**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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# **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 | 1 Connected Structure Only | \_ | NOT Included |
| 30 | 3-Phenykl-Allyl Triphenyl Phosphonium, Bromide | 1 Connected Structure Only | \_ | 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 |
| 43 | Toluene bromide | 1 Connected Structure Only | \_ | NOT Included |
| 44 | Cationic niobium | Uncommon Atom (Nb) | \_ | NOT Included |
| 46 | 1,1-Diphenylethane | Uncertain molecule representation | Need refactoring | Included but as |
| 46 | Thiphenylmethane | Invalid Name | Triphenylmethane | Included |
| 50 | 2-Naphthyl radical | Radical | \_ | NOT Included |
| 51 | 4,5-Methylene-phenathrene | Invalid Name | 1-methyl-2-(2-methylphenyl)benzene | Included |
| 55 | Fluorenes, substituted  X = | Invalid Functional Group (Checked on 1992ZHA/BOR). All values are similar | 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  Me3SiCH2, SiMe3, SiEt3, SiPh3 | Uncommon Atom (Si) | \_ | NOT Included |
| 55 | Fluorenes, substituted  Me3N+Cl-, PyN+Br-, Ph3P+Br-, nBu3P+Br- | Ionic Atom, 1 Connected Structure Only | \_ | 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), 1 Connected Structure Only | \_ | 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 |
| 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 | 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 |
| 68 | Chloroethylene | Uncertain BDE | \_ | NOT Included |
| 73 | Ethane-1,1-diol | Uncertain BDE | \_ | Included |
| 75 | Cyclo-hexyl methyl ether | Inconsistent Representation | Need refactoring with this Information (**H**-C-O) | 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-MeC(O)O | Unclear Representation | Need refactoring as MeC(=O)**O** or 4-**O**C(=O)Me | Included as C(=O)OC |
| 79 | 2-Alkyl-2HK3,4,5,6-tetra-hydropyrans: C6H11 | Lack of Information. Same information in the Original Paper | Need refactoring. Assumed to be C6H13 | 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 | 1 Connected Structure Only | \_ | 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 |
| 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 |
| 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 | 1 Connected Structure Only | \_ | NOT Included |
| 105 | Fluorenyl trimethylammonium bromide | 1 Connected Structure Only | \_ | NOT Included |
| 105 | Benzyl trimethylammonium | 1 Connected Structure Only | \_ | NOT 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 | 1 Connected Structure Only | \_ | NOT Included |
| 108 | 1-Acetonitrile pyridinium chloride | 1 Connected Structure Only | \_ | 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 | 1 Connected Structure Only | \_ | NOT Included |
| 120 | Ethyl-2-aminoacetate | Unclear BDE | Need refactoring | Convert to 81.0 ± 2 |
| 122 | 1,3-Oxazolidines, substituted (#2) | Incorrect structure representation | Need refactoring: R – C whose neighbors are O and N | Included |
| 127 | Adduct of BH3 and S(CH3)2 | Uncommon Atom (B) | \_ | NOT Included |
| 131 | 2,2,2-Trimethyl-1-(phenylfonyl)-2-silaethane | Uncommon Atom (Si) | \_ | NOT Included |
| 131 | 2,2,2-Triphenyl-1-(phenylfonyl)-2-silaethane | Uncommon Atom (Si) | \_ | NOT Included |
| 131 | Methyl N-(p-tolylsulfonyl) phenyloxosulfoximes (#2) | Uncommon Atom (Si) | \_ | NOT Included |
| 131 | 2,2-Dimethyl-1-(phenylsulfonyl)-2-sila-vinylpropane | Incorrect Structure and Name | Need refactoring | NOT Included |
| 131 | Benzyl dimethylsulfonium bromide | 1 Connected Structure Only | \_ | NOT Included |
| 131 | Benzyl dibutylsulfonium bromide | 1 Connected Structure Only | \_ | NOT Included |
| 131 | Phenyl methylene ketone dibutylsulfonium bromide | 1 Connected Structure Only | \_ | NOT Included |
| 131 | Benzyl dibutylsulfonium, substituted | Incorrect Name | Need refactoring: Benzyl dimethylsulfonium, substituted | Included |
| 132 | Benzyl dibutylsulfonium, substituted: p-MCO2 | Incorrect Functional Group: p-C(=O)OMe | Need refactoring | 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), Incorrect Method (SPST not SPTS) | 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) |
| 175 | 1,2-Dichlorobutane | Incorrect Name | Need refactoring: 1,3-Dichlorobutane | Included by Structure: Not reliable |
| 175 | 2-Chloro-3-methyl-butane | Incorrect Name | Need refactoring: 1-Chloro-3-methyl-butane | Included by Structure |
| 175 | 1-Bromohexane | Incorrect Name | Need refactoring: 1-Chlorohexane | Included by Structure: Not reliable |
| 175 | 2-Chlorohexane | Incorrect Name | Need refactoring: 1-Chlorohexane | Included by Structure: Not reliable |
| 184 | Chloroacetone | Incorrect Structure | Need refactoring | Included by Name |
| 187 | Propenoic acid | Uncertain result | Need refactoring | Convert to 100.0 ± 2 |
| 191 | Radical dimer | \_ | \_ | Not Included (No physical bond) |
| 192 | 2-Butynedinitrile | Incorrect Structure or Name ? | Need refactoring | Included by Structure |
| 196 | Diphenyl-CN-methyl dimer | \_ | \_ | Not Included (No physical bond) |
| 196 | Pyridine, substituted (#1) | Redundant & Undefined Text (HO(O)C-pyridyl) | \_ | Ignored. Broken bond: R-pyridine |
| 196, 197 | Pyridine, substituted (#2)  Pyridine, substituted (#3)  Pyrazines, substituted | 1) These result from SIL/MIR are built from crystal structure, which is out-of-scope  2) Incorrect Citation: 2000 SIL/MIR cannot be found in the reference | 1) Need refactoring  2) Need Extra Information; Is that 2005 SIL/MIR? | Not Included (Ignored) |
| 202 | Nitrozoamines (#4) | Incorrect Structure: Lack of “C” | Need refactoring: **(…)C**-CH2CH2N | Included |
| 203 | Nitrofluoroethanes | Incorrect Structure: Lack of “C” | Need refactoring: FC(NO2)2 | Included |
| 203 | Coenzyme B12, substituted | Uncommon Atom (Co, I) | \_ | Not Included |
| 213 | Fluoroiodomethane | Inconsistent BDE | Need refactoring | Included as Normal |
| 216-217 | F-C60 to F–C\*(O)CH2 | Radical | \_ | Not Included |
| 220 | Chloroiodomethane | Inconsistent BDE | Need refactoring | Included as Normal |
| 223 | 3-Chloro-1-propyne | Incorrect Structure | Need refactoring: Cl-CH2C#CH | Not Included |
| 224 | 4-Chlorobutene | Incorrect Structure (Similar Result at 4-Chloro-but-1-ene, page 225) | Need refactoring | Not Included |
| 227 | Chlorocyclohexane | Duplicated result at same reference at page 226 | Need refactoring | Not Included |
| 232-233 | Cl–C to Cl–C\*(O) | Radical | \_ | Not Included |
| 235, 236 | (Z)-1,2-dibromoethylene  (E)-1,2-dibromoethylene | Inconsistent BDE | Need refactoring | Included |
| 240 | Bromopentafluorobenzene | Inconsistent BDE | Need refactoring | Included |
| 240 | (1-Bromovinyl)benzene | Incorrect Structure | Need refactoring: CH2=C(Br)Ph | Included |
| 243 | Br-C to Br–CH2C\*HCH3 | Radical | \_ | Not Included |
| 244 | Difluorodiiodomethane | Inconsistent BDE | Need refactoring | Included |
| 250 | Pentafluoroiodobenzene | Inconsistent BDE | Need refactoring | Noy Included |
| 253 | I–C to I-CH2 | Radical | \_ | Not Included |
| 255 | Water, Oxygen deuteride, Oxygen tritide | Radical | \_ | Not Included |
| 257 | 1-Propanol | Inconsistent BDE | Need refactoring | Included |
| 257 | 2-Propanol | Inconsistent BDE | Need refactoring | 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: DOI: 10.1002/kin.20035 | Need refactoring: Isofulminic acid | Included |
| 261 | HOS radical | Uncommon Atom (S), Radical | \_ | Not Included |
| 261 | HOP radical | Uncommon Atom (P), Radical | \_ | Not Included |
| 261 | 2,2-Dimethylsilaethanol | Uncommon Atom (Si) | \_ | Not Included |
| 265 | Nicotinic acid, substituted | Incorrect Structure | Need refactoring: 3-N not 4-N | Included by reference |
| 266 | Hydroperoxy radical | Radical | \_ | Not Included |
| 273 | Norcamphor, oximes | \_ | \_ | Included base state: ON=C1C-C2CCC1C2 |
| 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 |
| 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 |
| 280 | 2,5-Dihydrioimidazole, substituted | Incorrect Core:  ON1C(C)(C)N(=O)=CC1(C)C | Need Refactoring | Included by the fix |
| 280 | Methanesulphovinates, substituted | 1 Connected Structure Only  Incorrect Reference: DOI: 10.1007/s10975-005-0140-6 | \_ | Not Included |
| 281 | Piperdin-1-ol | Inconsistent Name | \_ | Included by Structure |
| 283 | N-Hydroxyphthalimide (NHPI) | Inconsistent BDE | \_ | Included |
| 285 | Organomecury species | Uncommon Atom (Hg, Cl) | \_ | Not Included |
| 285 | Phenol | Swap the position in Sol. And Gas. | \_ | Included |
| 286 | Phenols, substituted | Incorrect Citation: 2004COR/GUF | Need refactoring: 2004COR/GUE | Followed |
| 288 - 289 | Phenols, substituted | Ionic Atom (O-) and Radical (O\*) | \_ | 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 |
| 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 |
| 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 (Se, Te) | \_ | Not Included |
| 296 | Tetrahydroquinoline, substituted | Base structure is not well-drawn | Need refactoring | Included |
| 299 | Phenols, substituted (p-RS) | Unclear Functional: The original is probucol | Need refactoring | Included |
| 301 | Methane, substituted | Incorrect Structure | \_ | 2,4: Included  3,5: Build a reverse |
| 302 | Silane, substituted | Uncommon Atom (Si) | \_ | Not Included |
| 303 | 4-((4-Hydroxyphenylthio)-methylthio)phenyl, substituted | Duplicated Result at page 299 (phenol, substituted: p-RS) | Need refactoring | Included & Remove at page 299 |
| 303 | 4-((4-Hydroxyphenylthio)-methylthio)phenyl, substituted | Unclear Drawn Structure | Need refactoring | Included |
| 304 | Galvinol | Unclear Drawn Structure | Need refactoring | Included |
| 304 | Silicoorganics | Uncommon Atom (Si) | \_ | Not Included |
| 305 | 4-Hydroxydiphenylaminyl radical | Radical | \_ | Not Included |
| 309 | Oxygen anion | Radical | \_ | Included |
| 310 | Hydroperoxy radical | Radical | \_ | Not Included |
| 310 | Dioxygen fluoride radical | Radical | \_ | Not Included |
| 310 | Dioxygen bromide radical | Radical | \_ | 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 | Alkyl hydroperoxide | Inconsistent BDE | \_ | Included as 45 ± 1 |
| 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 | Chlorofluorotrioxide | Radical | \_ | Not Included |
| 316 | Chlorotrioxide | Radical | \_ | Not Included |
| 316 | Tetrahydrofuran-2-yl-peroxy | Radical | \_ | Not Included |
| 316 | Dioxan-2-yl-peroxy | Radical | \_ | Not Included |
| 319 | Peroxydisulfuryl difluoride | Inconsistent BDE | \_ | Convert to 23.0 ± 1 |
| 320 | Flavins | Ring-bond, Unclear BDE | \_ | Not Included |
| 321 | Trifluoromethanol | Inconsistent BDE | \_ | Included |
| 326 | 1-Chloroethyl methyl ether | Duplicate Result in page 325 | Need refactoring: Remove result in page 325 | Convert to 88.5 ± 1.75 |
| 326 | 1-Chloroethyl ethyl ether | Incorrect Name | Need refactoring | Included by structure |
| 331 | 1-[(4-Benzolphenoxy)methyl]-naphthalene | Inconsistent BDE | \_ | Included |
| 336 | Acetic acid phenyl ester | ~ Phenyl acetate | \_ | Included |
| 338 - 341 | Peroxy | Radical | \_ | Not Included |
| 338 | Methyl peroxy | Inconsistent BDE, Radical | \_ | Not Included |
| 342 | Methanisocynate | Inconsistent Name | Need refactoring: Methan isocyanate | Included |
| 342 | Trifluoromethyl hypochlorite | Inconsistent BDE | \_ | 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 | Tungsten alkoxide | Uncommon Atom (W) | \_ | Not Included |
| 347 | CF3O–CO2 | Closed-shell molecules (not radical) | Need refactoring | Included |
| 347 | Nitric oxide | Radical | \_ | Not Included |
| 347 | Nitrogen dioxide | Radical | \_ | Not Included |
| 348 | Nitric oxide dimer | Dimer | \_ | Not Included (No physical bond) |
| 348 | Nitrosyl hydride | Incorrect Structure | Need refactoring: O-NH | Included |
| 349 | Iodomonitrooxy | Inconsistent BDE | \_ | Convert to 27.5 ± 4.8 and 24.0 ± 1 |
| 353 | Nitromethyl radical | Radical | \_ | Not Included |
| 357 | 2,3-Diazabicyclo[2.2.1]-hept-2-ene N-oxide | Duplication Result in Page 355 | Need Refactoring | Included |
| 358 | 2-Amino-3-quinoixalinecarbonitrile-1,4-dioxide (#1 and #2) | \_ | \_ | Combined with mean and range |
| 360 | Oxythio radical | Radical | \_ | Not Included |
| 363 | Methylthio peroxy | Radical | \_ | Not Included |
| 364 | Adduct | Inconsistent BDE | \_ | Convert to 14 ± 1 |
| 364 | Methylthiyl peroxy | Radical | \_ | Not Included |
| 364 | N,N-difluorohydroxylamine O-Fluorosulfate | Inconsistent BDE | \_ | Convert to 65 ± 1 |
| 365 | Difluorine monoxide (#2) | Radical | \_ | Not Included |
| 365 | Methyl hypofluorite | Inconsistent BDE | \_ | Included |
| 365 | Fluoro peroxy | Radical | \_ | Not Included |
| 365 | Fluorine dioxide | Radical | \_ | Not Included |
| 366 | Dichlorine monoxide (#2) | Radical | \_ | Not Included |
| 366 | Trifluoromethyl hypochlorite | Inconsistent BDE | \_ | Included |
| 366 | Chloro peroxy | Radical | \_ | Not Included |
| 366 | Chlorine dioxide | Radical | \_ | Not Included |
| 367 | Chloro trioxide | Radical | \_ | Not Included |
| 367 | Chloro trioxide | Radical | \_ | Not Included |
| 367 | Dibromine oxide | Radical | \_ | Not Included |
| 367 | Bromine dioxide | Radical | \_ | Not Included |
| 367 | Bromo peroxy | Radical | \_ | Not Included |
| 367 | Bromo trioxide | Radical | \_ | Not Included |
| 368 | Diiodo oxide | Radical | \_ | Not Included |
| 368 | Iodo peroxy | Radical | \_ | Not Included |
| 368 | Iodo rioxide | Typo, Radical | Need refactoring | Not Included |
| 369 | Ammonia | Radical | \_ | Not Included |
| 369 | Deuterated ammonias | Radical | \_ | Not Included |
| 370 | Hydrazoic acid | Inconsistent BDE | \_ | Included |
| 370 | Isocyanic acid | Inconsistent BDE | \_ | Included |
| 370 | Iso-thiocyanic acid | Inconsistent BDE | \_ | Included |
| 370 | Cyanoamino radical | Radical | \_ | Not Included |
| 370 | Methylamine | Inconsistent BDE | \_ | Included |
| 371 | Propylamine phosphonium bromide | 1 Connected Structure Only | \_ | Not Included |
| 371 | Hydrazine radical | Radical | \_ | Not Included |
| 372 | Methylhydrazine radical | Radical | \_ | Not Included |
| 372 | Amonomethanenitrile | Incorrect Name | Need refactoring: Cyanamide | Included |
| 373 | Hydroxylamine | Inconsistent BDE | \_ | Convert to 81.5 ± 0.5 |
| 373 | 2-Ethyl-pentanamide | Incorrect Name | Need refactoring: 2,2-diethylbutanamide | Included |
| 376 | Phenylphenylthioamine, substituted | Uncommon Atom (S, Br) | \_ | Not Included |
| 377 | Bis(1,1-dimethyl-1-silaethyl)-amine | Uncommon Atom (Si) | \_ | Not Included |
| 377-378 | \_ | Uncommon Atom (Rh), Radical | \_ | Not Included |
| 381 | Alkyloxy(2-nitrophenyl)amine | Duplicative Substances: N-alkoxyanilines in page 377 | Need refactoring | Not Included |
| 382 | 4-Phenylaminyl phenoxyl radical | Radical | \_ | Not Included |
| 382 | N,N’-diphenyl-1,4 phenylenediamine radical | Radical | \_ | Not Included |
| 383 | Phenylhydrazine | Duplicative Result: hydrazines in page 377 but difference reference | Need refactoring | Included |
| 383 | Aminotriphenylphosphonium bromides | 1 Connected Structure Only | \_ | Not Included |
| 383 | Aniline phosphonium bromide, substituted | 1 Connected Structure Only | \_ | Not Included |
| 384 | Diphenylamine, substituted | Radical (O) | \_ | Not Included |
| 384 | Diphenylamine, substituted | Duplicate Result at tert-Bu and Incorrect Citation (86.4) | Need refactoring | Convert to 86.05 ± 0.05 |
| 385 | Naphthylphenylamine | Duplicative Result: 1-Naphthylamine (#2) 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 |
| 393 | Phenothiazine, analogues | Uncommon Atom (Se) | \_ | 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 |
| 396 | Azide radical | Radical | \_ | Not Included |
| 396 | Azide cation | Invalid Structure | \_ | Not Included |
| 396 | Nitrogen dimer cation | Ionic Atom, Dimer | \_ | Not Included |
| 396 | Nitric oxide dimmer | Ionic Atom, Dimer | \_ | Not Included |
| 396 | Diazene | Inconsistent BDE | \_ | Included |
| 398-399 | Nitrozoamines (#1 & #6) | Duplication | Need refactoring | Convert to 39.5 ± 0.5 |
| 399 | N-methyl-nitrosobenzenesul forn-amides, substituted | Incorrect Citation: 2005: ZHU/HAO | Need refactoring | Included |
| 399 | N-methyl-nitrosobenzenesul forn-amides, substituted | Incorrect Functional Group: 2,5-2-Cl2 | Need refactoring: 2,5-Cl2 | Included |
| 402 | Hydrogen azide | Duplicated Structure in page 396 but different source | \_ | 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 | Inconsistent BDE | Need refactoring | Included |
| 404 | Isocyanic acid | Inconsistent BDE | Need refactoring | Not Included \* |
| 407 | Nitromethyl radical | Radical | \_ | Not Included |
| 411 | 1,1,1,2,2-Pentanitrofluoroethane | Incorrect Structure | Need refactoring: (NO2)2(F)CC(NO2)2-NO2 | Included |
| 411 | 2,2-Bis(difluoroamino) propane | Inconsistent BDE | \_ | Convert to 47 ± 1 |
| 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 |
| 417 | N,N-dimethylformamide | Inconsistent BDE | \_ | Convert to 80 ± 1 |
| 418 | Bis(1,1-dimethyl-silaethyl)-methylamine | Uncommon Atom (Si) | \_ | Not Included |
| 419 | \_ | Radical | \_ | Not Included |
| 419 | \_ | Radical | \_ | Not Included |
| **420** | **Thiazyl** | **Radical** | **\_** | **Not Included** |
| 420 | (Triaryl)nitrosothio | Uncommon Atom (Ar) | \_ | Not Included |
| 421 | Phenylphenylthiodiazene | Incorrect Highlight | Need refactoring | Included |
| 421 | Thiazyl fluoride | Too wide range | Need refactoring | Not Included |
| 421 | Thiocyanogen | Incorrect Structure and Bond | Need refactoring | Not Included |
| 421 | Bis(fluorosulfuryl)fluoramine | Incorrect Structure | Need refactoring: (FSO2)2–NF | Included |
|  |  |  |  |  |
| 422 | Nitrogen trifluoride (#2, #3) | Radical | \_ | Not Included |
| 422 | Nitrogen monochloride | Radical | \_ | Not Included |
| 422 | Nitrogen chlorofluoride | Inconsistent BDE | \_ | Convert to 32 ± 1 |
| 423 | Nitrogen monobromide | Radical | \_ | Not Included |
| 423 | Nitrogen iodide | Radical | \_ | Not Included |
| 425 | Mercapto radical | Radical | \_ | Not Included |
| 425 | Hydrogen sulfide-d2 | Inconsistent BDE, Isotope | Need refactoring | Included |
| 425 | Mercapto radical-d | Radical, Isotope | \_ | Not Included |
| 426 | Methylthiol (#2) | Isotope | \_ | Not Included |
| 428 | Oxythio radical | Radical | \_ | Not Included |
| 429 | Methylsulfone | Inconsistent BDE | Need refactoring | Included |
| 430 | Thio-a-tocopherol | Apply Structure in page 294 and PubChem (Vitamin E, CID 14985) | \_ | Included |
| 430 | Hydrogen disulfide radicals | Radical | \_ | Not Included |
| 431 | Thiocynic acid | Inconsistent BDE | Need refactoring | Included |
| 431 | \_ | Radical | \_ | Not Included |
| 432 | Difluoro disulfur | Inconsistent BDE | Need refactoring | Included |
| 432 | Dichlorodisulfane (#1) | Inconsistent BDE | Need refactoring | Not Included |
| 432 | Chlorodisulfane (#1) | Inconsistent BDE | Need refactoring | Not Included |
| 433 | Chlorodisulfane | Radical | \_ | Not Included |
| 435 | Hydro disulphide radicals -> Alkyl tetrasulphide radicals | Radical | \_ | Not Included |
| 435 | Dialkyl disulfide ions | Dimer-Radical Ionic Bond  Undeterministic Ionic Atom  Incorrect Structure: DOI 10.1016/S1387-3806(98)14072-1 | Need refactoring: R2S-SR2 | Not Included |
| 435 | Tetradialkyl disulfide ions (#4) | Undeterministic Ionic Atom | Need refactoring | Not Included |
| 436 | Methylthio radical | Radical | \_ | Not Included |
| 442 | Methyl sulphone radical | Radical | \_ | Not Included |
| 444 | Full page 444 | Radical | \_ | Not Included |
| 445 | Sulfur hexafluoride anion | Undeterministic Ionic Atom | Need refactoring | Not Included |
| 445 | Full page 444 | Radical | \_ | Not Included |
| 446 | Trimethyl sulfur pentafluoride | Inconsistent BDE | Need refactoring | Included |
| 446 | Trimethyl sulfur trifluoride | Inconsistent BDE | Need refactoring | Included |
| 446 | Sulfuryl fluorides | Too wide range (1958REE/DIB) | Need refactoring | Not Included |
| 447 | Sulfur dichlorides (#2) | Inconsistent BDE | Need refactoring | Included |
| 447 | Sulfur tetrafluoro chloride | Inconsistent BDE | Need refactoring | Included |
| 447 | Sulfur pentafluoro chloride | Inconsistent BDE | Need refactoring | Included |
| 447 | Thionyl chloride | Inconsistent BDE | Need refactoring | Included |
| 448 | Sulfuryl chlorides | Inconsistent BDE | Need refactoring | Included |
| 448 | Chloropropylsulfone | Incorrect Structure | Need refactoring: Cl-SO2C3H7 | Included |
| 449 | Sulfur pentafluoro bromide | Inconsistent BDE | Need refactoring | Included |
| 449 | Adduct | Inconsistent BDE | Need refactoring | Convert to 14 ± 1 |
| 481 | Radicals | Radical | \_ | Not Included |
| 482 | Phosphorus clusters | Clusters | \_ | Not Included |
| 483 | Phosphorus fluorides (#2, #3) | Radical | \_ | Not Included |
| 483 | Phosphorus chlorides (#1) | Inconsistent BDE | Need refactoring | Not Included |
| 483 | Phosphorus chlorides (#2, #3) | Radical | \_ | Not Included |
| 483 | Phosphorus bromides | Inconsistent BDE | \_ | Included |
| 483 | Phosphorus bromides | Radical | \_ | Not Included |
|  | Carbon phosphide | Radical \_ Not Included |  |  |
| 484 | Silicon phosphide | Uncommon Atom (Si) | \_ | Not Included |
| 484 | Phosphino silane | Uncommon Atom (Si) | \_ | Not Included |
| 485-486 | Trifluorophosphino-1-Thione -> Triphenylphosphino-1-thione | Duplication Result in page 449-450 (S-P) | \_ | Not Included |
| 493-496 | H-based | Incompatible with electron configuration or not 1 Connected Structure Only | \_ | 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 value 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 result are mainly derived from 1986 PED/NAY (small), 1994PED (large), 2002CRC (small). Several results have been adjusted based on other 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) | \_ | \_ |

**R-group Substances**:

Several molecules replace some substructures by keyword “R” to denotes specific-generalized structure that is not listed out such as alkyl hydroperoxides (page 268), hydroperoxides (#1, page 271), hydroperoxides (#2, page 271).

* Most of them are the ‘alkyl’ group: sequences of ‘-CH2-’. In this situation, we would replace by these groups: -CH3 (1 group), -C2H5 (1 group), and -C3H7 (2 groups).
* For the sulfur-chain, such as hydrogen polysulfide, hydrogen alkyl polysulfide, dialkyl polysulfide, and alkyl ethyl poly sulfide, we ensure that only at most eight sulfur atoms maximum, regardless of structure to guarantee the “localization” sphere

Those structures are 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 | \_ |
| 427 | Alkyl thiol | \_ |
| 430 | Hydrogen alkyl disulfide | \_ |
| 431 | Hydrogen polysulfide | \_ |
| 431 | Hydrogen alkyl polysulfide | \_ |
| 432 | Alkyl hydrodifulfide | \_ |
| 433 | Dialkyl disulphide | \_ |
| 434 | Alkyl hydrotrisulfide | \_ |
| 434 | Dialkyl tetrasulfide | \_ |
| 435 | Dialkyl polysulfide | \_ |
| 442 | Alkyl ethyl disulfide | \_ |
| 442 | Alkyl phenyl disulfide | \_ |
| 442 | Alkyl ethyl polysulfide | \_ |
|  |  |  |