students in high schools. Hence, for teaching and learning the organic chemistry in secondary schools, I collected the crystalline structural data of organic compounds from the CCDC database to demonstrate their structures clearly summarized as a checklist.

II. RESULTS

Collected articles are described as follow:

1. Alkane

1.1. Methane CH_4

1.1.1. Methane hydrate $(CH_4)(H_2O)_4$ [15]

1.1.2. Methane-C_{60}fullerene-nickel(II) octaethylporphrin-benzene $CH_4{\cdot}C_{60}{\cdot}NiC_{36}H_{44}N_4{\cdot}C_6H_6$ [16]

1.2. Ethane C_2H_6 [17]

1.3. Propane C_3H_8 [18]

1.4. Butane C_4H_{10} [18]

1.5. Hexane C_6H_{14} [18]

1.6. Octane C_8H_{18} [18]

2. Haloalkane

2.1. Chloromethane CH_3Cl [19]

2.2. Dichloromethane CH_2Cl_2 [20]

2.3. Chloroform $CHCl_3$ [21]

2.4. Tetrachloromethane CCl_4 [22]

2.5. Iodoform CHI_3 [23]

2.6. Iodoform-octasulfur $CHI_3{\cdot}3S_8$ [24]

2.7 1,2-Dibromoethane-7,16-(2,3-anthraceno)-7,16-dihydroheptacene $3C_2H_4Br_2{\cdot}C_{44}H_{26}$ [25]

3. Cycloalkane/Halocycloalkane

3.1. Cyclobutane C_4H_8 [26]

3.2. Cyclopentane C_5H_{10} [27]

3.3. Cyclohexane C_6H_{12} [28]

3.4. Hexachlorocyclohexane $C_6H_6Cl_6$ [29]

4. Alkene/Cycloalkene

4.1. Ethylene C_2H_4 [30]

4.2. Propene C_3H_6

4.2.1. Propene-iron(II) 2,5-dioxido-1,4-benzenedicarboxylate $C_3H_6\cdot Fe_2C_8O_6$ [31]

4.3. Butene C_4H_8

4.3.1. 1-Butene-cobalt (II) 2,5-dioxido-1,4-benzenedicarboxylate $CH_2{=}CHCH_2CH_3\cdot Co_2C_8O_6$[32]

4.3.2. *cis*-2-Butene-cobalt (II) 2,5-dioxido-1,4-benzenedicarboxylate $CH_2{=}CHCH_2CH_3\cdot Co_2C_8O_6$ [32]

4.3.3. *trans*-2-Butene-cobalt (II) 2,5-dioxido-1,4-benzenedicarboxylate $CH_2{=}CHCH_2CH_3\cdot Co_2C_8O_6$ [32]

4.4. Cyclohexene C_6H_{10} [33]

5. Alkyne

5.1. Acetylene C_2H_2 [34]

5.2. Propyne C_3H_4

5.2.1. Cadmium(II) [bis(-3,5-bis[3-(pyridin-4-yl)phenyl]-4H-1,2,4-triazol-4-amine) perchlorate-propyne $[Cd(C_{24}H_{18}N_6)_2(ClO_4)_2]\cdot 2C_3H_4$ [35]

5.3. 2-Butyne C_4H_6

5.3.1. 2-Butyne-hydrogen chloride $C_4H_6\cdot HCl$ [36]

6. Aliphatic alcohol

6.1. Methanol CH_3OH [37]

6.1-1. Methanol-chloroform $CH_3OH\cdot CHCl_3$ [38]

6.2. Ethanol C_2H_5OH [39]

6.2.1. Sodium ethoxide-ethanol $C_2H_5ONa\cdot 2C_2H_5OH$ [40]

6.3. Propanol C_3H_7OH

6.3.1. Sodium 1-propoxide-1-propanol $CH_3(CH_2)_2ONa\cdot 2CH_3(CH_2)_2OH$ [40]

6.3.2. Mono-2-*O*-(mesitylsulfonyl)-α-cyclodextrin 1-propanol nonahydrate $2CH_3(CH_2)_2OH\cdot C_{45}H_{60}O_{32}S\cdot 9H_2O$ [41]

6.3.3. 1-Propanol-vitamin B_{12} dodecahydrate $3CH_3(CH_2)_2OH\cdot C_{63}H_{88}CoN_{14}O_{14}P\cdot 12H_2O$ [42]

6.4. 2-Propanol $CH_3CH(OH)CH_3$ [43]

6.5. Butanol C_4H_9OH

6.5.1. 1-Butanol $CH_3(CH_2)_3OH$ [44]

6.5.2. 2-Butanol $CH_3CH(OH)CH_2CH_3$ [45]

6.5.3. 2-Methyl-1-propanol $(CH_3)_2CHCH_2OH$ [46]

6.5.4. 2-Methyl-2-propanol $(CH_3)_3COH$ [47]

6.6. Ethylene glycol $HOCH_2CH_2OH$ [48]

6.7. Glycerin $HOCH_2CH(OH)CH_2OH$ [49]

7. Aliphatic ether

7.1. Dimethyl ether $(CH_3)_2O$ [50]

7.2. Diethyl ether $(C_2H_5)_2O$ [51]

8. Aliphatic Aldehyde/ Ketone

8.1. Formaldehyde HCHO [52]

8.1.1. Formaldehyde-acetylene $HCHO\cdot C_2H_2$ [53]

8.2. Acetaldehyde CH_3CHO [54]

8.3. Propionaldehyde CH_3CH_2CHO [55]

8.4. Acetone $(CH_3)_2CO$ [56]

9. Aliphatic carboxylic acid/carboxylate/anhydride

9.1. Formic acid HCOOH [57]

9.1.1. Formic acid-hydrogen fluoride $HCOOH\cdot HF$ [58]

9.2. Acetic acid CH_3COOH [59]

9.3. Ethyl acetate $CH_3COOC_2H_5$ [60]

9.4. Sodium acetate trihydrate $CH_3COONa\cdot 3H_2O$ [61]

9.4.1. Calcium acetate monohydrate $Ca(CH_3COO)_2\cdot H_2O$ [62]

9.5. Acetic anhydride $(CH_3COO)_2O$ [63]

9.6. Propionic acid CH_3CH_2COOH [64]

9.7. Butyric acid $CH_3(CH_2)_2COOH$

9.7.1. Butyric acid-cytenamide $CH_3(CH_2)_2COOH\cdot C_{16}H_{13}NO$ [65]

9.8. Oxalic acid $(COOH)_2$ [66]

9.8.1. Oxalic acid dihydrate $(COOH)_2\cdot 2H_2O$ [67]

9.9. Sodium oxalate $(COONa)_2$ [68]

9.10. Calcium oxalate trihydrate $CaC_2O_4\cdot 3H_2O$ [69]

9.11. Ammonium hydrogen oxalate hemihydrate $NH_4HC_2O_4\cdot 0.5H_2O$ [70]

9.12. Oxalic acid-ammonium hydrogen oxalate dihydrate $(COOH)_2\cdot NH_4H(COO)_2\cdot 2H_2O$ [71]

9.13. Hexamethylenediammonium bis(monohydrogen oxalate) monohydrate $(CH_2CH_2CH_2NH_3)_2H(COO)_2\cdot H_2O$ [72]

9.14. Glutaric acid $HOOC(CH_2)_3COOH$

9.14.1. Glutaric acid-glycine $HOOC(CH_2)_3COOH\cdot H_3N^+CH_2COO^-$ [73]

9.15. Adipic acid $HOOC(CH_2)_4COOH$ [74]

9.15.1. Adipic acid-urea $HOOC(CH_2)_4COOH\cdot CO(NH_2)_2$ [75]

9.16. Maleic acid $C_2H_2(COOH)_2$ [76]

9.16.1 Maleic acid-L-lysine $HOOCCH=CHCOO^{-}H_3N^{+}C$-$H(CH_2CH_2CH_2CH_2NH_3^{+})COO^{-}$ [77]

9.17. Maleic anhydride $(CHCO)_2O$ [78]

9.18. Fumaric acid $C_2H_2(COOH)_2$ [79]

9.18.1. Fumaric acid- ethenzamide $C_2H_2(COOH)_2 \cdot C_9H_{11}N$-$O_2$ [80]

9.19. Methyl methacrylate $CH_2=C(CH_3)COOCH_3$ [81]

9.20. Stearic acid $C_{17}H_{35}COOH$ [82]

9.21. Stearin $C_3H_5(C_{18}H_{35}O_2)_3$ [83]

10. Organosulfate/Organonitrate

10.1. Sodium dodecyl sulfate $C_{12}H_{25}OSO_3Na$ [84]

10.1.1. Sodium dodecyl sulfate monohydrate $C_{12}H_{25}OSO_3$-$Na \cdot H_2O$ [85]

10.2. Nitroglycerin $C_3H_5(NO_3)_3$ [86]

11. Aliphatic amine/amide/nitrile

11.1. Hexamethylenediamine $H_2N(CH_2)_6NH_2$ [87]

11.2. ε-Caprolactam $C_6H_{11}NO$ [88]

11.3. Acetonitrile CH_3CN

11.3.1. Acetonitrile-acetylene $CH_3CN \cdot C_2H_2$ [53]

12. Aliphatic hydroxy acid/amino acid

12.1. Lactic acid $CH_3CH(OH)COOH$ [89]

12.2. Tartaric acid $HOOCCH(OH)CH(OH)COOH$ [90]

12.2.1. Sodium ammonium tartrate tetrahydrate $NaNH_4O$-$OCCH(OH)CH(OH)COO \cdot 4H_2O$ [91]

12.3. Glycine $H_3N^{+}CH_2COO^{-}$ [92]

12.4. Alanine $H_3N^{+}CH(CH_3)COO^{-}$ [93]

12.5. Serine $H_3N^{+}CH(CH_2OH)COO^{-}$

12.5.1. Serine hydrogen peroxide $H_3N^{+}CH(CH_2OH)$-$COO^{-} \cdot H_2O_2$ [94]

13. Sugar

13.1. α-D-Glucose $C_6H_{12}O_6$ [95]

13.2. β-D-Glucose $C_6H_{12}O_6$ [96]

13.3. Fructose $C_6H_{12}O_6$

13.3.1. Fructose-calcium chloride trihydrate $2C_6H_{12}O_6 \cdot Ca$-$Cl_2 \cdot 3H_2O$ [97]

13.4. α-Maltose $C_{12}H_{22}O_{11}$ [98]

13.5. Sucrose $C_{12}H_{22}O_{11}$ [99]

13.6. Cellulose $(C_6H_{10}O_5)_n$ [100]

14. Aromatic hydrocarbon

14.1. Benzene C_6H_6 [101]

14.2. Benzene ethane $C_6H_6 \cdot C_2H_6$ [102]

14.3. Benzene bromine $C_6H_6 \cdot Br_2$ [103]

14.4. Toluene $C_6H_5CH_3$ [104]

14.4.1. $C_6H_5CH_3 \cdot Br_2$ [105]

14.5. Xylene $C_6H_4(CH_3)_2$

14.5.1. *o*-Xylene $C_6H_4(CH_3)_2$ [106]

14.5.2. *m*-Xylene $C_6H_4(CH_3)_2$ [107]

14.5.3. *m*-Xylene acetylene $C_6H_4(CH_3)_2 \cdot C_2H_2$ [53]

14.5.3. *p*-Xylene $C_6H_4(CH_3)_2$ [108]

14.6. Styrene $C_6H_5CH=CH_2$ [109]

14.7. Naphthalene $C_{10}H_8$ [110]

14.7. Naphthalene-picric acid $C_{10}H_8 \cdot C_6H_2OH(NO_2)_3$ [111]

14.8. Anthracene $C_{14}H_{10}$ [112]

15. Aromatic halohydrocarbon

15.1. Chlorobenzene C_6H_5Cl [113]

15.2. *p*-Dichlorobenzene $C_6H_5Cl_2$ [114]

15.3. Bromobenzene

15.3.1. C_{60}Fullerene bromobenzene $C_{60} \cdot C_6H_5Br$ [115]

16. Aromatic nitrohydrocarbon

16.1. Nitrobenzene $C_6H_5NO_2$ [116]

16.2. *m*-Dinitrobenzene $C_6H_4(NO_2)_2$ [117]

16.3. 1,3,5-Trinitrobenzene

16.3.1. 1,3,5-Trinitrobenzene-azobenzene $2C_6H_3(NO_2)_3 \cdot$-C_6-$H_5N=NC_6H_5$ [118]

16.4. 2,4,6-Trinitrotoluene $CH_3C_6H_2(NO_2)_3$ [119]

16.4.2. 2,4,6-Trinitrotoluene-anthracene $CH_3C_6H_2(NO_2)_3$-$\cdot C_{14}H_{10}$ [120]

17. Aromatic sulfonic acid

17.1. Benzenesulfonic acid $C_6H_5SO_3H$ [121]

17.2. Oxonium benzenesulfonate $H_3OC_6H_5SO_3$ [122]

17.3. Guanidium *p*-dodecylbenzenesulfonate $H_2N=C$-$(NH_2)_2C_{18}H_{30}SO_3$ [123]

18. Phenol

18.1. Phenol [124]

18.2. 2,4,6-Tribromophenol $C_6H_3Br_3OH$

18.2.1. 2,4,6-Tribromophenol 4-dimethylaminopyridinium 2,4,6-tribromophenoxide $C_6H_3Br_3OH·(CH_3)_2NC_5H_4NHC_6H_3Br_3O$ [125]

18.2.2. Diammine bis(2,4,6-tribromophenoxide) copper(II) $[Cu(NH_3)_2(C_6H_3Br_3O)_2]$ [126]

18.3. Sodium phenoxide C_6H_5ONa [127-128]

18.3.1. Sodium phenoxide monohydrate $C_6H_5ONa·H_2O$ [129]

18.3.2. Sodium phenoxide trihydrate $C_6H_5ONa·3H_2O$ [129]

18.3.3. Sodium tetramethanolate phenoxide $[Na(CH_3OH)_4][OC_6H_5]$ [130]

18.3.4. Sodium phenoxide acetonitrile [131]

18.4. *o*-Cresol $C_6H_4(OH)CH_3$ [132]

18.5. *m*-Cresol $C_6H_4(OH)CH_3$

18.5.1. *m*-Cresol urea $C_6H_4(OH)CH_3·(NH_2)_2CO$ [133]

18.6. *p*-Cresol $C_6H_4(OH)CH_3$ [134]

18.7. Catechol $C_6H_4(OH)_2$ [135]

18.8. Resorcinol $C_6H_4(OH)_2$ [136]

18.9. Hydroquinone $C_6H_4(OH)_2$ [137]

18.9.1. Hydroquinone-carbon dioxide $C_6H_4(OH)_2·CO_2$ [138]

19. Aromatic alcohol/aldehyde/peroxide

19.1. Benzyl alcohol $C_6H_5CH_2OH$

19.1.1. β-Cyclodextrin-benzyl alcohol pentahydrate $(C_6H_{10}O_5)_7·C_6H_5CH_2OH·5H_2O$ [139]

19.2. Benzaldehyde C_6H_5CHO [140]

19.3. Cumene hydroperoxide $C_6H_5C(CH_3)_2OOH$

19.3.1. *cis*-1,3-Di-tert-butyl-2,4-bis(tert-butylamino)-1,3,-2,4-diazadiphosphetidine 2,4-dioxide-cumyl alcohol-cumene hydroperoxide $[((CH_3)_3CHN)O=P(\mu\text{-}NC(CH_3)_3)_2P=O(NHC(CH_3)_3)]·C_6H_5C(CH_3)_2OH·C_6H_5C(CH_3)_2OOH$ [141]

19.3.2. Cumene peroxide-(1,4,7,10-tetramethyl-1,4,7,10-tetraazacyclododecane)-lithium-cumyl alcohol $[LiC_6H_5C(CH_3)_2OO(C_{12}H_{28}N_4)]·C_6H_5C(CH_3)_2OOH$ [142]

20. Aromatic carboxylic acid/anhydride/salt/ester

20.1. Benzoic acid C_6H_5COOH [143]

20.2. Phthalic acid $C_6H_4(COOH)_2$ [144]

20.2.1. Phthalic acid sesquihydrate $C_6H_4(COOH)_2·1.5H_2O$ [145]

20.3. Phthalic anhydride $C_6H_4(CO)_2O$ [146]

20.4. Hexaamminecobalt(III) chloride bis(hydrogen phthalate) trihydrate $[Co(NH_3)_6]Cl(C_8H_5O_4)_2·3H_2O$ [147]

20.5. Isophthalic acid $C_6H_4(COOH)_2$ [148]

20.6. Terephthalic acid $C_6H_4(COOH)_2$ [149]

20.7. Salicylic acid $C_6H_4(OH)COOH$ [150]

20.8. Sodium salicylate $C_6H_4(OH)COONa$ [151]

20.9. Methyl salicylate $C_6H_4(OH)COOCH_3$

20.9.1. Bis(2,4,6-tris(4-pyridyl)-1,3,5-triazine)-hexaiodozinc-methyl salicylate $(ZnI_2)_3(C_{18}H_{12}N_6)_2·4.25C_8H_8O_3$ [152]

20.10. Acetyl salicylate $C_6H_4(OCOCH_3)COOH$ [153]

21. Aromatic amine/diazonium salt/amide/amino acid

21.1. Aniline $C_6H_5NH_2$ [154]

21.1.1. Aniline $C_6H_5NH_2·C_6H_4(OH)CH_3$ [155]

21.1.2. Aniline hydrochloride $C_6H_5NH_3Cl$ [156]

21.2. Benzene diazonium chloride $C_6H_5N_2Cl$ [157]

21.3. Acetanilide $C_6H_5NHCOCH_3$ [158]

21.4. Phenylalanine

21.4.1. Phenylalanine monohydrate $H_3N^+CH(CH_2C_6H_5)COO^-·H_2O$ [159]

22. Azo dye/phenolphthalein/ninhydrin

22.1. *p*-(Phenylazo)phenol $C_6H_5N=NC_6H_4OH$ [160]

22.1.1. Permethylated β-cyclodextrin-*p*-(phenylazo)phenol hexahydrate $C_{63}H_{112}O_{35}·C_6H_5N=NC_6H_4OH·6H_2O$ [161]

22.1.2. β-cyclodextrin-*p*-(phenylazo)phenol octahydrate $(C_6H_{10}O_5)_7·C_6H_5N=NC_6H_4OH·8H_2O$ [162]

22.2. 1-Phenylazo-2-naphthol $C_6H_5N=NC_{10}H_6OH$ [163]

22.3. Methyl orange $(CH_3)NC_6H_4N=NC_6H_4SO_3Na$

22.3.1. Methyl orange tetrahydrate $(CH_3)NC_6H_4N=NC_6H_4SO_3Na·4H_2O$ [164]

22.3.1.2. Protonated methyl orange without sodium ion $(CH_3)NC_6H_4N=NH^+C_6H_4SO_3^-$ [165]

22.4. Methyl red $(CH_3)NC_6H_4N=NC_6H_4COOH$ [166]

22.5. Phenolphthalein $C_{20}H_{14}O_4$ [167-168]

22.6. Ninhydrin $C_6H_4(CO)_2C(OH)_2$ [169]

III. DISCUSSION

Although liquid and gaseous organic molecules at room temperature were seemed to have few data of crystal structures, it has revealed that almost all the crystalline structural data of the organic molecules learned in secondary chemical education are available in CCDC database. However, even in the simplest organic molecule such as methane, the crystal structure of pure methane to be visualized clearly have not been available in CCDC database [170] or there are disorders in atoms [171]. Instead, as the case of methane, a theoretically predicted crystal structure of methane hydrate by the Monte-Carlo packing algorithm and density-functional theory (DFT) optimization [15] and the crystal structure of a single methane molecule encapsulated in a C_{60}fullerene cage [16] are selected for the purpose to be learned by students.

Contrarily, organic molecules learned in secondary schools have been known widely. Thus, it also seems that almost all of their crystallographic structural studies might have been finished until the 20th century. Is this idea true or not? Reported years of each data are also of interest. For example, from 2000 to 2009 (2000s), 37 structures; from 2010 to 2019 (2010s), 46 structures have been published. Therefore, it is elucidated that recent studies have contributed the clarifying the structures of organic molecules learned in secondary education in addition to the researches conducted in the latter half of the 20th century.

Generating checklists can offer new insights into the subject matter and teaching strategies [172]. Based on this objective, I am making these graphics of the structures of organic molecules be available with bibliographic data through the Internet (refer to URL in Acknowledgement). These structural data on organic molecules studied in secondary schools summarized herein will have a potential for developing further teaching ICT materials to be attractive for students. Besides, these findings summarized herein could be fundamental for application to also higher education of chemistry and materials engineering in the future.

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