Supplementary Materials
for
Nonorthogonal Tight-Binding Model with
H–C–N–O Parameterization

Mikhail M. Maslov, Alexei I. Podlivaev, Konstantin P. Katin

National Research Nuclear University “MEPhI”,
Kashirskoe sh. 31, Moscow 115409, Russia
Research Institute for the Development of Scientific and Educational Potential of Youth,
Aviatorov str. 14/55, Moscow 119620, Russia

Correspondence to: Mikhail M. Maslov (E-mail: Mike.Maslov@gmail.com)
Table S1. The binding energies (eV/atom) for various \( \text{H}_2\text{C}_n\text{N}_m\text{O}_k \) molecules calculated within the NTBM1 model along with the corresponding experimental values and the values calculated using AM1/PM3/PM7 and the set of the model parameters from Ref. [Zhao J, Lu JP. Phys. Lett. A. 2003;319:523-529.]. The experimental and AM1/PM3 values are taken from the original PM3 work [Stewart JJP. J. Comp. Chem. 1989;10:221-264.]. The AM1/PM3 binding energies for the carbon dimer, imidogene and \( C_{60} \) fullerene are obtained using GAMESS program package [Schmidt MW, Baldridge KK, Boatz JA, Elbert ST, Gordon MS, Jensen JH, Koseki S, Matsunaga N, Nguyen KA, Su SJ, Windus TL, Dupuis M, Montgomery JA. J. Comp. Chem. 1993;14:1347-1363.]. The PM7 binding energies are obtained using MOPAC2012 [Stewart JJP, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2012).], and experimental values for \( C_2 \) and \( C_{60} \) are taken from NIST database [Computational Chemistry Comparison and Benchmark DataBase http://cccbdb.nist.gov/].

| Formula | Name                  | Exper. | PM3      | PM7      | AM1      | Zhao-Lu | Present work |
|---------|-----------------------|--------|----------|----------|----------|---------|--------------|
| 1       | Hydrogen              | 2.240  | 2.530    | 2.934    | 2.353    | 2.421   | 2.364        |
| CH      | Methylidyne           | 1.721  | 1.625    | 1.791    | 1.664    | 1.903   | 1.816        |
| CH₂     | Methylene, triplet    | 2.618  | 2.859    | 2.813    | 2.784    | 2.801   | 2.690        |
| CH₃     | Methyl radical        | 3.147  | 3.201    | 3.221    | 3.185    | 3.336   | 3.145        |
| CH₄     | Methane               | 3.422  | 3.380    | 3.392    | 3.344    | 3.664   | 3.339        |
| C₂      | Carbon, dimer         | 3.120  | 1.778    | 3.043    | 2.688    | 5.575   | 3.090        |
| C₂H₂    | Acetylene             | 4.221  | 4.259    | 4.189    | 4.214    | 4.838   | 4.483        |
| C₂H₃    | Vinyl                 | 3.778  | 3.832    | 3.792    | 3.733    | 4.021   | 3.838        |
| C₂H₄    | Ethylene              | 3.863  | 3.832    | 3.852    | 3.834    | 4.169   | 3.900        |
| C₂H₅    | Methylmethylene       | 3.300  | 3.312    | 3.382    | 3.318    | 3.570   | 3.433        |
| C₂H₆    | Ethyl                 | 3.553  | 3.600    | 3.603    | 3.595    | 3.738   | 3.557        |
| C₂H₇    | Ethane                | 3.634  | 3.622    | 3.623    | 3.618    | 3.872   | 3.602        |
| C₃      | Carbon, trimer        | 4.544  | 4.390    | 4.744    | 4.307    | 5.015   | 4.663        |
| C₂H₄    | Allene                | 4.159  | 4.150    | 4.213    | 4.156    | 4.526   | 4.265        |
| C₂H₅    | Cyclopropene          | 4.031  | 4.019    | 4.050    | 3.978    | 4.191   | 3.937        |
| C₂H₆    | Propyne               | 4.166  | 4.192    | 4.156    | 4.173    | 4.587   | 4.292        |
| C₂H₇    | Allyl                 | 3.949  | 3.952    | 3.996    | 3.957    | 4.188   | 3.994        |
| C₂H₈    | Cyclopropane          | 3.891  | 3.874    | 3.894    | 3.867    | 4.036   | 3.805        |
| C₂H₉    | Propene               | 3.929  | 3.921    | 3.932    | 3.920    | 4.179   | 3.933        |
| C₃H₃    | i-Propyl radical      | 3.708  | 3.757    | 3.756    | 3.751    | 3.888   | 3.701        |
| C₃H₄    | Propane               | 3.739  | 3.734    | 3.732    | 3.737    | 3.957   | 3.707        |
| C₃H₅    | 1-Methylcycloprop-1-ene| 4.042  | 4.046    | 4.064    | 4.014    | 4.200   | 3.969        |
| C₃H₆    | Bicyclobutane         | 4.070  | 3.995    | 4.010    | 3.956    | 4.092   | 3.881        |
| C₃H₇    | 1,2-Butadiene         | 4.126  | 4.130    | 4.169    | 4.134    | 4.427   | 4.186        |
| C₃H₈    | 1-Butyne              | 4.123  | 4.140    | 4.114    | 4.132    | 4.465   | 4.201        |
| C₃H₉    | 2-Butyne              | 4.144  | 4.165    | 4.141    | 4.156    | 4.484   | 4.216        |
| C₄H₈    | Cyclobutene           | 4.132  | 4.131    | 4.133    | 4.096    | 4.250   | 4.059        |
| C₄H₉    | Methylene-cyclopropane| 4.087  | 4.102    | 4.129    | 4.088    | 4.269   | 4.052        |
| C₄H₁₀   | 1,3-Butadiene         | 4.182  | 4.160    | 4.177    | 4.165    | 4.436   | 4.206        |
| C₄H₁₁   | 1-Butene              | 3.953  | 3.946    | 3.953    | 3.951    | 4.180   | 3.947        |
| 1   | 2                              | 3     | 4     | 5     | 6     | 7     | 8     |
|-----|--------------------------------|-------|-------|-------|-------|-------|-------|
| C₂H₆ | cis-2-Butene                   | 3.959 | 3.961 | 3.967 | 3.960 | 4.182 | 3.892 |
| C₂H₆ | Cyclobutane                    | 3.928 | 3.966 | 3.960 | 3.956 | 4.079 | 3.936 |
| C₃H₆ | Isobutane                      | 3.968 | 3.964 | 3.973 | 3.956 | 4.176 | 3.948 |
| C₃H₆ | trans-2-Butene                 | 3.963 | 3.966 | 3.970 | 3.964 | 4.182 | 3.765 |
| C₃H₈ | Isobutyl                       | 3.805 | 3.840 | 3.835 | 3.830 | 3.960 | 3.767 |
| C₅H₁₀ | n-Butane                       | 3.802 | 3.798 | 3.795 | 3.804 | 4.006 | 3.756 |
| C₅H₁₀ | Isobutane                      | 3.808 | 3.799 | 3.797 | 3.799 | 4.000 | 4.453 |
| C₆H₆ | Cyclopentadiene                | 4.448 | 4.449 | 4.447 | 4.429 | 4.591 | 3.986 |
| C₆H₈ | 1,2-Dimethylcyclopropane       | 4.061 | 4.060 | 4.071 | 4.033 | 4.203 | 4.092 |
| C₆H₈ | Methylene cyclobutane          | 4.119 | 4.150 | 4.154 | 4.132 | 4.271 | 4.168 |
| C₆H₁₀ | 1, cis-3-Pentadiene            | 4.152 | 4.145 | 4.145 | 4.146 | 4.378 | 4.185 |
| C₆H₆ | Cyclopentene                   | 4.188 | 4.206 | 4.198 | 4.206 | 4.350 | 4.001 |
| C₆H₈ | Bicycl(2.1.0)-pentane         | 4.091 | 4.089 | 4.092 | 4.062 | 4.164 | 4.151 |
| C₆H₁₂ | 1,4-Pentadiene                | 4.131 | 4.127 | 4.141 | 4.133 | 4.368 | 3.951 |
| C₆H₈ | Spiropentane                  | 4.068 | 4.072 | 4.087 | 4.047 | 4.143 | 4.160 |
| C₆H₁₀ | 1, trans-3-Pentadiene         | 4.155 | 4.145 | 4.156 | 4.147 | 4.381 | 3.956 |
| C₆H₁₀ | 1-Pentene                     | 3.967 | 3.964 | 3.968 | 3.972 | 4.182 | 3.951 |
| C₆H₁₀ | 2-Methyl-1-butene              | 3.977 | 3.975 | 3.979 | 3.972 | 4.178 | 3.952 |
| C₆H₁₀ | 2-Methyl-2-butene              | 3.981 | 3.987 | 3.991 | 3.981 | 4.178 | 3.948 |
| C₆H₁₀ | 3-Methyl-1-butene              | 3.971 | 3.963 | 3.966 | 3.965 | 4.174 | 3.961 |
| C₆H₁₀ | cis-2-Pentene                 | 3.972 | 3.974 | 3.978 | 3.978 | 4.183 | 3.883 |
| C₆H₁₀ | cis-Dimethylcyclopropane      | 3.948 | 3.948 | 3.953 | 3.938 | 4.094 | 3.992 |
| C₆H₁₀ | Cyclopentane                  | 4.005 | 4.021 | 4.010 | 4.035 | 4.170 | 3.957 |
| C₆H₁₀ | trans-2-Pentene               | 3.975 | 3.977 | 3.980 | 3.980 | 4.183 | 3.799 |
| C₇H₁₂ | 2-Methylbutane                | 3.845 | 3.838 | 3.836 | 3.841 | 4.032 | 3.778 |
| C₇H₁₂ | Neopentane                    | 3.853 | 3.842 | 3.841 | 3.834 | 4.023 | 3.811 |
| C₇H₁₂ | n-Pentane                     | 3.840 | 3.839 | 3.836 | 3.848 | 4.038 | 4.764 |
| C₇H₆ | Benzene                       | 4.737 | 4.723 | 4.725 | 4.729 | 4.899 | 4.635 |
| C₇H₈ | Fulvene                       | 4.637 | 4.605 | 4.609 | 4.582 | 4.774 | 4.402 |
| C₈H₈ | 1,3-Cyclohexadiene            | 4.363 | 4.378 | 4.379 | 4.387 | 4.544 | 4.116 |
| C₈H₁₀ | 2,3-Dimethyl-1,3-butadiene    | 4.137 | 4.128 | 4.138 | 4.119 | 4.332 | 4.180 |
| C₈H₁₀ | Cyclohexene                   | 4.169 | 4.179 | 4.175 | 4.194 | 4.341 | 4.128 |
| C₈H₁₀ | 1,5-Hexadiene                 | 4.112 | 4.109 | 4.120 | 4.118 | 4.335 | 4.048 |
| C₈H₁₀ | 1,2-Dimethylcyclobutene       | 4.113 | 4.122 | 4.122 | 4.093 | 4.228 | 3.983 |
| C₈H₁₀ | Bicyclopentylpropyl          | 4.082 | 4.068 | 4.086 | 4.059 | 4.171 | 3.988 |
| C₈H₁₂ | Cyclohexane                   | 4.023 | 4.027 | 4.018 | 4.045 | 4.166 | 3.840 |
| C₈H₁₂ | n-Hexane                     | 3.867 | 3.867 | 3.864 | 3.878 | 4.060 | 4.556 |
| C₈H₆ | Cycloheptatriene              | 4.512 | 4.514 | 4.526 | 4.526 | 4.695 | 4.467 |
| C₈H₈ | Norbornadiene                 | 4.464 | 4.467 | 4.466 | 4.441 | 4.576 | 4.603 |
| C₈H₈ | Toluene                       | 4.602 | 4.596 | 4.599 | 4.595 | 4.751 | 4.125 |
| C₈H₁₂ | Norbornane                    | 4.161 | 4.164 | 4.154 | 4.165 | 4.272 | 3.854 |
| C₈H₁₂ | n-Heptane                    | 3.888 | 3.889 | 3.885 | 3.901 | 4.076 | 4.363 |
| C₈H₈ | Cubane                        | 4.405 | 4.500 | 4.468 | 4.399 | 4.325 | 4.738 |
| C₈H₈ | Styrene                       | 4.713 | 4.702 | 4.708 | 4.703 | 4.876 | 4.504 |
| C₈H₁₀ | Ethylbenzene                 | 4.506 | 4.500 | 4.502 | 4.502 | 4.657 | 4.146 |
| C₈H₁₂ | Bicycl(2.2.2)-octane         | 4.155 | 4.163 | 4.154 | 4.179 | 4.286 | 3.869 |
| C₈H₁₀ | n-Octane                     | 3.904 | 3.905 | 3.901 | 3.918 | 4.089 | 3.892 |
| C₁₀H₂₀ | n-Nonane                    | 3.916 | 3.918 | 3.914 | 3.932 | 4.099 | 3.882 |
### Table S1. (continued)

| 1       | 2                   | 3   | 4   | 5   | 6   | 7   | 8   |
|---------|---------------------|-----|-----|-----|-----|-----|-----|
| C_{10}H_{14} | Azulene            | 4.917 | 4.898 | 4.903 | 4.890 | 5.044 | 4.958 |
| C_{14}H_{10} | Naphthalene        | 5.007 | 4.996 | 4.998 | 4.996 | 5.115 | 5.029 |
| C_{12}H_{16} | Adamantane         | 4.269 | 4.273 | 4.263 | 4.288 | 4.368 | 4.252 |
| C_{17}H_{10} | Anthracene         | 5.137 | 5.125 | 5.127 | 5.123 | 5.218 | 5.157 |
| C_{14}H_{10} | Phenanthrene       | 5.147 | 5.137 | 5.138 | 5.133 | 5.227 | 5.167 |
| C_{20} | Buckminsterfullerene | 6.918 | 6.790 | 6.776 | 6.673 | 6.590 | 6.954 |
| OH      | Hydroxyl radical   | 2.193 | 2.334 | 2.242 | 2.380 | 2.356 | 2.076 |
| H_{2}O  | Water              | 3.182 | 3.118 | 3.182 | 3.202 | 3.387 | 2.859 |
| CO      | Carbon monoxide    | 5.540 | 5.395 | 5.365 | 5.091 | 4.607 | 5.059 |
| HCO     | H-C=O              | 3.908 | 4.193 | 4.095 | 4.073 | 3.836 | 3.965 |
| CH_{2}O | Formaldehyde       | 3.886 | 3.973 | 3.881 | 3.945 | 4.250 | 4.114 |
| CH_{3}O | Methanol           | 3.497 | 3.524 | 3.503 | 3.561 | 3.775 | 3.579 |
| C_{2}H_{3}O | Acetaldehyde     | 3.999 | 4.027 | 4.008 | 4.010 | 4.259 | 4.043 |
| C_{2}H_{4}O | Ethylene oxide    | 3.831 | 3.803 | 3.823 | 3.809 | 4.076 | 3.923 |
| C_{3}H_{6}O | Ethanol          | 3.688 | 3.690 | 3.686 | 3.719 | 3.923 | 3.711 |
| C_{3}H_{6}O | Acetone           | 4.038 | 4.044 | 4.053 | 4.026 | 4.251 | 4.005 |
| C_{3}H_{6}O | Propanal          | 4.010 | 4.027 | 4.012 | 4.022 | 4.241 | 4.026 |
| C_{4}H_{8}O | Trimethylene oxide| 3.896 | 3.929 | 3.923 | 3.924 | 4.150 | 4.004 |
| C_{4}H_{8}O | Isopropanol       | 3.786 | 3.782 | 3.793 | 3.796 | 3.988 | 3.763 |
| C_{3}H_{6}O | Furan             | 4.598 | 4.578 | 4.586 | 4.544 | 4.709 | 4.728 |
| C_{4}H_{8}O | 2-Butenal         | 4.231 | 4.244 | 4.238 | 4.238 | 4.484 | 4.263 |
| C_{5}H_{10}O | Butanal           | 4.008 | 4.027 | 4.014 | 4.029 | 4.222 | 4.017 |
| C_{6}H_{10}O | Tetrahydrofuran  | 3.992 | 4.016 | 4.008 | 4.040 | 4.188 | 4.091 |
| C_{6}H_{8}O | Diethyl ether     | 3.805 | 3.803 | 3.801 | 3.819 | 4.027 | 3.879 |
| C_{6}H_{8}O | 1,3-Butadiene    | 3.847 | 3.837 | 3.847 | 3.838 | 4.022 | 3.784 |
| C_{6}H_{10}O | Cyclopentanone   | 4.240 | 4.212 | 4.263 | 4.209 | 4.394 | 4.227 |
| C_{6}H_{10}O | Tetrahydrofuran  | 4.010 | 4.021 | 4.017 | 4.047 | 4.194 | 4.088 |
| C_{6}H_{12}O | 3-Pentanol       | 3.866 | 3.862 | 3.864 | 3.879 | 4.054 | 3.837 |
| C_{6}H_{8}O | Phenol            | 4.712 | 4.708 | 4.709 | 4.709 | 4.855 | 4.734 |
| C_{6}H_{10}O | Cyclohexanone    | 4.209 | 4.225 | 4.223 | 4.233 | 4.377 | 4.204 |
| C_{7}H_{10}O | Benzaldehyde     | 4.858 | 4.864 | 4.850 | 4.859 | 5.027 | 4.894 |
| C_{7}H_{10}O | Anisole           | 4.554 | 4.547 | 4.553 | 4.550 | 4.722 | 4.650 |
| C_{8}H_{10}O | 1-Naphthol       | 4.972 | 4.970 | 4.972 | 4.965 | 5.074 | 4.997 |
| C_{10}H_{10}O | 2-Naphthol       | 4.983 | 4.971 | 4.973 | 4.969 | 5.073 | 4.995 |
| O_{2}    | Oxygen(triplet)   | 2.559 | 2.650 | 2.743 | 3.144 | 2.181 | 2.471 |
| H_{2}O_{2} | Hydrogen peroxide | 2.751 | 2.841 | 2.727 | 2.782 | 3.083 | 2.579 |
| CO_{2}  | Carbon dioxide    | 5.525 | 5.393 | 5.386 | 5.320 | 5.465 | 5.074 |
| CH_{2}O_{2} | Formic acid      | 4.180 | 4.213 | 4.171 | 4.239 | 4.437 | 4.079 |
| C_{2}H_{2}O_{2} | Acetic acid    | 4.164 | 4.157 | 4.158 | 4.162 | 4.378 | 3.994 |
| C_{2}H_{2}O_{2} | Ethylene glycol | 3.738 | 3.744 | 3.821 | 3.797 | 3.962 | 3.790 |
| C_{2}H_{2}O_{2} | beta-Propiolactone | 4.349 | 4.363 | 4.316 | 4.365 | 4.606 | 4.268 |
| C_{2}H_{2}O_{2} | Proponic acid   | 4.126 | 4.118 | 4.119 | 4.129 | 4.328 | 3.981 |
| C_{2}H_{2}O_{2} | Methyl acetate  | 4.085 | 4.070 | 4.080 | 4.079 | 4.320 | 4.072 |
| C_{4}H_{2}O_{2} | Diacetyl        | 4.288 | 4.307 | 4.305 | 4.276 | 4.486 | 4.255 |
| C_{4}H_{2}O_{2} | Diethyl peroxide | 3.689 | 3.672 | 3.681 | 3.668 | 3.920 | 3.737 |
| C_{4}H_{2}O_{2} | Acetylacetone   | 4.256 | 4.259 | 4.272 | 4.242 | 4.441 | 4.226 |
| C_{4}H_{2}O_{2} | p-Benzooquinone | 4.967 | 4.975 | 4.964 | 4.952 | 5.170 | 5.010 |
| C_{4}H_{6}O_{2} | Benzoic acid   | 4.882 | 4.871 | 4.871 | 4.876 | 5.033 | 4.804 |
Table S1. (continued)

| 1  | 2                                      | 3  | 4  | 5  | 6  | 7  | 8  |
|----|----------------------------------------|----|----|----|----|----|----|
| C₄H₇O₃ | Malic anhydride                         | 5.088 | 5.063 | 5.026 | 4.997 | 5.255 | 4.930 |
| C₅H₉O₄ | Acetic anhydride                        | 4.351 | 4.344 | 3.627 | 4.333 | 4.606 | 4.230 |
| NH   | Imidogen                               | 1.703 | 1.960 | 1.826 | 1.874 | -    | 1.577 |
| NH₂  | Amidogen                               | 2.462 | 2.608 | 2.507 | 2.565 | -    | 2.384 |
| NH₃  | Ammonia                                | 3.019 | 2.934 | 2.946 | 2.979 | -    | 2.871 |
| CN   | Cyanide                                | 3.874 | 3.353 | 3.879 | 3.648 | -    | 3.592 |
| CHN  | Hydrogen cyanide                       | 4.366 | 4.355 | 4.401 | 4.384 | -    | 4.302 |
| CH₄N | Methyl amine anion                     | 3.316 | 3.379 | 3.561 | 3.297 | -    | 3.339 |
| CH₃N | CH₃-NH                                 | 3.269 | 3.339 | 3.282 | 3.290 | -    | 3.268 |
| CH₃N | Methylamine                            | 3.385 | 3.383 | 3.372 | 3.397 | -    | 3.370 |
| C₂H₅N | Acetonitrile                           | 4.241 | 4.224 | 4.261 | 4.253 | -    | 4.187 |
| C₂H₆N | Methyl isocyanide                      | 4.135 | 3.997 | 4.111 | 4.028 | -    | 4.026 |
| C₂H₇N | Ethyleneimine(Azirane)                 | 3.690 | 3.683 | 3.679 | 3.675 | -    | 3.570 |
| C₂H₈N | Ethylamine                             | 3.581 | 3.585 | 3.580 | 3.597 | -    | 3.562 |
| C₂H₉N | Dimethylamine                          | 3.560 | 3.566 | 3.550 | 3.556 | -    | 3.558 |
| C₂H₁₀N | Acrylonitrile                         | 4.545 | 4.508 | 4.548 | 4.540 | -    | 4.537 |
| C₂H₁₁N | Ethyl cyanide                         | 4.187 | 4.156 | 4.180 | 4.183 | -    | 4.117 |
| C₂H₁₂N | Isopropylamine                        | 3.695 | 3.691 | 3.687 | 3.693 | -    | 3.652 |
| C₂H₁₃N | Trimethylamine                         | 3.650 | 3.665 | 3.649 | 3.634 | -    | 3.646 |
| C₂H₁₄N | n-Propylamine                          | 3.684 | 3.688 | 3.683 | 3.702 | -    | 3.660 |
| C₂H₁₅N | Pyrrole                               | 4.446 | 4.441 | 4.444 | 4.386 | -    | 4.475 |
| C₂H₁₆N | Pyrrolidine                            | 3.899 | 3.933 | 3.913 | 3.928 | -    | 3.917 |
| C₂H₁₇N | t-Butylamine                           | 3.767 | 3.757 | 3.755 | 3.747 | -    | 3.701 |
| C₂H₁₈N | Pyridine                               | 4.678 | 4.695 | 4.690 | 4.689 | -    | 4.704 |
| C₂H₁₉N | Aniline                                | 4.566 | 4.564 | 4.564 | 4.567 | -    | 4.589 |
| C₂H₂₀N | Phenyl cyanide                         | 5.037 | 5.014 | 5.030 | 5.031 | -    | 5.033 |
| NO   | Nitrogen oxide                          | 3.251 | 3.399 | 3.236 | 3.694 | -    | 3.375 |
| HNCO | Hydrogen isocyanate                    | 4.527 | 4.430 | 4.518 | 4.429 | -    | 4.528 |
| CH₂NO | Formamide                              | 3.911 | 3.891 | 3.908 | 3.913 | -    | 3.943 |
| C₂H₂NO | Dimethylformamide                     | 3.936 | 3.932 | 3.929 | 3.904 | -    | 3.953 |
| NO₂  | Nitrogen dioxide                       | 3.218 | 3.347 | 3.412 | 3.549 | -    | 3.493 |
| HNO₂ | Nitrous acid, trans                    | 3.263 | 3.221 | 3.315 | 3.486 | -    | 3.127 |
| CH₄NO₂ | Nitromethane                          | 3.553 | 3.540 | 3.548 | 3.503 | -    | 3.733 |
| CH₅NO₂ | Methyl nitrite                         | 3.540 | 3.498 | 3.561 | 3.639 | -    | 3.635 |
| C₂H₆NO₂ | Glycine                               | 4.001 | 4.011 | 3.999 | 4.035 | -    | 3.863 |
| C₂H₇NO₂ | 1-Nitropropane                      | 3.778 | 3.767 | 3.771 | 3.757 | -    | 3.851 |
| C₂H₈NO₂ | 2-Nitropropane                      | 3.788 | 3.768 | 3.773 | 3.749 | -    | 3.839 |
| C₂H₉NO₂ | Alanine                               | 4.049 | 4.015 | 4.008 | 4.028 | -    | 3.884 |
| C₂H₁₀NO₂ | 1-Nitrobutane                    | 3.822 | 3.816 | 3.818 | 3.811 | -    | 3.877 |
| C₂H₁₁NO₂ | 2-Nitrobutane                    | 3.835 | 3.815 | 3.822 | 3.805 | -    | 3.869 |
| C₂H₁₂NO₂ | Nitrobenzene                   | 4.628 | 4.631 | 4.619 | 4.597 | -    | 4.729 |
| C₂H₁₃NO₂ | 2-Nitrotoluene                  | 4.524 | 4.536 | 4.525 | 4.504 | -    | 4.596 |
| NO₃  | Nitrate radical                      | 2.955 | 2.891 | 2.841 | 2.779 | -    | 3.065 |
| HNO₃ | Nitric acid                           | 3.238 | 3.289 | 3.256 | 3.284 | -    | 3.210 |
| C₂H₅NO₃ | Ethyl nitrate                       | 3.646 | 3.644 | 3.654 | 3.647 | -    | 3.712 |
| C₂H₆NO₃ | Nitroethanol                         | 3.797 | 3.743 | 3.734 | 3.755 | -    | 3.878 |
| N₂   | Nitrogen                              | 4.881 | 4.499 | 4.165 | 4.638 | -    | 4.788 |
| N₂H₂ | Diazene                               | 3.170 | 3.150 | 3.089 | 3.219 | -    | 3.251 |
Table S1. (continued)

|     | 1                | 2                | 3    | 4    | 5    | 6    | 7    | 8    |
|-----|------------------|------------------|------|------|------|------|------|------|
| N₂H₄ | Hydrazine        | 2.955            | 2.971| 3.009| 3.021| -    | 2.911|      |
| CH₃N₂| Methylhydrazine  | 3.289            | 3.311| 3.328| 3.314| -    | 3.257|      |
| C₂N₂ | Cyanogen         | 5.329            | 5.289| 5.354| 5.393| -    | 5.393|      |
| C₂H₆N₂| 1,1-Dimethylhydrazine | 3.464           | 3.482| 3.490| 3.449| -    | 3.425|      |
| C₂H₅N₂| 1,2-Dimethylhydrazine | 3.457           | 3.480| 3.487| 3.458| -    | 3.433|      |
| C₂H₄N₂| Dicyanoacetylene | 5.630            | 5.619| 5.630| 5.679| -    | 5.882|      |
| C₂H₃N₂| Fumaronitrile    | 5.028            | 5.002| 5.048| 5.057| -    | 5.021|      |
| C₂H₅N₂| Pyridazine       | 4.534            | 4.580| 4.592| 4.583| -    | 4.517|      |
| C₂H₆N₂| Pyrimidine       | 4.619            | 4.658| 4.648| 4.632| -    | 4.534|      |
| C₂H₅N₂| Pyrazine         | 4.619            | 4.652| 4.630| 4.631| -    | 4.590|      |
| C₂H₆N₄| n-Nitrodimethylamine | 3.601           | 3.585| 3.599| 3.511| -    | 3.758|      |
| C₂H₅N₂| Para nitroaniline| 4.492            | 4.507| 4.501| 4.478| -    | 4.584|      |
| C₂H₅N₄| 1,1-Dinitroethane| 3.729            | 3.705| 3.696| 3.652| -    | 3.873|      |
| C₂H₅N₄| 1,1-Dinitropropane| 3.779            | 3.768| 3.764| 3.731| -    | 3.899|      |
| C₂H₅N₄| 1,3-Dinitropropane| 3.796            | 3.781| 3.788| 3.759| -    | 3.957|      |
| C₂H₅N₄| 2,2-Dinitropropane| 3.782            | 3.771| 3.763| 3.720| -    | 3.858|      |
| C₂H₅N₄| 1,1-Dinitrobutane| 3.828            | 3.811| 3.808| 3.784| -    | 3.914|      |
| C₂H₅N₄| 1,4-Dinitrobutane| 3.839            | 3.824| 3.832| 3.812| -    | 3.962|      |
| C₆H₆N₂| m-Dinitrobenzene | 4.545            | 4.551| 4.529| 4.486| -    | 4.702|      |
| N₃  | Azide            | 3.450            | 3.348| 3.335| 3.328| -    | 3.454|      |
| HN₃ | Hydrazoic acid   | 3.458            | 3.404| 3.426| 3.399| -    | 3.606|      |
| C₂H₅N₄| 1,1,1-trinitropropane | 3.772            | 3.745| 3.737| 3.678| -    | 3.874|      |
| C₂H₅N₄| 2,4,6-Trinitrotoluene | 4.394            | 4.414| 4.398| 4.335| -    | 4.581|      |
| C₂H₅N₄| Glycerol trinitrate | 3.742            | 3.716| 3.729| 3.704| -    | 3.822|      |
| CH₃N₄| [1-H]Tetrazole   | 3.988            | 3.948| 4.018| 3.804| -    | 3.970|      |
| CN₃O₅| Tetranitromethane| 3.582            | 3.622| 3.549| 3.467| -    | 3.719|      |
Table S2. The bond lengths (in Angstroms) for various \( \text{H}_2\text{C}_n\text{N}_m\text{O}_n \) molecules calculated within the NTBM1 model along with the corresponding experimental values and the values calculated using AM1/PM3/PM7 and the set of the model parameters from Ref. [Zhao J, Lu JP. Phys. Lett. A. 2003;319:523-529.]. The experimental and AM1/PM3 values are taken from the original PM3 work [Stewart JJP. J. Comp. Chem. 1989;10:221-264.]. The AM1/PM3 bond lengths for the cubane \( \text{C}_8\text{H}_8 \), imidogen NH, and amidogen NH\(_2\) are obtained using GAMESS program package [Schmidt MW, Baldridge KK, Boatz JA, Elbert ST, Gordon MS, Jensen JH, Koseki S, Matsunaga N, Nguyen KA, Su SJ, Windus TL, Dupuis M, Montgomery JA. J. Comp. Chem. 1993;14:1347-1363.]. The PM7 bond lengths are obtained using MOPAC2012 [Stewart JJP, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2012).], and experimental values for cubane, imidogen, and amidogen are taken from NIST database [Computational Chemistry Comparison and Benchmark DataBase http://cccbdb.nist.gov/].

| Formula | Name                  | Bond type | Exper. | PM3  | PM7  | AM1 | Zhao-Lu | Present work |
|---------|-----------------------|-----------|--------|------|------|-----|---------|--------------|
|         |                       |           | 1      | 2    | 3    | 4   | 5       | 6            | 7   | 8   | 9       |
| \( \text{H}_2 \) | Hydrogen              | H-H       | 0.741  | 0.699| 0.76 | 0.677| 0.745  |              |     |     | 0.745  |
| \( \text{CH} \)  | Methylidyne           | CH        | 1.120  | 1.088| 1.08 | 1.106| 1.089  | 1.081        |     |     |         |
| \( \text{CH}_3 \) | Methylene, triplet    | CH        | 1.029  | 1.064| 1.02 | 1.063| 1.079  | 1.080        |     |     |         |
| \( \text{CH}_4 \) | Methane               | CH        | 1.094  | 1.087| 1.08 | 1.112| 1.089  | 1.099        |     |     |         |
| \( \text{C}_2 \)  | Carbon, dimer         | CC        | 1.242  | 1.189| 1.17 | 1.164| 1.159  | 1.230        |     |     |         |
| \( \text{C}_2\text{H}_2 \) | Acetylene          | CC        | 1.203  | 1.190| 1.21 | 1.195| 1.201  | 1.226        |     |     |         |
| \( \text{C}_2\text{H}_4 \) | Ethylene            | CC        | 1.339  | 1.322| 1.33 | 1.326| 1.319  | 1.327        |     |     |         |
| \( \text{C}_2\text{H}_6 \) | Ethane              | CC        | 1.536  | 1.504| 1.53 | 1.500| 1.542  | 1.476        |     |     |         |
| \( \text{C}_3\text{H}_4 \) | Allene             | CC        | 1.308  | 1.297| 1.30 | 1.298| 1.312  | 1.323        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Cyclopropene        | \(\text{C}_2\text{C}_3\) | 1.509  | 1.484| 1.50 | 1.489| 1.585  | 1.537        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propyne             | \(\text{C}_2\text{C}_3\) | 1.296  | 1.314| 1.32 | 1.318| 1.297  | 1.326        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propyne             | \(\text{C}_2\text{H}\) | 1.072  | 1.073| 1.04 | 1.069| 1.065  | 1.074        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propyne             | \(\text{C}_2\text{C}_3\) | 1.206  | 1.191| 1.21 | 1.197| 1.206  | 1.235        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | C=C                  | \(\text{C}_2\text{H}\) | 1.056  | 1.064| 1.03 | 1.060| 1.064  | 1.079        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Cyclopropane        | \(\text{C}_2\text{C}_3\) | 1.459  | 1.433| 1.43 | 1.427| 1.492  | 1.446        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propene             | \(\text{C}_2\text{H}\) | 1.105  | 1.098| 1.10 | 1.121| 1.099  | 1.106        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propene             | C=C       | 1.336  | 1.328| 1.34 | 1.331| 1.327  | 1.341        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propene             | C–C       | 1.501  | 1.480| 1.43 | 1.476| 1.545  | 1.479        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propene             | \(\text{C}_2\text{H}\) | 1.085  | 1.098| 1.09 | 1.118| 1.091  | 1.096        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propene             | HC        | 1.090  | 1.097| 1.09 | 1.103| 1.096  | 1.098        |     |     |         |
| \( \text{C}_3\text{H}_6 \) | Propene             | HC        | 1.091  | 1.087| 1.08 | 1.098| 1.096  | 1.104        |     |     |         |
Table S2. (continued)

| 1      | 2             | 3   | 4   | 5   | 6   | 7   | 8   | 9   |
|--------|---------------|-----|-----|-----|-----|-----|-----|-----|
| C₂H₆   | Propane       | CC  | 1.526 | 1.512 | 1.53 | 1.507 | 1.557 | 1.495 |
|        | C₂H₅          | 1.115 | 1.108 | 1.10 | 1.122 | 1.097 | 1.104 |
|        | C₂H₄          | 1.096 | 1.097 | 1.10 | 1.117 | 1.093 | 1.101 |
| C₃H₆   | Bicyclobutane | C₃C₂ | 1.498 | 1.507 | 1.52 | 1.510 | 1.599 | 1.552 |
|        |               | C₃C₃ | 1.497 | 1.481 | 1.49 | 1.495 | 1.544 | 1.517 |
|        |               | C₃H₂ | 1.071 | 1.083 | 1.06 | 1.079 | 1.062 | 1.074 |
|        |               | C₃H₁ | 1.093 | 1.095 | 1.08 | 1.105 | 1.084 | 1.092 |
| C₄H₆   | 2-Butyne      | C₄C₃ | 1.213 | 1.193 | 1.21 | 1.198 | 1.211 | 1.242 |
|        |               | C₄C₂ | 1.467 | 1.432 | 1.43 | 1.425 | 1.494 | 1.447 |
|        |               | CH   | 1.115 | 1.098 | 1.10 | 1.121 | 1.099 | 1.107 |
| C₅H₆   | 1,3-Butadiene | C₅C₄ | 1.344 | 1.331 | 1.33 | 1.335 | 1.335 | 1.347 |
|        |               | C₅C₃ | 1.467 | 1.456 | 1.46 | 1.451 | 1.526 | 1.475 |
| C₅H₈   | 1-Butene      | C₅C₄ | 1.347 | 1.328 | 1.34 | 1.331 | 1.326 | 1.338 |
|        |               | C₅C₂ | 1.508 | 1.489 | 1.50 | 1.484 | 1.564 | 1.500 |
| C₆H₈   | Cyclobutane   | CC   | 1.548 | 1.542 | 1.55 | 1.543 | 1.613 | 1.541 |
|        |               | CH   | 1.105 | 1.100 | 1.09 | 1.110 | 1.086 | 1.094 |
| C₆H₈   | Isobutene     | C₆C₄ | 1.330 | 1.333 | 1.34 | 1.336 | 1.335 | 1.355 |
|        |               | C₆C₃ | 1.507 | 1.487 | 1.50 | 1.484 | 1.562 | 1.500 |
| C₆H₁₀  | n-Butane      | C₆C₄ | 1.533 | 1.512 | 1.53 | 1.507 | 1.556 | 1.492 |
|        |               | C₆C₃ | 1.533 | 1.521 | 1.53 | 1.514 | 1.576 | 1.517 |
| C₆H₁₀  | Isobutane     | CC   | 1.525 | 1.520 | 1.53 | 1.514 | 1.572 | 1.514 |
| C₆H₈   | 1,4-Pentadiene| C₆C₄ | 1.339 | 1.328 | 1.33 | 1.331 | 1.325 | 1.338 |
|        |               | C₆C₃ | 1.511 | 1.489 | 1.50 | 1.484 | 1.568 | 1.502 |
| C₇H₁₂  | Neopentane    | CC   | 1.539 | 1.527 | 1.54 | 1.521 | 1.584 | 1.532 |
|        |               | CH   | 1.120 | 1.098 | 1.09 | 1.116 | 1.092 | 1.099 |
| C₈H₆   | Benzene       | CC   | 1.399 | 1.391 | 1.39 | 1.395 | 1.424 | 1.407 |
|        |               | CH   | 1.084 | 1.095 | 1.08 | 1.100 | 1.091 | 1.095 |
| C₉H₆   | Fulvene       | C₉C₄ | 1.476 | 1.471 | 1.48 | 1.476 | 1.569 | 1.504 |
|        |               | C₉C₃ | 1.355 | 1.355 | 1.35 | 1.363 | 1.359 | 1.376 |
|        |               | C₉C₂ | 1.470 | 1.478 | 1.48 | 1.483 | 1.547 | 1.480 |
|        |               | C₉C₁ | 1.349 | 1.331 | 1.33 | 1.332 | 1.338 | 1.358 |
| C₁₀H₁₀  | Cyclohexene   | C₁₀C₂ | 1.335 | 1.334 | 1.33 | 1.337 | 1.333 | 1.348 |
|        |               | C₁₀C₁ | 1.504 | 1.487 | 1.49 | 1.483 | 1.562 | 1.506 |
|        |               | C₁₀C₄ | 1.515 | 1.521 | 1.53 | 1.517 | 1.573 | 1.507 |
|        |               | C₁₀C₃ | 1.550 | 1.519 | 1.53 | 1.514 | 1.570 | 1.490 |
| C₁₀H₁₂  | Cyclopentane  | CC   | 1.536 | 1.521 | 1.54 | 1.515 | 1.575 | 1.506 |
|        |               | CH   | 1.121 | 1.107 | 1.11 | 1.121 | 1.096 | 1.104 |
| C₁₂H₈   | Cubane        | CC   | 1.571 | 1.568 | 1.58 | 1.576 | 1.649 | 1.570 |
|        |               | CH   | 1.097 | 1.088 | 1.06 | 1.086 | 1.073 | 1.082 |
| C₂₀[60] | [60]Fullerene | CC   | 1.458 | 1.457 | 1.46 | 1.464 | 1.530 | 1.481 |
|        |               | CC   | 1.401 | 1.383 | 1.38 | 1.385 | 1.418 | 1.412 |
| OH     | Hydroxyl radical | OH | 0.970 | 0.937 | 0.97 | 0.949 | 0.985 | 0.982 |
| H₂O    | Water         | OH   | 0.957 | 0.951 | 0.96 | 0.961 | 0.960 | 0.974 |
| CO     | Carbon monoxide | CO | 1.128 | 1.135 | 1.14 | 1.171 | 1.156 | 1.110 |
| CH₃O   | Formaldehyde  | CO   | 1.208 | 1.202 | 1.21 | 1.227 | 1.207 | 1.190 |
|        |               | CH   | 1.116 | 1.091 | 1.10 | 1.110 | 1.088 | 1.109 |
Table S2. (continued)

| 1 | 2            | 3   | 4   | 5   | 6   | 7   | 8   | 9   |
|---|--------------|-----|-----|-----|-----|-----|-----|-----|
| CH₄O | Methanol | CO  | 1.425 | 1.395 | 1.42 | 1.410 | 1.380 | 1.343 |
|     |           | CH  | 1.094 | 1.097 | 1.09 | 1.119 | 1.089 | 1.103 |
|     |           | OH  | 0.945 | 0.949 | 0.97 | 0.964 | 0.962 | 0.978 |
| C₂H₂O | Furan    | CO  | 1.362 | 1.378 | 1.38 | 1.395 | 1.410 | 1.334 |
|     |           | C₂C₂ | 1.361 | 1.373 | 1.37 | 1.380 | 1.349 | 1.401 |
| O₂ | Oxygen, triplet | O=O | 1.216 | 1.169 | 1.14 | 1.086 | 1.215 | 1.230 |
| H₂O₂ | Hydrogen peroxide | O=O | 1.475 | 1.482 | 1.43 | 1.300 | 1.405 | 1.397 |
|     |           | OH  | 0.950 | 0.945 | 0.99 | 0.983 | 0.968 | 0.991 |
| CO₂ | Carbon dioxide | CO  | 1.162 | 1.181 | 1.17 | 1.189 | 1.157 | 1.202 |
| CH₂O₂ | Formic acid | C=O | 1.202 | 1.211 | 1.20 | 1.230 | 1.265 | 1.273 |
|     |           | C–O | 1.343 | 1.344 | 1.35 | 1.357 | 1.229 | 1.293 |
|     |           | OH  | 0.972 | 0.953 | 0.99 | 0.971 | 0.960 | 0.980 |
| C₂H₄O₂ | 3-Benzophenone | C₂=O₂ | 1.477 | 1.487 | 1.49 | 1.479 | 1.499 | 1.480 |
|     |           | C₂C₂ | 1.322 | 1.335 | 1.33 | 1.338 | 1.363 | 1.360 |
|     |           | CO  | 1.222 | 1.217 | 1.21 | 1.236 | 1.272 | 1.252 |
| NH | Imidogen   | NH  | 1.036 | 0.974 | 0.98 | 0.988 | -    | 1.044 |
| NH₂ | Amidogen   | NH  | 1.024 | 0.987 | 0.99 | 0.996 | -    | 1.014 |
| NH₃ | Ammonia    | NH  | 1.012 | 0.999 | 0.99 | 0.998 | -    | 1.012 |
| CN | Cyanide    | CN  | 1.175 | 1.157 | 1.14 | 1.148 | -    | 1.157 |
| CHN | Hydrogen cyanide | CN  | 1.154 | 1.156 | 1.15 | 1.160 | -    | 1.166 |
|     |           | CH  | 1.063 | 1.070 | 1.04 | 1.069 | -    | 1.069 |
| CH₃N | Methylamine | CN  | 1.474 | 1.469 | 1.47 | 1.432 | -    | 1.394 |
|     |           | NH  | 1.011 | 0.999 | 1.01 | 1.000 | -    | 1.011 |
| C₂H₃N | Acetonitrile | CC  | 1.458 | 1.440 | 1.44 | 1.439 | -    | 1.421 |
|     |           | CH  | 1.104 | 1.098 | 1.10 | 1.120 | -    | 1.108 |
| CH₃N | Methyl isocyanide | CN– | 1.124 | 1.433 | 1.41 | 1.395 | -    | 1.376 |
|     |           | CH  | 1.101 | 1.097 | 1.11 | 1.125 | -    | 1.101 |
|     |           | CN  | 1.166 | 1.181 | 1.18 | 1.181 | -    | 1.165 |
| C₂H₅N | Trimethylamine | CN  | 1.451 | 1.480 | 1.48 | 1.445 | -    | 1.433 |
| C₂H₆N | Pyrrole | CN  | 1.370 | 1.397 | 1.39 | 1.392 | -    | 1.367 |
|     |           | C₂C₂ | 1.382 | 1.390 | 1.39 | 1.402 | -    | 1.405 |
|     |           | C₂C₃ | 1.417 | 1.390 | 1.40 | 1.402 | -    | 1.445 |
| NO | Nitrogen oxide | NO  | 1.151 | 1.127 | 1.13 | 1.115 | -    | 1.177 |
| HNCO | Hydrogen isocyanate | NH  | 0.987 | 0.985 | 0.99 | 0.985 | -    | 0.994 |
|     |           | CN  | 1.207 | 1.251 | 1.22 | 1.232 | -    | 1.223 |
|     |           | CO  | 1.171 | 1.181 | 1.17 | 1.202 | -    | 1.172 |
| CH₂NO | Formamide | CN  | 1.376 | 1.413 | 1.39 | 1.367 | -    | 1.309 |
|     |           | NH  | 1.002 | 0.994 | 0.99 | 0.986 | -    | 1.010 |
|     |           | CH  | 1.102 | 1.102 | 1.09 | 1.114 | -    | 1.091 |
|     |           | CO  | 1.193 | 1.217 | 1.21 | 1.243 | -    | 1.254 |
| NO₂ | Nitrogen dioxide | NO  | 1.197 | 1.181 | 1.18 | 1.159 | -    | 1.205 |
| HNO₃ | Nitric acid | N=O | 1.206 | 1.203 | 1.21 | 1.195 | -    | 1.270 |
|     |           | N–O | 1.405 | 1.410 | 1.41 | 1.333 | -    | 1.272 |
|     |           | OH  | 0.960 | 0.953 | 1.00 | 0.982 | -    | 0.981 |
Table S2. (continued)

|   | 2             | 3     | 4     | 5     | 6     | 7     | 8     | 9     |
|---|---------------|-------|-------|-------|-------|-------|-------|-------|
| N\textsubscript{2} | Nitrogen     | NN    | 1.094 | 1.098 | 1.11  | 1.106 | -     | 1.135 |
| N\textsubscript{2}H\textsubscript{4} | Hydrazine   | NN    | 1.449 | 1.440 | 1.45  | 1.378 | -     | 1.321 |
|               | NH           |       | 1.022 | 1.001 | 1.02  | 1.014 | -     | 1.013 |
| C\textsubscript{2}N\textsubscript{2} | Cyanogen    | CN    | 1.154 | 1.159 | 1.15  | 1.162 | -     | 1.179 |
|               | CC           |       | 1.389 | 1.382 | 1.39  | 1.384 | -     | 1.398 |
| N\textsubscript{3} | Azide       | NN    | 1.181 | 1.174 | 1.18  | 1.177 | -     | 1.218 |
Table S3. The valence angles (in degrees) for various $H_xC_{y}N_{m}O_{n}$ molecules calculated within the NTBM1 model along with the corresponding experimental values and the values calculated using AM1/PM3/PM7 and the set of the model parameters from Ref. [Zhao J, Lu JP. Phys. Lett. A. 2003;319:523-529.]. The experimental and AM1/PM3 values are taken from the original PM3 work [Stewart JJP. J. Comp. Chem. 1989;10:221-264]. The PM7 valence angles are obtained using MOPAC2012 [Stewart JJP, Stewart Computational Chemistry, Colorado Springs, CO, USA, HTTP://OpenMOPAC.net (2012)].

| Formula | Name                  | Angle type | Exper. | PM3  | PM7  | AM1  | Zhao-Lu | Present work |
|---------|-----------------------|------------|--------|------|------|------|---------|--------------|
| CH$_2$  | Methylene, triplet    | HCH        | 144.7  | 144.7| 175.5| 148.3| 113.0   | 140.1       |
| C$_2$H$_4$ | Ethylene          | HCC        | 121.2  | 123.1| 123.6| 122.7| 123.7   | 122.0       |
| C$_2$H$_6$ | Ethane            | HCC        | 110.9  | 111.6| 114.1| 110.7| 111.0   | 110.4       |
| C$_3$H$_4$ | Allene            | HCC        | 120.9  | 122.3| 123.6| 122.3| 124.4   | 123.1       |
| C$_5$H$_4$ | Cyclopentene      | HCC$_2$   | 149.9  | 151.5| 153.6| 151.9| 154.6   | 154.0       |
| C$_4$H$_4$ | Propyne           | HCC        | 111.0  | 110.7| 111.9| 110.5| 112.0   | 111.8       |
| C$_6$H$_6$ | Propene           | CCC        | 124.3  | 123.4| 123.6| 124.3| 127.4   | 127.7       |
| C$_4$H$_8$ | Propane           | CCC        | 112.4  | 111.7| 111.2| 111.8| 113.8   | 115.5       |
| C$_5$H$_6$ | Bicyclobutane     | C$_2$H$_2$ | 121.7  | 120.0| 120.4| 122.0| 133.8   | 133.4       |
| C$_6$H$_6$ | 2-Butyne          | HCC        | 110.7  | 110.7| 111.7| 110.6| 112.1   | 112.0       |
| C$_6$H$_6$ | 1,3-Butadiene     | CCC        | 122.9  | 122.3| 122.7| 123.4| 127.2   | 126.7       |
| C$_6$H$_6$ | 1-Butene          | CCC        | 123.8  | 122.6| 122.8| 123.4| 127.0   | 126.8       |
| C$_6$H$_6$ | Isobutene         | C$_2$H$_2$ | 122.4  | 122.1| 122.5| 122.4| 123.4   | 122.6       |
| C$_{10}$H$_{10}$ | n-Butane     | CCC        | 112.8  | 111.6| 111.0| 111.6| 113.3   | 114.5       |
| C$_6$H$_8$ | 1,4-Pentadiene   | C–C=C     | 115.5  | 123.1| 123.4| 123.9| 127.0   | 126.6       |
| C$_{12}$H$_{12}$ | Neopentane | HCC        | 110.0  | 111.3| 111.3| 110.3| 110.2   | 109.6       |
| C$_{10}$H$_{10}$ | Cyclohexene | C$_2$H$_2$C$_4$ | 21.8  | 27.8| 28.8| 27.2| 24.4     | 24.0        |
| H$_2$O   | Water               | HOH        | 104.5  | 107.7| 104.6| 103.5| 128.4   | 112.7       |
| CH$_2$O  | Formaldehyde       | HCO        | 121.8  | 121.8| 121.2| 122.2| 119.0   | 117.2       |
| CH$_3$O  | Methanol           | HCO        | 108.5  | 112.2| 110.4| 110.9| 107.3   | 107.3       |
| C$_2$H$_2$O | Furan            | CCC        | 110.7  | 110.2| 106.4| 110.1| 107.5   | 105.9       |
| H$_2$O$_2$ | Hydrogen peroxide | HOO        | 94.8   | 96.5 | 97.7 | 96.0 | 107.3   | 103.8       |
| CH$_2$O$_2$ | Formic acid      | OCO        | 124.9  | 117.1| 121.6| 117.6| 117.6   | 134.9       |
| C$_5$H$_8$O$_2$ | p-Benzoquinone | CCC        | 121.1  | 121.6| 121.4| 121.9| 120.6   | 121.0       |
| NH$_3$   | Ammonia             | HNH        | 106.7  | 108.1| 110.1| 109.1| -       | 120.1       |
| CH$_3$N  | Methylamine        | HNC        | 112.0  | 109.8| 111.4| 111.3| -       | 119.8       |
| C$_2$H$_3$N | Acetonitrile      | HCC        | 109.5  | 110.4| 111.9| 110.1| -       | 112.2       |
| C$_3$H$_5$N | Methyl isocyanide | HCN        | 109.1  | 109.7| 110.9| 110.1| -       | 108.1       |
Table S3. (continued)

| 1 | 2               | 3    | 4    | 5    | 6    | 7    | 8    | 9    |
|---|----------------|------|------|------|------|------|------|------|
| C₃H₇N | Trimethylamine | CNC  | 110.9| 112.3| 110.6| 113.0| -    | 118.4|
| C₅H₅N | Pyrrole | CNC  | 107.7| 109.7| 108.8| 108.8| -    | 112.5|
| HNCO    | Hydrogen isocyanate | CNH | 128.1| 123.7| 137.9| 127.2| -    | 179.8|
|         |            | OCN  | 180.0| 168.7| 166.9| 166.7| -    | 180.0|
| CH₃NO  | Formamide | OCN  | 123.8| 118.5| 119.6| 121.9| -    | 119.3|
| NO₂    | Nitrogen dioxide | ONO | 136.0| 137.8| 139.7| 136.4| -    | 151.1|
| HNO₃ | Nitric acid | O=N=O | 130.0| 132.7| 131.6| 129.0| -    | 121.0|
|        |            | NOH  | 102.0| 109.0| 108.9| 109.7| -    | 106.2|
| N₂H₄ | Hydrazine | HNN  | 112.0| 106.5| 105.5| 107.4| -    | 116.2|
|        |            | HNNH | 90.0 | 180.3| 106.4| 180.2| -    | 101.3|
Geometries of the peptides employed in this study optimized at the B3LYP/6-311G level of theory

Bradykinin

| C | 7.4124056373 | -0.8107633345 | 1.3524528185 |
| C | 3.9419327292 | 0.6202533156 | 1.7733270579 |
| C | 1.6450083034 | -2.8184826584 | -0.6919016673 |
| C | 3.7104686532 | 1.7270804666 | 0.4670894266 |
| C | 0.1312392570 | -0.4566925276 | -0.1492059101 |
| C | 2.3740563641 | -1.5346390049 | -0.2304717991 |
| C | 3.204545040 | 2.8625282474 | 4.9286424782 |
| C | -0.5341560201 | -6.3796206366 | -0.7657525317 |
| C | -10.5679037071 | -2.9201786267 | 0.1178945667 |
| C | -0.3410587576 | -6.6939323247 | -2.2125052728 |
| C | 3.7595443537 | -1.5147726050 | -2.2402995964 |
| C | 1.6504124476 | -0.3448906667 | -2.2106302938 |
| C | 2.0977044326 | 2.7861406384 | 5.7680166241 |
| C | 3.8483035531 | 4.1121261452 | 4.9343219116 |
| C | -0.6178660506 | -5.7475808243 | -3.2242611041 |
| C | -0.5498577398 | -7.5086808366 | 0.2641758655 |
| C | 4.4092827494 | -0.3324477743 | -2.6082170520 |
| C | 2.2970550986 | 0.8364731562 | -2.5755262976 |
| C | 3.6807556851 | 0.8470366102 | -2.7755365698 |
| C | 1.6447481782 | 3.7065827130 | 6.5986944991 |
| C | 3.3976820740 | 5.1436190697 | 5.7092621797 |
| C | -0.3295310424 | -0.0982629586 | -4.6887368887 |
| C | 2.2963116262 | 4.9420334080 | 6.9807931985 |
| C | -0.0948746424 | -0.8245145529 | -6.7159508053 |
| H | 7.7828351934 | 1.1320723423 | 0.9216633453 |
| H | -0.6891133606 | -6.1184799180 | 1.6691760027 |
| H | -0.2136956495 | 2.5993688215 | -0.8767868063 |
| H | -10.5619892098 | 2.6835266808 | -2.2699671633 |
| H | -9.3966192465 | 3.2578371363 | -3.3568369254 |
| H | 3.3977319795 | -3.4744106491 | 0.1094401722 |
| H | 5.8618953751 | 0.9000157303 | 2.4823755557 |
| H | 1.3848758916 | 1.3191560671 | 2.6354953128 |
| H | 1.4416681784 | -5.6155852037 | -0.4368419297 |
| H | -9.4271037902 | -4.2248107734 | 1.2793023616 |
| H | -8.5939894516 | -3.5644492986 | -0.0720055972 |
| H | -12.5418676620 | -2.7903178774 | 0.5790511427 |
| H | -11.8946570847 | -4.3607511538 | 0.8160413037 |
| H | 0.3392102715 | -6.8178808899 | -7.1403948975 |
| H | 0.9970468946 | -5.6986045061 | -2.6504670408 |
| H | -0.395829087 | -2.8206491126 | -6.8293971349 |
| H | -0.3095113986 | -3.5754644755 | -3.6684324348 |
| H | -5.6725084466 | 5.2619884665 | -2.2916942768 |
| H | -6.1228206978 | 6.6116295324 | -0.3840161216 |
| H | -4.4567972925 | 6.2161327569 | 0.0574987292 |
| H | -1.4441212989 | 3.5939991399 | -2.4290901447 |
| H | -5.1643603262 | 4.7614583092 | 1.7688168296 |
| H | -6.7497327972 | 5.0571011029 | 1.5862237262 |
| H | -5.8696179688 | 2.7961363650 | 0.7207599068 |
| H | -7.5250789479 | 3.4183503062 | 0.7924762768 |
| H | 0.0744338112 | 5.4062690432 | -2.9338234918 |
| H | -0.5843691123 | 6.3981716950 | -1.6309229754 |
| H | -4.0353593390 | 6.1837422108 | -0.3805943347 |
| Bradykinin (continued) |
|-----------------------|
| H -3.3722951437       | 7.0186840856 -1.9633512328 |
| H -1.8646601182       | 5.8853199202 -4.3629915948 |
| H -1.6118992882       | 7.4438580744 -3.5721706114 |
| H -8.8402232300       | 2.8703545387 -0.5123435958 |
| H 4.3504692575        | -4.5493856228 2.1037594476 |
| H -7.4666484798       | 0.8320496893 -1.0505633330 |
| H -8.1505455007       | 0.8384141301 -2.6741450342 |
| H 3.7860017096        | -5.0478233335 1.8627741478 |
| H 2.6696923092        | -3.6873528745 4.4297819207 |
| H 4.4577788892        | -2.8162574248 5.8207751542 |
| H 5.7003235835        | -3.6304242262 4.8659933909 |
| H 8.1755317110        | -1.3979612296 3.9359390207 |
| H 4.0666026781        | -1.1775528103 4.0734513207 |
| H -9.7980090742       | 0.6197972154 -0.0801939997 |
| H -10.4584576203      | 0.5262007833 -1.7025060637 |
| H -0.4035949789       | 1.9622867079 1.5372489788 |
| H -0.3817608690       | 3.6949421533 1.8627741478 |
| H 5.7253854466        | -0.5996152396 0.0770191283 |
| H -9.1619025066       | -1.5507334842 -2.1251363172 |
| H -8.4932668179       | -1.4591918722 -0.4910989292 |
| H 0.8980861069        | -2.133682388 0.2504393397 |
| H 3.9159226463        | 2.7444197574 2.1361084168 |
| H 7.6606116759        | -0.7833854465 2.4209129681 |
| H 7.8059626020        | -1.7288573426 0.9269449095 |
| H 0.7067169464        | -2.8393286291 -2.2503802635 |
| H 2.2250574177        | -3.6771915874 -2.0426172254 |
| H 4.7903586034        | 1.6257198060 4.2138087414 |
| H 3.2656197451        | 0.7925478982 4.4198140558 |
| H -1.4957058595       | -5.8606147446 -0.6883026056 |
| H -1.0050520450       | -7.7209886756 -2.3784814707 |
| H 0.6787261535        | -2.2546651785 -2.3287568281 |
| H 4.3374004533        | -2.4198777302 -2.1095459030 |
| H 0.5754275326        | -0.3518917794 -2.0671065605 |
| H 1.589651169         | 1.7206121092 5.7772863131 |
| H 4.7019022851        | 4.2824362217 4.2885276803 |
| H -1.6593365936       | -5.4234953988 -3.1490343259 |
| H -0.0097240652       | -4.8747049928 -2.9855173769 |
| H 5.4794913106        | -0.3387950736 -2.7731891861 |
| H 1.7285262175        | 1.7494156561 -2.7066250075 |
| H 4.1816760119        | 1.7645185313 -3.0557985199 |
| H 0.7889223947        | 3.5428667573 7.2403054891 |
| H 3.8986178821        | 6.1017235459 5.7470853821 |
| H -1.0128298633       | -6.8981429604 -5.0138814859 |
| H 0.6946763774        | -6.4998558063 -4.7763850552 |
| H 1.9468971009        | 5.7406094432 7.2389366841 |
Colistin
| Colistin (continued) |  |  |  |
|----------------------|-----------------|-----------------|
| H 3.2498978216 -0.3864879939 4.5126242292 | H -5.9687683441 3.0177801426 -1.1160855010 |
| H 4.8412648206 -2.1739156982 4.4441639505 | H -0.1356305776 -1.2998038101 -2.488128256 |
| H 1.1287090119 3.2274382237 0.1670645032 | H -0.2802078029 -1.3618079072 -0.7366248937 |
| H 6.4345857231 -4.603579799 -0.9697478365 | H -7.279436192 4.3955211744 9.5026225046 |
| H 0.9330366821 1.3008177362 -1.7203351464 | H -5.6520392646 4.8391113259 8.9844988971 |
| H 1.8804103586 -2.1549931115 5.6075126309 | H -6.5035469610 3.5062488994 8.1993189072 |
| H 2.0789308788 -0.7652723201 6.6805327644 | H 1.6093824112 0.3628340675 -6.9005786231 |
| H 0.5525568116 -1.0087401896 5.8257324116 | H -0.0012777966 -0.3638685349 -6.8678186860 |
| H 2.2680890728 1.5406264694 5.7913114314 | H 0.4655685465 0.7352037120 -5.5811019867 |
| H 0.8172034397 1.4556070351 4.7878146244 | H -2.8066414187 0.9389722296 7.2010439492 |
| H 2.3700347473 1.8758205443 4.0633657879 | H -4.3541097175 0.2525408662 3.2598868074 |
| H -0.4084463431 3.9142640495 2.6778726334 | H -2.9039884030 -0.7626300277 3.1342849095 |
| H 1.3382625504 3.6513712434 2.6196348942 | H -6.4881899936 5.2916912743 -2.0768756765 |
| H 6.6404373204 -1.1339552902 5.8141365088 | H -6.3821156628 5.9838809662 -0.4590835655 |
| H 6.2784518158 -2.7697159832 6.3757295300 |  |  |
Geometries of the peptides employed in this study optimized within the NTBM1 model

**Bradykinin**

| O      | -3.96260455 | 3.05143124 | -1.12237337 |
|--------|-------------|-------------|-------------|
| C      | -7.03116095 | 3.94023427 | -3.14735128 |
| N      | -1.51275856 | 5.14294274 | 5.50054077  |
| C      | 5.07173156  | -2.58787301| 0.22742707  |
| C      | 1.59718056  | -2.85851179| 2.24720448  |
| O      | 8.04068275  | 0.54150537 | 1.35942520  |
| C      | 2.23406285  | 3.98515188 | 0.10460174  |
| N      | 3.49976417  | 0.44045303 | 0.75793462  |
| C      | -1.09353134 | -3.98981096| -0.2659246  |
| C      | 0.24084143  | -7.44859247| 1.25251273  |
| N      | -1.23151834 | -8.83690426| 0.04931048  |
| C      | -3.03036671 | 4.94224289 | -1.8107491  |
| N      | -5.63912063 | 3.99715112 | -0.98171407 |
| C      | -4.72431253 | -2.48791883| 2.40122969  |
| C      | -0.42155837 | 3.26798902 | 0.05648896  |
| O      | -9.40979447 | 2.73637755 | -2.8435906  |
| C      | 2.39741870  | -3.58963658| 0.31437913  |
| C      | 5.38785764  | 0.49124549 | 1.95460713  |
| C      | 2.12636838  | 2.15463227 | 2.2970162  |
| N      | -10.35030820| -1.76054100| -0.4659018  |
| C      | -3.38431227 | -5.64586702| -0.57820491 |
| N      | -9.53838589 | -3.81599915| 0.42043041  |
| O      | -11.76190791| -3.51452459| 0.49664189  |
| N      | -0.63800084 | -5.12535153| -5.4820559  |
| C      | -0.40766957 | -0.03800210| -7.49042064 |
| C      | -0.32209026 | -3.72078071| -7.45819631 |
| C      | -5.45103192 | 4.97553181 | -1.24083415 |
| C      | -5.52341495 | 5.85727093 | 0.0052622  |
| C      | -1.69563495 | 4.31320153 | -1.78397944 |
| O      | -6.06473464 | 4.96583197 | 1.10547353  |
| C      | -6.69229005 | 3.76793223 | 0.43443142  |
| O      | -0.86069093 | 5.17452338 | -2.72840453 |
| C      | -2.99184108 | 6.29595380 | -2.32740796 |
| C      | -4.13653629 | 4.28433534 | -1.40256762 |
| C      | -1.65643174 | 4.63549543 | -3.01820830 |
| C      | -7.32550541 | 5.35372871 | -1.97147127 |
| C      | -1.20374164 | 4.26012680 | -0.36878350 |
| C      | -8.52573904 | 2.67198843 | -1.72319377 |
| C      | 3.88274363 | 3.70266647 | 2.29526889  |
| O      | -8.19592458 | 1.21154474 | -1.38666345 |
| C      | 3.74706255 | -4.19140380 | 3.73306647 |
| C      | 4.56524400 | -3.14225537 | 4.63615436 |
| C      | 4.86082837 | -2.02008549 | 3.76342338 |
| O      | -9.43084824 | 0.40220605 | -1.07657658 |
| C      | 0.01825895 | 3.07563039 | 1.44124214 |
| C      | 5.24025164 | -1.90831818 | 1.29994066 |
| C      | 2.58517557 | -3.36345960 | 1.61831518 |
| C      | 5.98464460 | -0.61162733 | 1.22756227 |
| C      | -9.16628211 | -1.06682926 | -0.84362125 |
| C      | 1.49819603 | 3.08088238 | 1.56524911 |
| C      | 1.18615148 | -3.27278467 | -0.42153865 |
| C      | 3.56019232 | 2.09642238 | 2.52291517 |
| C      | 7.44291309 | -0.66276818 | 1.63123189 |
| C      | 4.14539304 | 0.97296886 | 1.71980212 |
| C      | 1.55941181 | -2.89989818 | -1.85791121 |
| C      | 3.83958228 | 2.00238559 | 4.01952879 |
| C      | 0.12723015 | -4.33919630 | -0.39017846 |
| C      | 2.35337538 | -1.62409093 | -1.98467475 |
| C      | 3.22236452 | 3.11750026 | 8.25882235 |
| C      | -0.70586669 | -6.62943540 | -0.77104678 |
| C      | -10.48866446| -3.03619218 | 0.15843797 |

-17-
**Bradykinin (continued)**

| H   | -3.08791336 | 6.98937166 | -1.47789416 |
| H   | -1.79286711 | 6.55436780 | -4.09711900 |
| H   | -1.12198412 | 7.31908695 | -2.63243513 |
| H   | -9.10599819 | 3.08557973 | -0.88416124 |
| H   | 4.45745269  | -4.41672742 | 1.68825738 |
| H   | -7.52887736 | 1.20052399 | -0.51169236 |
| H   | -7.66496082 | 0.75798672 | -2.3850607 |
| H   | 4.27428018  | -5.15047686 | 3.85109241 |
| H   | 2.68915774  | -4.34324269 | 3.99395902 |
| H   | 3.62117484  | -2.76905246 | 5.35676891 |
| H   | 5.20078865  | -3.58208218 | 5.20333836 |
| H   | 5.91950177  | -1.78832192 | 3.94143852 |
| H   | 4.24461264  | -1.11517929 | 3.87404094 |
| H   | -9.0591032  | 0.81730362 | -0.17222460 |
| H   | -10.14044225| 0.49880667 | -1.91530566 |
| H   | -0.41344676 | 2.11750983 | 1.74543841 |
| H   | -0.41402615 | 3.90694023 | 1.99124761 |
| H   | 5.97568232  | -0.30511598 | 0.16800164 |
| H   | -8.78474059 | -1.53112746 | -1.7718945 |
| H   | -8.41297093 | -1.19063598 | -0.04343910 |
| H   | 0.75595805  | -2.39415376 | 0.08398972 |
| H   | 3.94926836  | 3.05183503 | 2.13892715 |
| H   | 7.58444315  | -0.81607160 | 2.71861279 |
| H   | 8.01950902  | -1.37948493 | 1.02548141 |
| H   | 0.61907073  | -2.78269878 | -2.42032364 |
| H   | 2.12152320  | -3.73792439 | -2.29709716 |
| H   | 4.93292637  | 2.02767012 | 4.15536272 |
| H   | 3.46931070  | 1.03297233 | 4.38863052 |
| H   | -1.65014579 | -6.11641099 | -0.53960651 |
| H   | -1.56004604 | -7.76377400 | -2.37546297 |
| H   | 0.21914576  | -7.61958959 | -2.44460853 |
| H   | 4.28468774  | -2.60304820 | -2.26844134 |
| H   | 0.62241239  | -3.1475712 | -1.74834116 |
| H   | 1.63423321  | 1.89103852 | 5.68627621 |
| H   | 4.65723357  | 4.62830301 | 4.17480903 |
| H   | -1.85733087 | 5.49545361 | -3.11101625 |
| H   | -0.12154991 | -5.13533453 | -2.89372195 |
| H   | 5.55013797  | -0.48621423 | -2.58299519 |
| H   | 1.90626423  | 1.79240428 | -2.06475000 |
| H   | 4.37043084  | 1.71876025 | -2.49129248 |
| H   | 0.66452535  | 3.73024407 | 7.05084117 |
| H   | 3.67463668  | 6.45557834 | 5.54804202 |
| H   | -1.32332933 | -7.00789870 | -4.98539576 |
| H   | 0.43422995  | -6.71308505 | -4.72906573 |
| H   | 1.68040270  | 6.01660218 | 6.99475107 |
Colistin (continued)

| H  | 3.18326175 | -0.42938841 | 4.47458330 |
| H  | 4.90410898 | -2.27089087 | 4.46894167 |
| H  | 1.21025180 | 3.34022801 | 0.08152991 |
| H  | 6.56669028 | -4.47497786 | -0.95461541 |
| H  | 0.11939144 | 1.13037817 | -1.49511114 |
| H  | 1.80910781 | -2.11070814 | 5.53231180 |
| H  | 2.09810664 | -0.72483885 | 6.63117316 |
| H  | 0.50399394 | -0.91780052 | 5.83212748 |
| H  | 2.37449639 | 1.50953309 | 5.76486167 |
| H  | 0.88529663 | 1.54562552 | 4.76967249 |
| H  | 2.48769164 | 1.81483774 | 4.00832368 |
| H  | -0.43130257 | 3.87794571 | 2.58514305 |
| H  | 1.35110329 | 3.74459911 | 2.58931077 |
| H  | 6.62247063 | -1.21948503 | 5.81304797 |
| H  | 6.30715603 | -2.90371212 | 6.34028325 |
| H  | 7.78805643 | -2.51927109 | 5.40374372 |
| H  | 5.55391364 | -4.59527960 | 4.68845049 |
| H  | 6.98740735 | -4.33282699 | 3.64337367 |
| H  | 5.33818026 | -4.13496097 | 2.97065357 |
| H  | 1.04703862 | 3.70375242 | -1.95347926 |
| H  | 0.64288352 | 3.18169713 | -3.59692499 |
| H  | 4.12585769 | -5.84851758 | 0.26605293 |
| H  | 5.80662789 | -5.82834903 | 0.88851105 |
| H  | 5.48254111 | -4.40656709 | -5.28938716 |
| H  | -2.30736977 | 0.52126238 | -0.96769406 |
| H  | 3.01722573 | 2.85960389 | -2.84048515 |
| H  | 2.44230312 | 1.56298105 | -1.72761429 |
| H  | -5.44709792 | 6.27350470 | 6.89809381 |
| H  | -6.96638033 | 4.09867790 | 5.41281854 |
| H  | -5.43276995 | 3.97379445 | 6.31831153 |
| H  | 3.30534653 | -0.65559092 | -5.48587252 |
| H  | 0.61789650 | 6.06620240 | 2.50297383 |
| H  | -0.26961557 | 5.75978278 | 0.96496942 |
| H  | -4.41667457 | 5.38597060 | 4.66988507 |
| H  | -5.92031239 | 5.46208398 | 3.71377031 |
| H  | 2.83253867 | -5.22013017 | -3.99153247 |
| H  | 3.10768780 | -5.05291235 | -5.75124831 |
| H  | -4.01171703 | 1.66531702 | 0.43459666 |
| H  | -2.58772238 | -2.04944144 | -2.60566500 |
| H  | -2.63068870 | -1.90198650 | -0.82376228 |
| H  | 4.90040572 | -7.10577767 | -1.73612112 |
| H  | 6.55823175 | -7.16419309 | -1.03392239 |
| H  | -7.42652463 | 6.45232132 | 8.27540805 |
| H  | -8.23732153 | 5.15406887 | 7.35979954 |
| H  | 0.49792883 | -1.77303060 | -5.03178961 |
| H  | -6.53662578 | 4.32341103 | 1.41314443 |
| H  | -4.01014004 | 3.19942284 | 4.42492016 |
| H  | -5.56259608 | 2.99337389 | 3.55050639 |
| H  | -2.83616267 | -0.50650957 | 0.82945539 |
| H  | -7.27221949 | 7.81787915 | 6.34262233 |
| H  | -7.95052901 | 6.61792740 | 5.19796148 |
| H  | -6.32219876 | 7.31472227 | 4.91552567 |
| H  | 4.64159073 | -6.94436908 | -3.90632061 |
| H  | 4.79627225 | -6.82628019 | -5.69579544 |
| H  | -7.15590948 | 3.39659807 | -0.79197576 |

-20-