**AIP-BDET-v2: Remove Undirected Edge Training in Bond Dissociation Energy Prediction with Smaller Model by Counting and Blind-Match Searching**

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**Table of Contents**

[**Exp-BDEs: Data Collection** 2](#_Toc94130941)

[**Learning Rate Scaling** 19](#_Toc94130942)

[**Working Progress (Tracking)** 20](#_Toc94130943)

[**Technical Configuration** 21](#_Toc94130944)

[**Additional Information** 21](#_Toc94130945)

[**References** 21](#_Toc94130946)

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# **Exp-BDEs: Data Collection**

In the process of collecting the experimental BDE, some values needed to be in careful consideration in which all of them would be removed or accepted despite some subjective issues about SMILES converter and bond identifier. The main book/article used to extract is “Comprehensive Handbook of Bond Dissociation Energies” by Yu Ran Luo, written in 2007.

**Table S1**: Molecules that may have uncommon behavior which may require extra validation

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Page** | **Molecule / Name** | **Issue(s)** | **How to Resolve** | **Our Solution** |
| 24 | X ~ | Uncommon Atom, Ionic Atom | \_ | NOT Included |
| 30 | Allyl Triphenyl Phosphonium Bromide | Uncommon Atoms | \_ | NOT Included |
| 30 | 3-Phenykl-Allyl Triphenyl Phosphonium, Bromide | Uncommon Atoms | \_ | NOT Included |
| 32 | 1-Phenyl-cyclo-buten-3-yl | Radical | \_ | NOT Included |
| 37 | Norboradine | \_ | Change to 2,5-Norbornadiene | Included |
| 37 | Bicyclo-octane | \_ | Change to Bicyclo[2.2.2]octane | Included |
| 40 | Phenyl | Radical | \_ | NOT Included |
| 40 | 3,5-Didehydrophenyl | Radical | \_ | NOT Included |
| 40 | 5-Dehydro-1,3-quinodimethane | Radical | \_ | NOT Included |
| 40, 41 | Benzene, substituted  Y = Num  Y = 4-Br | Ionic atom / functional group  Uncommon Atom | \_ | NOT Included |
| 41 | Toluene, substituted  F, Cl, Br | Uncommon Atom | \_ | NOT Included |
| 41 | Toluene, substituted  Y = 4- ; Cl | Uncommon Atom | \_ | NOT Included |
| 41 | Toluene, substituted  Y = 4-Pr | Inconsistent order | Need refactoring: Assumed to be 4-nPr | Included with provided Name |
| 42 | Toluene, other-substituted | Radical | \_ | NOT Included |
| 43 | Toluene bromide | Uncommon & Ionic Atom | \_ | NOT Included |
| 43 | Ethylbenzene, substituted  Y = 4-Br | Uncommon Atom | \_ | NOT Included |
| 44 | Cationic niobium | Uncommon Atom | \_ | NOT Included |
| 46 | 1,1-Diphenylethane | Uncertain molecule representation | Need refactoring | Included but as |
| 46 | Thiphenylmethane | Invalid Name | Triphenylmethane | Included |
| 46 | Thiphenylmethane, substituted | Uncommon Atom (F) | \_ | NOT Included |
| 47 | Indene, substituded  Y = 2-Br, 3-MeS, 2-PhS | Uncommon Atom (Br, S) | \_ | NOT Included |
| 49 | 2-Naphthyl anion | Ionic Atom | \_ | NOT Included |
| 50 | 2-Naphthyl radical | Radical | \_ | NOT Included |
| 51 | 2-Methyl-naphthalene | Uncommon Atom (S) | \_ | NOT Included |
| 51 | 4,5-Methylene-phenathrene | Invalid Name | 1-methyl-2-(2-methylphenyl)benzene | Included |
| 52 | Xanthene, subsititued  Y = ;  Y = ; | Uncommon Atom (S, Cl, F) | \_ | NOT Included |
| 53 | Fluorenes | WARNING ONLY: Fluorenes is not available in PubChem | \_ | \_ |
| 53 | Fluorenes, substituted  Y =  Y = ; | Uncommon Atom (Sulfur, Bromide)  Duplicated Found | \_  Need refactoring | NOT Included |
| 54 | Fluorenes, substituted  X = 9; 9-PhS  X = | Uncommon Atom (Sulfur, Florua) | \_ | NOT Included |
| 55 | Fluorenes, substituted  X = | Invalid Functional Group | Need refactoring by both References | NOT Included |
| 55 | Fluorenes, substituted | Invalid Functional Group (Checked on 1994 ZHA/BOR (c)). The reference author is correctly written. | Need refactoring by Book’s Author | Included followed by Origin |
| 55 | Fluorenes, substituted  MeS, EtS, iPrS, tert-BuS, PhS, MeSO2, EtSO2, iso-PrSO2, PhSO2, (p-BrPh)SO2, Me3SiCH2, SiMe3, SiEt3, SiPh3 | Uncommon Atom (S, Br, Si) | \_ | NOT Included |
| 55 | Fluorenes, substituted  Me3N+Cl-, PyN+Br-, Ph3P+Br-, nBu3P+Br- | Ionic Atom | \_ | NOT Included |
| 56 | Fluorenes, substituted  Ph3As+Br-, Me2S+Br-, Me2Se+Br-, tBu2Te+Br-, Me3N+ (2-PhSO2)Br- | Ionic Atom, Uncommon Atom (S, As, Se, Te) | \_ | NOT Included |
| 56 | Fluorenes, substituted  π-Cr(CO)3, π-+Mn(CO)3, π-+Fe(C5H5) | Ionic Atom, Uncommon Atom (Cr, Fe, Mn) | \_ | NOT Included |
| 58 | 9-Anthracenylmethanes  Y = PhS, PhSO2 | Uncommon Atom (S) | \_ | NOT Included |
| 58 | Anthracenes  Y = Cl, PhS | Uncommon Atom (S, Cl) | \_ | NOT Included |
| 59 | 9-Phenanthrenylmethane | Warning: Old name ??? | PubChem: 9-Methylphenanthrene | Included |
| 59 | Benzanthrene | Lack of Sufficient Information | Need refactoring to be 7H-Benzanthrene | Included |
| 59 | Triphenylene radical cation | Ionic Atom, Radical | \_ | NOT Included |
| 59 | Phenalene, Benzanthrene | Incorrect Author Name in Citation: 1990BAU/GOS | 1990BAU/DOB | Included |
| 59 | 1,2-Benzofluorence | Invalid Name | Need refactoring to be 1,2-Benzofluorene | Included |
| 60 | 2,3-Benzofluorence | Invalid Name | Need refactoring to be 2,3-Benzofluorene | Included |
| 60 | Methylbenzo(b)phenanthrene | Invalid Name | Need refactoring to be 1-methylbenzo[a]anthracene | Included |
| 73 | Ethane-1,1-diol | Uncertain BDE | \_ | Included |
| 74 | Difluoromethyl  trifluoromethyl ether | Uncommon Atom (F) | \_ | NOT Included |
| 74 | Bis(difluoromethyl) ether | Uncommon Atom (F) | \_ | NOT Included |
| 74 | Methyl trifluoromethyl ether | Uncommon Atom (F) | \_ | NOT Included |
| 75 | Cyclo-hexyl methyl ether | Inconsistent Representation | Need refactoring with this Information (**H**-C-O) | Included |
| 75 | Benzyl methyl ether, substituted: 3-Cl, 4-Cl, 4-Br | Uncommon Atom (Cl, Br) | \_ | NOT Included |
| 75 | Diphenylmethyl methyl ether, substituted: 3-Cl, 4-Br | Uncommon Atom (Cl, Br) | \_ | NOT Included |
| 76 | Diphenylmethyl methyl ether, substituted: 4-MeC(O)O | Unclear Representation | Need refactoring as MeC(=O)**O** or 4-**O**C(=O)Me | Included as C(=O)OC |
| 76 | Dialkyloxymethenes  **C**CC(C)C and sec-C5H11 | Inconsistent behavior of sec-C5H11 as it can be sec-2 or sec-3 | Need better refactoring | Included sec as sec-2 |
| 77 | Dimethoxyphenylmethane, substituted: 4-Cl, 4-Br | Uncommon Atom (Cl, Br) | \_ | NOT Included |
| 77 | Dimethoxyphenylmethane, substituted: OME | Warning: Incorrect Name | \_ | Included |
| 77 | Dimethoxyphenylmethane, substituted: 4-MeC(O)O | Unclear Representation | Need refactoring as MeC(=O)**O** or 4-**O**C(=O)Me | Included |
| 79 | 2-Alkyl-2HK3,4,5,6-tetra-hydropyrans: C6H11 | Lack of Information | Need refactoring. Assumed to be C6H13 | Included |
| 83 | Formyl fluoride | Uncommon Atom (F) | \_ | NOT Included |
| 84 | Benzaldehyde, substituted: 3-Cl, 4-Cl, 3-Br | Uncommon Atom (Cl, Br) | \_ | NOT Included |
| 85 | Acetyl fluoride | Uncommon Atom (F) | \_ | NOT Included |
| 85 | Acetyl chloride | Uncommon Atom (Cl) | \_ | NOT Included |
| 86 | 1,1,1-Trifluoroacetone | Uncommon Atom (F) | \_ | NOT Included |
| 87 | Methyl trimethylphenyl ketone | Unclear structure representation and name | Need better refactoring as 1-(2,4,6-trimethylphenyl)ethanone | Included |
| 87 | Methyl phenyl ketone bromide | Ionic Atom, Uncommon Atom (Br) | \_ | NOT Included |
| 89 | Anthracenyl-2 phenyl ketone  Anthracenyl-9 phenyl ketone | Warning: Old name | 2-Benzoylanthracene  9-Benzoylanthracene | Included |
| 89 | Naphthyl-1 phenyl ketone  Naphthyl-2 phenyl ketone | Warning: Old name | 1-Benzoylnaphthylene  2-Benzoylnaphthylene | Included |
| 89 | Phenyl pyridyl ketone | Inconsistent Structure Name | Need both refactoring. Expect Py(2) (2-phenacylpyridine) | Included but should be warned |
| 89 | Chromium tricarbonyl  complexes | Uncommon Atom (Cr) | \_ | NOT Included |
| 93 | Acetic ion | Ionic Atom | \_ | NOT Included |
| 93 | Chloroacetic acid | Uncommon Atom (Cl) | \_ | NOT Included |
| 96 | Methyl pebtanoate | Typo: Name + Incorrect Structure | Methyl pentanoate - Need refactoring: (CH2)2 | Included |
| 96 | Ethyl butylanoate | Incorrect Structure | Need refactoring: (CH2)2 | Included |
| 96 | Ethyl pentanoate | Incorrect Structure | Need refactoring: (CH2)3 | Included |
| 96 | Propyl pebtanoate | Typo: Name + Incorrect Structure | Propyl pentanoate - Need refactoring: (CH2)3 | Included |
| 97 | Iso-Propyl pebtanoate | Typo: Name + Incorrect Structure | Iso-Propyl pentanoate - Need refactoring: (CH2)3 | Included |
| 97 | Tert-butyl-2,2-dimethyl propanoate | Incorrect Structure | Need refactoring: **(CH3)3**CC(O) | Included |
| 100 | Diethyl 2-(1,1-dimethyl-1silaethyl) propane-1,3-dioate | Uncommon Atom (Si) | \_ | NOT Included |
| 100 | Ethyl methyl 2-(1,1-dimethyl-1silaethyl) propane-1,3-dioate | Uncommon Atom (Si) | \_ | NOT Included |
| 101 | Ethyl octafluoro-fluorene-9 carboxylate | Uncommon Atom (F) | \_ | NOT Included |
| 105 | N,N-Dimethylaniline, substituted: 4-Cl, 4-CF3 | Uncommon Atom (Cl, F) | \_ | NOT Included |
| 105 | N,N-Dimethylaniline, substituted: 2,2-Me2 | Invalid structure | Need refactoring to author: o,o- or 2,5- | Included with new structure |
| 105 | Benzyl trimethylammonium, chloride | Ionic Atom, Uncommon Atom (Cl) | \_ | NOT Included |
| 105 | Fluorenyl trimethylammonium bromide | Ionic Atom, Uncommon Atom (F) | \_ | NOT Included |
| 105 | Benzyl trimethylammonium | Ionic Atom, Uncommon Atom (Br) | \_ | NOT Included |
| 106 | Prop-2-enenitrile | Invalid Structure | Need refactoring to C=CC#N as Author | Included |
| 106 | Prop-2-ynenitrile | Invalid Structure | Need refactoring to C#CC#N as Author | Included |
| 107 | Pentafluorophenyl acetonitrile | Uncommon Atom (F) | \_ | NOT Included |
| 107 | Di(pentafluorophenyl)-acetonitrile | Uncommon Atom (F) | \_ | NOT Included |
| 108 | Phenylmethane-1,1-dicarbonitrile | Inconsistent Structure | Need refactoring as N#CC(Ph)C#N | Included |
| 108 | 1-Acetonitrile trimethylammonium chloride | Ionic Atom, Uncommon Atom (Cl) | \_ | NOT Included |
| 108 | 1-Acetonitrile pyridinium chloride | Ionic Atom, Uncommon Atom (Cl) | \_ | NOT Included |
| 111 | 1-Phenylnitroethanes, substituted: 4-F | Uncommon Atom (F) | \_ | NOT Included |
| 115 | 1,4-Dihydropyridines, substituted: 4-Cl, 4-Br, 4-CF3 | Uncommon Atom | \_ | NOT Included |
| 118 | (1Z)-2-Aza-2-methoxy-1,1 phenylvinylamine | Undetermined cis-trans (1Z) | Need refactoring | Included as RDKit’s canonical system |
| 119 | Phenyl pyridyl ketone | Duplicate in page 89 | Need refactoring | NOT Included |
| 119 | Phenyl methylene ketone trimethylammonium bromide | Ionic Atom, Uncommon Atom (Br) | \_ | NOT Included |
| 120 | Ethyl-2-aminoacetate | Unclear BDE | Need refactoring | Convert to 81.0 ± 2 |
| 121 | Ethyl-2-cyano-2 phenylacetates, substituted: Y=F, Cl, CF3 | Uncommon Atom (Cl, F) | \_ | NOT Included |
| 121 | Ethyl-2-cyano-2 pentafluorophenyl-acetate | Uncommon Atom (F) | \_ | NOT Included |
| 122 | 1,3-Oxazolidines, substituted (#2) | Incorrect structure representation | Need refactoring: R – C whose neighbors are O and N | Included |
| 123 | NADH | Text overflow, Uncommon Atom (P) | \_ | NOT Included |
| 123 | NADH+\* | Text overflow, Uncommon Atom (P), Ionic atom | \_ | NOT Included |
| 152 | 2,3,4-trimethylpentane | Wrong name | Need refactoring: 2,2,4-trimethylpentane | Included by structure |
| 152 | 2,3-Trimethylpentane | Wrong name | Need refactoring: 2,3,3-trimethylpentane | Included by structure |
| 155 | 2-Butyne | Incorrect structure | Need refactoring | Included by name |
| 156 | 2-Ethyl-1-pentyne | Incorrect name (may be old style) | Need refactoring: 5-Ethyl-1-pentyne | Included by structure |
| 160 | 5-Methyl-1-hexene | Incorrect name (may be old style) | Need refactoring: 2-Methyl-1-hexene | Included by structure |
| 166 | Phenalenyl pi-dimer & sigma-dimer | \_ | \_ | Not Included (No physical bond) |
| 166 | Phenalenyl, substituted pi-dimer | Inconsistent citation (2004 SMA/ZAI) | Need refactoring | Not Included (No physical bond) |
| 166 | Phenalenyl, substituted sigma-dimer | \_ | \_ | Not Included (No physical bond) |
| 178 | 2,2,2-Trifluoroethanol | Uncommon Atom (F) | \_ | Not Included |
| 178 | 3,3,3-Trifluoro-1-propanol | Uncommon Atom (F) | \_ | Not Included |
| 178 | 2,2,3,3-Tetrafluoro-1-propanol | Uncommon Atom (F) | \_ | Not Included |
| 181 | Ketenylidene | Ionic Atom | It would be better if we have ‘ethynol’ instead | Not Included |
| 181 | Trichloroacetaldehyde | Uncommon Atom (Cl) | \_ | Not Included |
| 181 | Acetyl fluoride | Uncommon Atom (F) | \_ | Not Included |
| 181 | Acetyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 182 | Trichloroacetyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 182 | Dichloroacetyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 182 | Chloroacetyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 182 | Propanoyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 183 | Benzonyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 183 | Propanal chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 183 | Bromoacetone | Uncommon Atom (Br) | \_ | Not Included |
| 184 | Chloroacetone | Incorrect Structure | \_ | Not Included |
| 185 | Trifluoromethyl phenyl ketone | Uncommon Atom (F) | \_ | Not Included |
| 186 | Oxalyl chloride | Uncommon Atom (Cl) | \_ | Not Included |
| 187 | Trifluoroacetic acid | Uncommon Atom (F) | \_ | Not Included |
| 187 | Trichloroacetic acid | Uncommon Atom (Cl) | \_ | Not Included |
| 187 | Chloroacetic acid | Uncommon Atom (Cl) | \_ | Not Included |
| 187 | Bromoacetic acid | Uncommon Atom (Br) | \_ | Not Included |
| 187 | Propenoic acid | Uncertain result | Need refactoring | Included by means (1 std) |
| 187 | 2-Chloropropanoinc acid | Uncommon Atom (Cl) | \_ | Not Included |
| 188 | Pentafluoro-benznic acid | Uncommon Atom (F) | \_ | Not Included |
| 189 | Methyl-2,2,2- trifluoroacetate | Uncommon Atom (F) | \_ | Not Included |
| 189 | Chloroacetic acid methyl ester | Uncommon Atom (Cl) | \_ | Not Included |
| 189 | Pentafluoropropanoic acid methyl ester | Uncommon Atom (F) | \_ | Not Included |
| 190 | 1-Chloro-ropropanoic acid methyl ester | Uncommon Atom (Cl) | \_ | Not Included |
| 191 | 2-Chlorooxirane | Uncommon Atom (Cl) | \_ | Not Included |
| 191 | Radical dimer | \_ | \_ | Not Included (No physical bond) |
| 192 | Thioformyl cyanide | Uncommon Atom (S) | \_ | Not Included |
| 192 | Trifluoroacetonitrile | Uncommon Atom (F) | \_ | Not Included |
| 192 | 2-Butynedinitrile | Incorrect Structure or Name ? | Need refactoring | Included by Structure |
| 196 | Pyridine, substituted (#1) | Redundant & Undefined Text (HO(O)C-pyridyl) | \_ | Ignored. Broken bond: R-pyridine |
| 196 | Pyridine (#2) | Crystal Structure | Need Extra Information | Not Included (Ignored) |
| 196 | Pyridine (#3) | Crystal Structure; Incorrect Citation: 2000 SIL/MIR cannot be found in the reference | Need Extra Information; Is that 2005 SIL/MIR? | Not Included (Ignored) |
| 197 | Pyridine (#2) | Crystal Structure | Need Extra Information | Not Included (Ignored) |
| 196 - 197 | Pyridine | Result Conflict; Crystalline Structure | \_ | Not Included (Ignored) |
| 202 | Nitrozoamines (#4) | Incorrect Structure: Lack of “C” | Need refactoring: **(…)C**-CH2CH2N | Included |
| 203 | Nitrofluoroethanes | Uncommon Atom (F) | \_ | Not Included |
| 203 | Coenzyme B12, substituted | Uncommon Atom (Co, I) | \_ | Not Included |
| 255 | Water, Oxygen deuteride, Oxygen tritide | Radical | \_ | Not Included |
| 255 | Hypofluorous acid | Uncommon Atom (F) | \_ | Not Included |
| 256 | Hypochlorous acid | Uncommon Atom (Cl) | \_ | Not Included |
| 256 | Hypobromous acid | Uncommon Atom (Br) | \_ | Not Included |
| 256 | Hypoiodomous acid | Uncommon Atom (I) | \_ | Not Included |
| 256 | Trifluoromethanol | Uncommon Atom (F) | \_ | Not Included |
| 257 | Ethanol (C2H5O-D) | Inconsistent BDE | Need refactoring | Included as Normal |
| 257 | 2,2,2-Trifluoroethan-1-ol | Uncommon Atom (F) | \_ | Not Included |
| 257 | 1-Propanol | Inconsistent BDE | Need refactoring | Included as Normal |
| 257 | 2-Propanol | Inconsistent BDE | Need refactoring | Included as Normal |
| 257 | 1,1-Dimethyl-2 chloropropanol | Uncommon Atom (Cl) | \_ | Not Included |
| 260 | Enols | Uncommon Atom (Si) | \_ | Not Included |
| 261 | Hydroxylamine | Inconsistent BDE | Need refactoring | Included as 76 ± 1 |
| 261 | Hyponitrite | Contain Cis-Trans Isomer | \_ | Included both state with equal BDE |
| 261 | Isocyanic acid | Incorrect Name | Need refactoring: Formaldoxime | Included |
| 261 | HOS radical | Uncommon Atom (S), Radical | \_ | Not Included |
| 261 | Sulfuric acid | Uncommon Atom (S) | \_ | Not Included |
| 261 | HOP radical | Uncommon Atom (P), Radical | \_ | Not Included |
| 261 | Metaphosphoric acid | Uncommon Atom (P) | \_ | Not Included |
| 261 | 2,2-Dimethylsilaethanol | Uncommon Atom (Si) | \_ | Not Included |
| 262 | Chloroacetic acid | Uncommon Atom (Cl) | \_ | Not Included |
| 262 | Trifluoroacetic acid | Uncommon Atom (F) | \_ | Not Included |
| 264 | Benzoic acids, substituted | Uncommon Atom (Br, Cl) | \_ | Not Included |
| 265 | Nicotinic acid, substituted | Incorrect Structure | Need refactoring: 3-N not 4-N | Included by reference |
| 265 | Pyridium carboxyled species | Ionic Atom | \_ | Not Included |
| 266 | Hydroperoxy radical | Radical | \_ | Not Included |
| 266 | Trifluoromethyl hydroperoxide | Uncommon Atom (F) | \_ | Not Included |
| 266 | Fluoromethyl hydroperoxide | Uncommon Atom (F) | \_ | Not Included |
| 266 | Trichloromethyl hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 267 | Dichloromethyl hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 267 | Chloromethyl hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 267 | Tribromomethyl hydroperoxide | Uncommon Atom (Br) | \_ | Not Included |
| 267 | Bromomethyl hydroperoxide | Uncommon Atom (Br) | \_ | Not Included |
| 267 | 2-Chloroethyl hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 267 | 2,2-Dichloroethyl hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 267 | 1,1,1-Trifluoro-2-chloroethyl  hydroperoxide | Uncommon Atom (F) | \_ | Not Included |
| 268 | 1,1,2,2-Tetrachloroethyl  hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 268 | Pentachloroethyl hydroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 268 | Alkyl hydroperoxides | \_ | \_ | Included but need further standardization \* |
| 269 | Phenyl hydroperoxide, substituted (Cl, CO2) | Uncommon Atom (Cl), Ionic Atom | \_ | Not Included |
| 269 | 2,2-Dichloro–2 hydroperoxyethane | Uncommon Atom (Cl) | \_ | Not Included |
| 270 | a-CO2-methyl hydro - peroxide | Ionic Atom | \_ | Not Included |
| 270 | a-CO2-chloromethyl hydroperoxide | Uncommon Atom (Cl), Ionic Atom | \_ | Not Included |
| 270 | a-CO2-dichloromethyl  hydroperoxide | Uncommon Atom (Cl), Ionic Atom | \_ | Not Included |
| 270 | 2,2-Dichloro-2-  hydroperoxyethanenitrile | Ionic Atom | \_ | Not Included |
| 272 | Oximes (CF3) | Uncommon Atom (F) | \_ | Not Included |
| 273 | Norcamphor, oximes | \_ | \_ | Included base state: ON=C1C-C2CCC1C2 |
| 274 | (Hydroxyimino)-2,7-dibromofluorenylmethane | Uncommon Atom (Br) | \_ | Not Included |
| 274 | (Hydroxyimino)-2-PhSO2-fluorenylmethane | Uncommon Atom (S) | \_ | Not Included |
| 274 | Oximes, substituted (#1, #2) | Uncommon Atom (Cl, Br, F) | \_ | Not Included |
| 274 | Hydroxylamines, substituted | Uncommon Atom (F) | \_ | Not Included |
| 275 | Hydroxylamines, substituted (tBu) | Inconsistent BDE | Need Refactoring | Not Included |
| 275 | Hydroxamic acids, substituted (#2) | Uncommon Atom (Br) | \_ | Not Included |
| 276 | Hydroxamic acids, substituted (#1) – Line 4 | \_ | Structure should be drawn instead of basic formula | Included |
| 276 | Hydroxamic acids, substituted (#2) | Incorrect Structure | Need Refactoring: 3,5-(NO2)2-C6H3 | Included by reference |
| 277 | 2,5-Dihydropyrrole, substituted | Uncommon Atom (Cl, Br) | \_ | Not Included |
| 277 | 2,5-Dihydropyrrole, substituted | Uncommon Atom (Br) | \_ | Not Included |
| 278 | 1-Hydroxy-tetrahydro-imidazole | Uncommon Atom (F) | \_ | Not Included |
| 278 | 1-Hydroxy-tetrahydro-imidazole (#2) (Line 2) | Redundant hydrogen | Need Refactoring | Included by reference’s structure (1995) |
| 279 | Hydroimidazole, substituted | Uncommon Atom (Cl, F) | \_ | Not Included |
| 279 | Hydroimidazole, substituted:  CH3C6H4 | Incorrect Structure | Need Refactoring:  p-MeC6H4 | Included by reference’s structure (1995) |
| 279 | 2,5-Dihydrioimidazole, substituted | Incorrect Core:  ON1C(C)(C)N(=O)=CC1(C)C | Need Refactoring | Included by the fix |
| 279 - 280 | 2,5-Dihydrioimidazole, substituted | Uncommon Atom (Cl, Br, F) | \_ | Not Included |
| 280 | 2,5-Dihydrioimidazole, substituted | Incorrect Core:  ON1C(C)(C)N(=O)=CC1(C)C | Need Refactoring | Included by the fix |
| 279 | Methanesulphovinates, substituted | Unable to validate | Need Refactoring | Not Included |
| 280 | Piperdin-1-ol, substituted (#1) | Uncommon Atom (Cl) | \_ | Not Included |
| 281 | Piperdin-1-ol, substituted (#2) | Uncommon Atom (Cl, Br) | \_ | Not Included |
| 281 | 1-Hydroxy-piperidn-4-one, substituted | Uncommon Atom (Cl, Br) | \_ | Not Included |
| 283 | N-Hydroxyphthalimide (NHPI) | Inconsistent BDE | \_ | Not Included |
| 283 | N-Hydroxyphthalimide (NHPI), substituted (#2) | Uncommon Atom (F) | \_ | Not Included |
| 284 | 1,2-Dihydroquinoline, substituted | Uncommon Atom (F) | \_ | Not Included |
| 285 | Organomecury species | Uncommon Atom (Hg, Cl) | \_ | Not Included |
| 285 | Phenol | Swap the position in Sol. And Gas. | \_ | Included |
| 285 | Pentafluorophenol | Uncommon Atom (F) | \_ | Not Included |
| 285 - 286 | Phenols, substituted | Uncommon Atom (F, Cl, Br, I) | \_ | Not Included |
| 286 | Phenols, substituted | Incorrect Citation: 2004COR/GUF | Need refactoring: 2004COR/GUE | Followed |
| 287 | Phenols, substituted | Uncommon Atom (F) | \_ | Not Included |
| 288 | Phenols, substituted | Uncommon Atom (S) | \_ | Not Included |
| 288 | Phenols, substituted | Ionic Atom (COO-) | \_ | Not Included |
| 288 - 289 | Phenols, substituted | Ionic Atom (O-) and Radical (O\*) | \_ | Not Included |
| 289 | Phenols, substituted | Ionic Atom (N-) | \_ | Not Included |
| 289 | Phenols, di-substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 289 | Phenols, di-substituted | Incorrect Citation: 2004COR/GUF | Need refactoring: 2004COR/GUE | Followed |
| 289 | Phenols, di-substituted | Unclear Functional Group: 2,2-(OH)2 | Need refactoring: 2,6-(OH2) | Included |
| 290 | Phenols, tri-substituted | Unclear Functional Group: 1,3-tBu2-5-OH | Need refactoring: 2,4-tBu2-6-OH | Included |
| 290 | Phenols, tri-substituted | Uncommon Atom (Cl, S) | \_ | Not Included |
| 291 | Phenols, tri-substituted | Incorrect Functional Group:  4-C3H7-2,5-di-OH  4-C8H17-2,5-di-OH | Need refactoring:  4-C(O)OC3H7-2,6-di-OH  4-C(O)OC8H17-2,6-di-OH | Included |
| 291 | Phenols, substituted (#1) | Gas added first, Solution added later. Small deviation (<= 2 kcal/mol). | \_ | Included by reference order |
| 292 | Phenols, tetra-substituted | Duplicated Result in page 291: Phenols, tri-substituted | Need refactoring | Not Included |
| 292 | Biphenols | Ionic Atom (O-) | \_ | Not Included |
| 294 | All–rac-a-selenotocopherol | Uncommon Atom (Se) | \_ | Included |
| 295 | 5,7-Dimethyl-tocol, DMT | \_ | Need Extra Information as rac-5,7-dimethyltocol | Included |
| 295 | Ubiquinol-10 | Gas added first, Solution added later. Small deviation (<= 2 kcal/mol). | \_ | Included by reference order |
| 296 | 2,3-dihydrobenzo(b)furan-5-ol, substituted | Uncommon Atom (S, Se, Te) | \_ | Not Included |
| 296 | Tetrahydroquinoline, substituted | Base structure is not well-drawn | Need refactoring | Included |
| 296 | Hydroxynaphthalene, substituted | Uncommon Atom (Br) | \_ | Not Included |
| 297 | 2,4-Dichlorophenoxy-10,50-dichloro-phenyl-6, 20-ether | Uncommon Atom (Cl) | \_ | Not Included |
| 298 | Phenols, substituted | Uncommon Atom (Cl, S) | \_ | Not Included |
| 298 | Phenols, substituted: 4-NC | Incorrect Structure | Need refactoring: 4-C#N or 4-CN | Not Included |
| 299 | Phenols, substituted | Uncommon Atom (S) | \_ | Not Included |
| 301 | Methane, substituted | Incorrect Structure | \_ | 2,4: Included  3,5: Build a reverse |
| 302 | Silane, substituted | Uncommon Atom (Si) | \_ | Not Included |
| 302 | Sulfide, substituted (#1) | Uncommon Atom (S) | \_ | Not Included |
| 302 | Sulfide, substituted (#2) | Uncommon Atom (S) | \_ | Not Included |
| 302 | Sulfide, substituted (#1) | Uncommon Atom (S) | \_ | Not Included |
| 302 | Sulfide, substituted (#2) | Uncommon Atom (S) | \_ | Not Included |
| 303 | Sulfide, substituted (#1) | Uncommon Atom (S) | \_ | Not Included |
| 303 | Sulfide, substituted (#2) | Uncommon Atom (S) | \_ | Not Included |
| 303 | 4-((4-Hydroxyphenylthio)-methylthio)phenyl, substituted | Uncommon Atom (S) | \_ | Not Included |
| 304 | Silicoorganics | Uncommon Atom (Si) | \_ | Not Included |
| 305 | 4-Hydroxydiphenylaminyl radical | Radical | \_ | Not Included |
| 309 | Oxygen cation | Ionic Atom | \_ | Not Included |
| 309 | Oxygen anion | Ionic Atom | \_ | Not Included |
| 310 | Hydroperoxy radical | Radical | \_ | Not Included |
| 310 | Fluoride hydroperoxide | Uncommon Atom (F) | \_ | Not Included |
| 310 | Bromine hydroperoxide | Uncommon Atom (Br) | \_ | Not Included |
| 310 | Difluoroperoxide | Uncommon Atom (F) | \_ | Not Included |
| 310 | Dioxygen fluoride radical | Uncommon Atom (F), Radical | \_ | Not Included |
| 310 | Dioxygen bromide radical | Uncommon Atom (Br), Radical | \_ | Not Included |
| 310 | Dichloroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 311 | Chloroperoxide | Uncommon Atom (Cl) | \_ | Not Included |
| 311 | Dichlorine trioxide | Uncommon Atom (Cl) | \_ | Not Included |
| 311 | Bromoperoxide | Uncommon Atom (Br) | \_ | Not Included |
| 311 | Diiodoperoxide | Uncommon Atom (I) | \_ | Not Included |
| 311 | trans-Perp-peronitrous acid | Inconsistent BDE | \_ | Included as Alternative Reference |
| 311 | trans-Perp-peronitrous acid  cis-cis-Peronitrous acid | 3D-Conformer | \_ | Included as canonical SMILES 2D |
| 311 | Hydroperoxy methyl | Negative BDE. Unable to verify the structure | \_ | Not Included |
| 312 | Trifluoromethyl hydroperoxide | Uncommon Atom (F) | \_ | Not Included |
| 312 | Alkyl hydroperoxide | Inconsistent BDE | \_ | Included as 45 ± 1 |
| 313 | Ditrifluoromethyl peroxide | Uncommon Atom (F) | \_ | Not Included |
| 314 | Di-tert-nonafluorobutyl peroxide | Uncommon Atom (F) | \_ | Not Included |
| 314 | Dialkyl peroxide | Uncommon Atom (Cl) | \_ | Not Included |
| 315 | Peroxides, substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 315 | di(Sulfur pentafluoro) peroxide | Uncommon Atom (F, S) | \_ | Not Included |
| 315 | Sulfur peroxide | Uncommon Atom (F, S) | \_ | Not Included |
| 315 | di(Sulfur pentafluoro) trioxide | Uncommon Atom (F, S) | \_ | Not Included |
| 315 | tert-Butyl 1,1-dimethyl-1-  silaethyl peroxide | Uncommon Atom (Si) | \_ | Not Included |
| 315 | 2,2-Diethyl-2-germabutyl tertbutyl peroxide | Uncommon Atom (Ge) | \_ | Not Included |
| 315 | 2,2-Diethyl-2-stannabutyl tertbutyl peroxide | Uncommon Atom (Sn) | \_ | Not Included |
| 315 | HOOO radical | Radical | \_ | Not Included |
| 316 | Trioxygen bromide radical | Uncommon Atom (Br), Radical | \_ | Not Included |
| 316 | ROOO radical | Radical | \_ | Not Included |
| 316 | Trifluoromethoxy-trifluoromethyl peroxide | Uncommon Atom (F) | \_ | Not Included |
| 316 | Chlorofluorotrioxide | Uncommon Atom (F, Cl) | \_ | Not Included |
| 316 | Chlorotrioxide | Uncommon Atom (Cl), Unclear BDE | \_ | Not Included |
| 316 | Tetrahydrofuran-2-yl-peroxy | Radical | \_ | Not Included |
| 316 | Dioxan-2-yl-peroxy | Radical | \_ | Not Included |
| 316 | Bifluoroformyloxy | Uncommon Atom (F) | \_ | Not Included |
| 316 | Perfluorinated peroxide | Uncommon Atom (F) | \_ | Not Included |
| 317 | Bis(trifluoroacetyl) peroxide | Uncommon Atom (F) | \_ | Not Included |
| 317 | Perfluorinated peroxide | Uncommon Atom (F) | \_ | Not Included |
| 317 | Bis(trifluoromethyl) peroxydicarbonate | Uncommon Atom (F) | \_ | Not Included |
| 318 | Acyl peroxides | Uncommon Atom (Cl, Br) | \_ | Not Included |
| 319 | Acyl peroxides (#3) | Uncommon Atom (Cl, Br) | \_ | Not Included |
| 319 | Acyl peroxides (#4) | Uncommon Atom (Cl) | \_ | Not Included |
| 319 | Peroxydisulfuryl difluoride | Uncommon Atom (F, S) | \_ | Not Included |
| 319 | Peroxodiphosphate | Uncommon Atom (P), Ionic Molecules | \_ | Not Included |
| 319 | Peroxodisulfate | Uncommon Atom (S), Ionic Molecules | \_ | Not Included |
| 320 | Flavins | Ring-bond, Unclear BDE | \_ | Not Included |
| 321 | Trifluoromethanol | Uncommon Atom (F) | \_ | Not Included |
| 321 | Trifluoromethylhypofluorite | Uncommon Atom (F) | \_ | Not Included |
| 321 | 2,2,2-Trifluoroethanol | Uncommon Atom (F) | \_ | Not Included |
| 323 | Pentafluorophenol | Uncommon Atom (F) | \_ | Not Included |
| 323 | 1-Hydroxy-1,3,4-trichloro cyclo-pentadiene | Uncommon Atom (Cl) | \_ | Not Included |
| 325 | Iodomethyl methyl ether | Uncommon Atom (I) | \_ | Not Included |
| 325 | 2-Chloroethyl methyl ether | Uncommon Atom (Cl) | \_ | Not Included |
| 325 | 2-Chloroethyl vinyl ether | Uncommon Atom (Cl) | \_ | Not Included |
| 326 | 2-Chloroethyl ethyl ether | Uncommon Atom (Cl) | \_ | Not Included |
| 326 | 1-Chloroethyl methyl ether | Uncommon Atom (Cl) | \_ | Not Included |
| 326 | 1-Chloroethyl ethyl ether | Uncommon Atom (Cl) | \_ | Not Included |
| 329 | Anisoles, substituted | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 330 | Anisoles, substituted | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 331 | 1-[(4-Benzolphenoxy)methyl]-naphthalene | Inconsistent BDE | \_ | Included |
| 332 | Tropylium phenoxides, substituted | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 333 | Thiphenylmethylium phenoxides, substituted | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 335 | Ethyl chloroformate | Uncommon Atom (Cl) | \_ | Not Included |
| 336 | Acetic acid phenyl ester | ~ Phenyl acetate | \_ | Included |
| 338 | Bis(trifluoromethyl) peroxide | Uncommon Atom (F) | \_ | Not Included |
| 338 - 341 | Peroxy | Radical | \_ | Not Included |
| 338 | Methyl peroxy | Inconsistent BDE | \_ | Not Included |
| 338 | Trifluoromethyl peroxy | Uncommon Atom (F) | \_ | Not Included |
| 338 | Chlorodifluoromethyl peroxy | Uncommon Atom (Cl) | \_ | Not Included |
| 339 | Dichlorofluoromethyl peroxy | Uncommon Atom (Cl) | \_ | Not Included |
| 339 | Chloromethyl peroxy | Uncommon Atom (Cl) | \_ | Not Included |
| 339 | Dichloromethyl peroxy | Uncommon Atom (Cl) | \_ | Not Included |
| 339 | Trichloromethyl peroxy | Uncommon Atom (Cl) | \_ | Not Included |
| 342 | Carbon monoxide | Ionic Atom | \_ | Not Included |
| 342 | Carbon oxysulfide | Uncommon Atom (S) | \_ | Not Included |
| 342 | Formaldehyde, halogened | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 342 | Methanisocynate | Inconsistent Name | Need refactoring: Methan isocyanate | Included |
| 342 | Trifluoromethyl hypochlorite | Uncommon Atom (Cl), Inconsistent BDE | \_ | Not Included |
| 344 | 1-Methoxy-1,1-dimethyl-1-silaethane | Uncommon Atom (Si) | \_ | Not Included |
| 344 | 1-Ethoxy-1,1-dimethyl-1-silaethane | Uncommon Atom (Si) | \_ | Not Included |
| 345 | 1-Nitroadamantane | Incorrect Positional Placement: The bond is C-N, not O-C | \_ | Included |
| 345 | Methoxy-1-thiol | Uncommon Atom (S) | \_ | Not Included |
| 345 | Methoxymethylthio | Uncommon Atom (S) | \_ | Not Included |
| 345 | Cinnamyl-4-nitrobenzene sulfonate | Uncommon Atom (S) | \_ | Not Included |
| 345 | Tungsten alkoxide | Uncommon Atom (W) | \_ | Not Included |
| **347** | **Nitric oxide** | **Radical** | **\_** | **Not Included** |
| **347** | **Dinitrogen oxide** | **Charged bond** | **\_** | **Not Included** |
| **347** | **Nitrogen dioxide** | **Radical** | **\_** | **Not Included** |
| **348** | **Nitrate** | **Charged bond** | **\_** | **Not Included** |
| **348** | **Dinitrogen tetroxide** | **Charged bond** | **\_** | **Not Included** |
| **348** | **Nitric oxide dimer** | **\_** | **\_** | **Not Included (No physical bond)** |
| **348** | **Dinitrogen pentoxide** | **Charged bond** | **\_** | **Not Included** |
| 348 | Nitrosyl hydride | Incorrect Structure | Need refactoring: O-NH | Included |
| 348 | Fluoronitrooxy | Uncommon Atom (F) | \_ | Not Included |
| 348 | cis-Chloronitrooxy | Uncommon Atom (Cl) | \_ | Not Included |
| 349 | trans-Chloronitrooxy | Uncommon Atom (Cl) | \_ | Not Included |
| 349 | cis-Bromonitrooxy | Uncommon Atom (Br) | \_ | Not Included |
| 349 | Fluoronitrooxy | Uncommon Atom (F) | \_ | Not Included |
| 349 | Chloronitrooxy | Uncommon Atom (Cl) | \_ | Not Included |
| 349 | Bromonitrooxy | Uncommon Atom (Br) | \_ | Not Included |
| 349 | Iodomonitrooxy | Uncommon Atom (I) | \_ | Not Included |
| 350 | Alkyl nitrate | Charged Bond | \_ | Not Included |
| 350 | Nitric acid | Charged Bond | \_ | Not Included |
| 351-352 | Methyl nitrate -> 1-Methylvinyl nitroperoxy | Charged Bond | \_ | Not Included |
| 351 | Trifluoromethyl nitroperoxy | Uncommon Atom (F) | \_ | Not Included |
| 351 | Chlorodifluoromethyl nitroperoxy | Uncommon Atom (F, Cl) | \_ | Not Included |
| 351 | Dichlorofluoromethyl nitroperoxy | Uncommon Atom (F, Cl) | \_ | Not Included |
| 351 | Trichloromethyl nitroperoxy | Uncommon Atom (Cl) | \_ | Not Included |
| 352 | Nitroso benzoate, substituted | Uncommon Atom (Br) | \_ | Not Included |
| 352 | N,N-Difluorohydroxylamine O-fluorosulfate | Uncommon Atom (F) | \_ | Not Included |
| 353 | Nitro compounds (#1, #2) | Charged Bond | \_ | Not Included |
| 353 | Trialkyl-N-oxides | Charged Bond | \_ | Not Included |
| 353 | Nitrobenzyl compounds | Charged Bond | \_ | Not Included |
| 353 | Nitromethyl radical | Radical | \_ | Not Included |
| 353 | Alkyl nitrate | Charged Bond | \_ | Not Included |
| 354 | 1-Nitropiperidine | Charged Bond | \_ | Not Included |
| 354 | N-Nitromorpholine | Charged Bond | \_ | Not Included |
| 354 | Furazan N-oxides, substituted | Dative Bond | \_ | Not Included |
| 354 | Furoxans | Dative Bond | \_ | Not Included |
| 354 - 355 | Pyridine N-oxides, substituted | Charged Bond | \_ | Not Included |
| 355 | Benzonitrile N-oxide, substituted | Charged Bond | \_ | Not Included |
| 355 | 2,3-Diazabicyclo[2.2.1]-hept-2-ene N-oxide | Charged Bond | \_ | Not Included |
| 355 | Benzofurazan N-oxides, substituted | Charged Bond | \_ | Not Included |
| 356 | Azoxy compounds | Charged Bond | \_ | Not Included |
| 356 | Azoxybenzenes, substituted | Charged Bond | \_ | Not Included |
| 356 | Benzylidene N-oxides, substituted | Charged Bond | \_ | Not Included |
| 357 | di-N-Oxides | Charged Bond | \_ | Not Included |
| 357 | 2,3-Diazabicyclo[2.2.1]-hept-2-ene N-oxide | Charged Bond | \_ | Not Included |
| 357 | 4,4’-Dinitroazoxyfurazan | Charged Bond | \_ | Not Included |
| 357 | 4,4’-Diaminoazoxyfurazan | Charged Bond | \_ | Not Included |
| 357 | di-N-Oxides | Charged Bond | \_ | Not Included |
| 358 | Quinoline N-oxides, substituted | Charged Bond | \_ | Not Included |
| 358 | 2-Amino-3-quinoixalinecarbonitrile-1,4-dioxide | Charged Bond | \_ | Not Included |
| 358 | 2-Amino-3-quinoixalinecarbonitrile-1,4-dioxide | Charged Bond | \_ | Not Included |
| 358 | Phenazine N-oxide | Charged Bond | \_ | Not Included |
| 359 | 2-Hydroxyphenazine-di-Noxide (#1) | Charged Bond | \_ | Not Included |
| 359 | 2-Hydroxyphenazine-di-Noxide (#2) | Charged Bond | \_ | Not Included |
| 359 | 2-Hydroxyphenazine-di-Noxide (#3) | Charged Bond | \_ | Not Included |
| 359-360 | Benzo furoxans | Charged Bond | \_ | Not Included |
| 369 | Ammonia | Radical | \_ | Not Included |
| 369 | Deuterated ammonias | Radical | \_ | Not Included |
| 370 | Hydrazoic acid | Ionic Atom | \_ | Not Included |
| 370 | Isocyanic acid | Inconsistent BDE | \_ | Included All |
| 370 | Iso-thiocyanic acid | Uncommon Atom (S) | \_ | Not Included |
| 370 | Cyanoamino radical | Radical | \_ | Not Included |
| 370 | Methylamine | Inconsistent BDE | \_ | Included All |
| 371 | Propylamine phosphonium bromide | Uncommon Atom (P, Br), Ionic Atom | \_ | Not Included |
| 371 | Hydrazine radical | Radical | \_ | Not Included |
| 372 | Methylhydrazine radical | Radical | \_ | Not Included |
| 372 | Amonomethanenitrile | Incorrect Name | Need refactoring: Cyanamide | Included |
| 372 | Thiourea | Uncommon Atom (S) | \_ | Not Included |
| 372 | 1-Aminoethane-1-thione | Uncommon Atom (S) | \_ | Not Included |
| 372 | Aminophenylmethane-1-thione | Uncommon Atom (S) | \_ | Not Included |
| 372 | Bis(phenylamino)methane-1-thione | Uncommon Atom (S) | \_ | Not Included |
| 373 | Benzylphenylthioamine | Uncommon Atom (S) | \_ | Not Included |
| 373 | Hydroxylamine | Inconsistent BDE | \_ | Convert to 81.5 ± 0.5 |
| 373 | 2-Ethyl-pentanamide | Incorrect Name | Need refactoring: 2,2-diethylbutanamide | Included |
| 374 | Benzenesulfonamide | Uncommon Atom (S) | \_ | Not Included |
| 374 | Hydrazinophenyl sulfone | Uncommon Atom (S) | \_ | Not Included |
| 375 | (Tert-buytl)phenylthioamine | Uncommon Atom (S) | \_ | Not Included |
| 376 | N-[(1E)-1-aza-2-phenylprop-1-enyl]aminoamide, substituted | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 376 | Phenylphenylthioamine, substituted | Uncommon Atom (S, Br) | \_ | Not Included |
| 376-377 | Phenyl(phenylsulfonyl)-amine, substituted | Uncommon Atom (S, Cl, Br) | \_ | Not Included |
| 377 | Hydrazines, substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 377 | Bis(1,1-dimethyl-1-silaethyl)-amine | Uncommon Atom (Si) | \_ | Not Included |
| 377-378 | \_ | Uncommon Atom (Rh), Radical | \_ | Not Included |
| 378 | Anilines, mono-substituted | Uncommon Atom (F, Cl, Br, I) | \_ | Not Included |
| 379 | Anilines, mono-substituted | Uncommon Atom (F, S) | \_ | Not Included |
| 380 | Anilines, di-and trisubstituted | Uncommon Atom (F, Cl) | \_ | Not Included |
| 381 | Alkyloxy(2-nitrophenyl)amine | Duplicative Substances: N-alkoxyanilines in page 377 | Need refactoring | Not Included |
| 381 | N-phenylacetamide, substituted (#1) | Uncommon Atom (F, Cl, Br) | \_ | Not Included |
| 381 | N-phenylacetamide, substituted (#2) | Uncommon Atom (F, Cl, Br, I) | \_ | Not Included |
| 382 | Diethyl(phenylamino)-phosphino-1-one, substituted | Uncommon Atom (P, Cl, Br) | \_ | Not Included |
| 382 | 4-Phenylaminyl phenoxyl radical | Radical | \_ | Not Included |
| 382 | N,N’-diphenyl-1,4 phenylenediamine radical | Radical | \_ | Not Included |
| 382 | Phenyl(phenylsulfonyl)amine | Uncommon Atom (S) | \_ | Not Included |
| 383 | 2,2,2-Trifluoro-N-phenylacetamide | Uncommon Atom (F) | \_ | Not Included |
| 383 | Phenylphenylthioamine | Uncommon Atom (S) | \_ | Not Included |
| 383 | Phenyl(phenylamino) methane-1-thione | Uncommon Atom (S) | \_ | Not Included |
| 383 | Phenylhydrazine | Duplicative Result: hydrazines in page 377 but difference reference | Need refactoring | Included |
| 383 | Aminotriphenylphosphonium bromides | Uncommon Atom (Br), Ionic Atom | \_ | Not Included |
| 383 | Aniline phosphonium bromide, substituted | Uncommon Atom (P, Br), Ionic Atom | \_ | Not Included |
| 384 | Diphenylamine, substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 384 | Diphenylamine, substituted | Radical (O) | \_ | Not Included |
| 384 | Diphenylamine, substituted | Duplicate Result at tert-Bu | Need refactoring | Convert to 86.05 ± 0.05 |
| 385 | Diphenylamine, substituted | Uncommon Atom (Br) | \_ | Not Included |
| 385 | Naphthylphenylamine | Duplicative Result: 1-Naphthylamine in page 385 | Need refactoring | Convert to 84.25 ± 0.05 |
| 386 | p-Phenyl-endiamines, substituted (#4) | Duplicative Result: N,N’-di-2-naphthylp-phenylendiamine in page 386 but different reference | Need refactoring + Lack information (1-naphthyl or 2-naphthyl) | Not Included |
| 389 | Urazole, 4-substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 390 | 2-Piperidone, analogues | Uncommon Atom (S) | \_ | Not Included |
| 390 | 4-Pyridone, analogues | Uncommon Atom (S) | \_ | Not Included |
| 390 | 4-Pyridone, analogues | Uncommon Atom (S) | \_ | Not Included |
| 391 | 1,4-Dihydropyridine, substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 392 | 2-Quinolone, analogues | Uncommon Atom (S) | \_ | Not Included |
| 393 | Carbazole | Uncommon Atom (Br) | \_ | Not Included |
| 393 | Phenothiazine, analogues | Uncommon Atom (S, Se) | \_ | Not Included |
| 393 | Phenothioazine, substituted | Uncommon Atom (S) | \_ | Not Included |
| 394 | 2,6-Diaryl-4-phenyl-1,2,3,4-tetrahydro-sym-tetrazines | Uncommon Atom (Cl) | \_ | Not Included |
| 394 | FeII(H2bim) H2bimZ2,20-bi-imidazoline | Uncommon Atom (Fe) | \_ | Not Included |
| 395 | CoII(H2bim) H2bimZ2,20-bi-imidazoline | Uncommon Atom (Co) | \_ | Not Included |
| 395 | FeII(H2bip) H2bipZ2,20-bi(tetrahydro) pyrimidine | Uncommon Atom (Fe) | \_ | Not Included |
| 395 | [Rh(trop2NH)(bipy)]C tropZ5-H dibenzo[a,d]cycloheptene-5-yl | Uncommon Atom (Rh) | \_ | Not Included |
| 395 | Nitrogen anion | Ionic Atom | \_ | Not Included |
| 395 | Nitrogen cation | Ionic Atom | \_ | Not Included |
| 396 | Azide radical | Radical | \_ | Not Included |
| 396 | Azide cation | Ionic Atom | \_ | Not Included |
| 396 | Nitrogen dimer cation | Ionic Atom, Dimer | \_ | Not Included |
| 396 | Dinitrogen oxide | Ionic Atom | \_ | Not Included |
| 396 | Nitric oxide dimmer | Ionic Atom, Dimer | \_ | Not Included |
| 396 | Dinitrogen trioxide | Ionic Atom | \_ | Not Included |
| 396 | Dinitrogen tetroxide | Ionic Atom | \_ | Not Included |
| 396 | Diazene | Inconsistent BDE | \_ | Included |
| 397 | Dinitrogen difluororide (#1) | Uncommon Atom (F) | \_ | Not Included |
| 397 | Dinitrogen difluororide (#2) | Uncommon Atom (F) | \_ | Not Included |
| 397 | Tetrafluorohydrazine | Uncommon Atom (F) | \_ | Not Included |
| 398 | Nitroamine -> Nitrozoamines | Charged Bond (NO2) | \_ | Not Included |
| 399 | N-nitroso-acetanilides | Uncommon Atom (Cl) | \_ | Not Included |
| 399 | N-methyl-nitrosobenzenesul forn-amides, substituted | Uncommon Atom (S, Cl, Br) | \_ | Not Included |
| 400 | Amino-N-nitroso-N-phenylamide, substituted | Uncommon Atom (Cl, Br, I) | \_ | Not Included |
| 400 | Nitrosophenyl(phenylsolfonyl)-amine, substituted | Uncommon Atom (S, Cl) | \_ | Not Included |
| 400 | Diethyl(nitrosophenylamino)-phosphino-1-one, substituted | Uncommon Atom (P, Cl, Br) | \_ | Not Included |
| 401 | 3,6-Dibromo-9-nitrosocarbazole | Uncommon Atom (Br) | \_ | Not Included |
| 402 | Nitrosodiphenylamine, substituted | Uncommon Atom (Cl) | \_ | Not Included |
| 402-403 | Azide group | Ionic Atom (N) | \_ | Not Included |
| 403 | Azo-N,N-dioxides | Ionic Atom (N) | \_ | Not Included |
| 403 | Azobenzene-N,N-dioxides, substituted | Ionic Atom (N) | \_ | Not Included |
| 403 | CN radical | Radical | \_ | Not Included |
| 404 | Halogened cyanide | Uncommon Atom (F, Cl, Br, I) | \_ | Not Included |
| 404 | CH2N radicals | Radical | \_ | Not Included |
| 404 | CNN radicals | Radical | \_ | Not Included |
| 404 | Diazomethylene | Ionic Atom (N), Inconsistent BDE | Need refactoring | Not Included |
| 404 | Isocyanic acid | Inconsistent BDE, Lack reference | Need refactoring | Not Included |
| 404-405 | Azide group | Ionic Atom (N) | \_ | Not Included |
| 405-406 | Cyanide group | Ionic Atom (N, C) | \_ | Not Included |
| 406 | Nitroso-trifluoromethane | Ionic Atom (F) | \_ | Not Included |
| 406 | Nitroso-trichloromethane | Ionic Atom (Cl) | \_ | Not Included |
| 406 | 2-Chloro-2-nitrosopropane | Ionic Atom (Cl) | \_ | Not Included |
| 407-411 | Nitromethane -> 2-Nitrofuran | Charged bond |  |  |
| 407 | Nitroso-pentafluorobenzene | Ionic Atom (F) | \_ | Not Included |
| 407 | Nitromethyl radical | Radical | \_ | Not Included |
| 407 | 1,1-Dichloro-1-nitro-propane | Ionic Atom (Cl) | \_ | Not Included |
| 409 | Dinitrodifluoromethane | Ionic Atom (F) | \_ | Not Included |
| 410 | Trinitrofluoromethane | Ionic Atom (F) | \_ | Not Included |
| 410 | Trinitrochloromethane | Ionic Atom (Cl) | \_ | Not Included |
| 410 | Trinitrobromomethane | Ionic Atom (Br) | \_ | Not Included |
| 411 | 1,1,1,2,2-Pentanitrofluoroethane | Ionic Atom (F) | \_ | Not Included |
| 411 | Difluoro(trifluoromethyl)-amine | Ionic Atom (F) | \_ | Not Included |
| 411 | Tert-butyldifluoroamine | Ionic Atom (F) | \_ | Not Included |
| 411 | N,N-difluorobenzylamine | Ionic Atom (F) | \_ | Not Included |
| 411 | 2,2-Bis(difluoroamino) propane | Ionic Atom (F) | \_ | Not Included |
| 413 | a-Methylbenzylamine | Incorrect Structure | Need Refactoring: C6H5CH(CH3)-NH2 | Included by reference |
| 415 | 1-Methylpyrrile | Incorrect Name | Need Refactoring: 1-Methylpyrrole | Included by reference |
| 416 | Dimethyl phenylamine | Duplicative Result: 1-Naphthylamine in page 416 | Need refactoring | Merged as one |
| 416 | Dimethyl benzylamine | Duplicative Result: Benzyl dimethylamine in page 415 | Need refactoring | Merged as one |
| 416 | Azohexafluoroethane | Ionic Atom (F) | \_ | Not Included |
| 417 | N,N-dimethylformamide | Inconsistent BDE | \_ | Convert to 80 ± 1 |
| 418 | Bis(1,1-dimethyl-silaethyl)-methylamine | Uncommon Atom (Si) | \_ | Not Included |
| 419 | Methanisothiocyanate | Ionic Atom (S) | \_ | Not Included |
| 419 | \_ | Ionic Atom (F, S) | \_ | Not Included |
| 419 | \_ | Radical | \_ | Not Included |
| 419 | \_ | Ionic Atom (F) | \_ | Not Included |
| 419 | \_ | Ionic Atom (N) | \_ | Not Included |

Note

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Page** | **Molecule / Name** | **Issue(s)** | **How to Resolve** | **Our Solution** |
| 166 | Cyclo-hexane | Ring-Bond | \_ | Included |
| 166 | Tetralin | Ring-Bond | \_ | Included |
| 320 | Ascaeidole | Ring-bond  Incorrect Name | Need refactoring: Ascaridole | Included |
| 320 | DPA-O2 | Ring-bond | \_ | Included |
| 320 | DMA-O2 | Ring-bond | \_ | Included |
| 320 | Artemisinin | Ring-bond | \_ | Included |
| 344 | 2H-3,4-Dihydropyran | Ring-bond | \_ | Included |
| 344 | 2,3-Dihydro-1,4-dioxin | Ring-bond | \_ | Included |
| 344 | Chromane | Ring-bond | \_ | Included |
| 344 | 2,3-Dihydro-1,4-benzodioxin | Ring-bond | \_ | Included |

Cause: There is a gap in BDE values ranging from around 0.5 kcal/mol to 1.5 kcal/mol (some can be 2.0 kcal/mol) between version 2002 and 2007. Those results are mainly derived from 1986 PED/NAY (small), 1994PED (large), and 2002CRC (small). Several results have been adjusted based on another issue such as numerical precision.

Need Refactoring: Since the change is minor, and the result can be affected due to the update of several conversion constants and could be calculated, we only add the result in version 2007 (whose BDE is relatively larger than itself in version 2002).

Suggestion

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Page** | **Molecule / Name** | **Issue(s)** | **How to Resolve** | **Our Solution** |
| 160 | Cyclo-pentene, 3-methyl | Just a note (by PubChem) | Use this name: 3-Methyl-1-cyclopentene: | CC1C=CCC1 |
| 161 | 3-Cyclo-pentylpropene | Just a note (by PubChem) | \_ | C=CCC1CCCC1 |
| 161 | Vinyl-cyclo-hexane | Just a note (by PubChem) | \_ | C=CC1CCCCC1 |
| 182 | Hexanal | We are lacking this | \_ | \_ |
| 188 | Naphthlene-1-carboxylic acid | \_ | Use this name: 1-Naphthoic acid | \_ |
| 189 | Naphthlene-2-carboxylic acid | \_ | Use this name: 2-Naphthoic acid | \_ |
| 199 | 2-(2-pyridyl)pyridine | This may contain cis-trans isomer (chirality) | \_ | \_ |
|  |  |  |  |  |

**Considering substance**

**R-group Substances**:

* Several molecules replace some substructures with the keyword “R” to denote specific-generalized structure that is not listed out such as alkyl hydroperoxides (page 268), and hydroperoxides (#1, page 271), hydroperoxides (#2, page 271). Most of them are the ‘alkyl’ group: sequences of ‘-CH2-’. In this situation, we would replace these groups: -CH3 (1 group), -C2H5 (1 group), -C3H7 (2 groups), -C4H9 (4 groups), -C5H11 (8 groups), and -C6H13 (1 group), which are 17 total functional groups by order
* Those structures are in the following table:

|  |  |  |
| --- | --- | --- |
| **Page** | **Molecule / Name** | **Note** |
| 268 | alkyl hydroperoxides | \_ |
| 271 | hydroperoxides | #1 |
| 271 | hydroperoxides | #2 |
| 312 | Alkyl hydroperoxide | \_ |
| 350 | Alkyl nitrite | \_ |
| 350 | Alkyl nitrate | Charged Bond |