**A New Database and Benchmark of the Bond Energies of Noble-Gas Containing Molecules**

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Five Tables.

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Table S1. The single level performance (MUE in kcal/mol) on the NGBE59 database, MGAE109 database, and all 168 energies. The root-mean-square deviations and maximum absolute errors are shown in parentheses and brackets.

|  |  |  |  |
| --- | --- | --- | --- |
| Method | NGBE59  | MGAE109 | Total 168 |
| MP2/aptz | 10.3 (13.8) [30.3] | 7.1 (8.8) [24.1] | 8.2 (10.8) [30.3] |
| MP2/ptz | 8.1 (10.3) [22.6] | 7.8 (9.8) [26.6] | 7.9 (9.9) [26.6] |
| MP2/apdz | 6.6 (8.9) [20.6] | 27.3 (32.1) [67.8] | 20.1 (26.3) [67.8] |
| MP2/pdz | 15.9 (19.0) [20.6] | 35.1 (39.7) [76.9] | 28.3 (34.0) [76.9] |
| B3LYP/aptz | 3.3 (4.3) [12.8] | 5.6 (8.4) [31.6] | 4.8 (7.2) [31.6] |
| B3LYP/ptz | 4.2 (5.4) [11.2] | 5.2 (8.0) [31.0] | 4.9 (7.2) [31.0] |
| B3LYP/apdz | 4.0 (5.3) [17.5] | 13.3 (17.2) [65.2] | 10.0 (14.1) [65.2] |
| B3LYP/pdz | 10.9 (12.9) [23.6] | 13.8 (17.6) [68.1] | 12.8 (16.1) [68.1] |
| MPW1B95/aptz | 2.1 (2.6) [7.4] | 3.0 (4.6) [19.4] | 2.7 (4.0) [19.4] |
| MPW1B95/ptz | 3.9 (4.9) [11.5] | 3.4 (4.9) [18.3] | 3.6 (4.9) [18.3] |
| MPW1B95/apdz | 2.8 (3.7) [12.1] | 7.3 (10.3) [51.7] | 5.7 (8.6) [51.7] |
| MPW1B95/pdz | 11.0 (12.7) [22.4] | 7.9 (11.6) [58.0] | 9.0 (12.0) [58.0] |
| MPW1PW91/aptz | 2.8 (3.6) [10.4] | 5.3 (7.4) [34.0] | 4.4 (6.3) [34.0] |
| MPW1PW91/ptz | 5.0 (6.2) [16.0] | 5.2 (7.4) [33.3] | 5.1 (7.0) [33.3] |
| MPW1PW91/apdz | 4.0 (5.1) [15.1] | 12.4 (15.4) [67.6] | 9.5 (12.7) [67.6] |
| MPW1PW91/pdz | 12.3 (14.4) [26.5] | 13.4 (16.8) [74.8] | 13.0 (16.0) [74.8] |
| B98/aptz | 3.0 (3.7) [8.7] | 4.7 (6.5) [24.6] | 4.1 (5.7) [24.6] |
| B98/ptz | 3.9 (5.0) [11.2] | 4.5 (6.2) [23.7] | 4.3 (5.8) [23.7] |
| B98/apdz | 3.3 (4.4) [13.4] | 12.6 (15.7) [58.8] | 9.4 (12.8) [58.8] |
| B98/pdz | 10.2 (12.1) [22.5] | 13.6 (16.9) [65.6] | 12.5 (15.3) [65.6] |
| BMK/aptz | 2.5 (3.3) [9.2] | 3.2 (4.5) [20.0] | 3.0 (4.1)[20.0] |
| BMK/ptz | 4.7 (5.7) [12.9] | 3.5 (4.9) [19.4] | 3.9 (5.2) 19.4] |
| BMK/apdz | 4.8 (5.9) [14.8] | 10.4 (13.2) [54.2] | 8.5 (11.1) [54.2] |
| BMK/pdz | 13.3 (15.7) [27.8] | 12.0 (15.1) [61.2] | 12.5 (15.3) [61.2] |
| M06-2X/aptz | 5.2 (6.2) [12.1] | 2.8 (4.2) [18.6] | 3.6 (4.9) [18.6] |
| M06-2X/ptz | 7.6 (8.8) [15.1] | 3.0 (4.4) [19.1] | 4.6 (6.3) [19.1] |
| M06-2X/apdz | 7.8 (9.1) [16.5] | 10.0 (12.5) [45.8] | 9.3 (11.4) [45.8] |
| M06-2X/pdz | 16.4 (18.8) [29.3] | 10.8 (13.8) [56.0] | 12.8 (15.7) [56.0] |
| B2GP-PLYP/aptz | 2.1 (2.8) [9.0] | 6.5 (7.5) [19.2] | 4.9 (6.2) [19.2] |
| B2GP-PLYP/ptz | 6.3 (7.6) [14.4] | 7.7 (8.8) [21.4] | 7.2 (8.3) [21.4] |
| B2GP-PLYP/apdz | 5.3 (6.3) [13.5] | 21.6 (24.6) [59.2] | 15.9 (20.1) [59.2] |
| B2GP-PLYP/pdz | 17.6 (20.2) [31.4] | 25.4 (28.8) [76.5] | 22.7 (26.0) [76.5] |
| DSD-BLYP/aptz | 2.0 (2.6) [8.4] | 4.6 (5.8) [21.5] | 3.7 (4.9) [21.5] |
| DSD-BLYP/ptz | 5.5 (6.8) [12.5] | 6.0 (7.2) [23.5] | 5.8 (7.0) [23.5] |
| DSD-BLYP/apdz | 4.5 (5.6) [14.1] | 21.0 (24.0) [56.0] | 15.2 (19.6) [56.0] |
| DSD-BLYP/pdz | 17.3 (19.9) [30.7] | 25.4 (28.8) [75.2] | 22.5 (25.9) [75.2] |

Table S2 The performance (MUE in kcal/mol) and optimized coefficients of selected MC-DFT methods on the NGBE59 database, MGAE109 database, and all 168 energies. The root-mean-square deviations and maximum absolute errors are shown in parentheses and brackets.

|  |  |  |  |
| --- | --- | --- | --- |
|  | NGBE59 | MGAE109 | Total 168 |
| Method | MUE | c1 | c2 | MUE | c1 | c2 | MUE | c1 | c2 |
|  M06-2X/apdz/aptz | 3.1 (4.0)[10.1] | 2.323 |  | 2.1 (3.5)[18.5] | 1.214 |  | 3.0 (4.3)[18.9] | 1.251 |  |
| MPW1B95/apdz/aptz | 2.0 (2.5)[5.9] | 1.429 |  | 3.0 (4.6)[20.3] | 0.975 |  | 2.7 (4.0)[20.1] | 0.979 |  |
| MPW1PW91/apdz/aptz | 2.2 (2.7)[6.9] | 2.402 |  | 3.6 (4.9)[18.5] | 1.599 |  | 3.2 (4.3)[18.4] | 1.604 |  |
| BMK/apdz/aptz | 2.1 (2.8)[7.9] | 1.444 |  | 2.8 (4.2)[22.0] | 1.205 |  | 2.6 (3.8)[22.1] | 1.217 |  |
| B2GP-PLYP/apdz/aptz | 1.7 (2.3)[8.7] | 1.349 |  | 1.9 (2.8)[9.6] | 1.373 |  | 1.9 (2.6)[9.6] | 1.373 |  |
| DSD-BLYP/apdz/aptz | 2.0 (2.6)[8.2] | 1.038 |  | 2.2 (3.6)[17.7] | 1.220 |  | 2.2 (3.3)[17.5] | 1.215 |  |
| B98/apdz/aptz | 3.0 (3.7)[8.2]  | 1.112 |  | 2.5 (3.7) [17.6] | 1.508 |  | 2.7 (3.8)[17.4] | 1.484 |  |
| B3LYP/apdz/aptz | 3.2 (4.1)[11.2] | 1.325 |  | 3.8 (6.1)[25.6] | 1.436 |  | 3.6 (5.5)[25.6] | 1.436 |  |
| M06-2X/pdz/apdz/aptz | 3.1 (4.0)[9.9] | 0.933 | 2.559 | 1.9 (3.3)[18.6] | 1.279 | 1.193 | 2.6 (4.1)[18.7] | 1.254 | 1.218 |
| MPW1B95/pdz/apdz/aptz | 1.7 (2.2)[23.7] | 0.868 | 1.943 | 2.7 (4.2)[18.7] | 1.421 | 0.940 | 2.7 (4.0)[20.3] | 0.998 | 0.975 |
| MPW1PW91/pdz/apdz/aptz | 2.1 (2.8)[30.2] | 0.908 | 2.664 | 3.3 (4.3)[11.6] | 1.697 | 1.584 | 3.1 (4.3)[17.8] | 1.068 | 1.598 |
| BMK/pdz/apdz/aptz | 1.9 (2.5)[27.9] | 0.851 | 1.848 | 2.7 (4.0)[22.2] | 1.415 | 1.128 | 2.6 (3.8)[22.1] | 1.016 | 1.206 |
| B2GP-PLYP/pdz/apdz/aptz | 1.6 (2.3)[10.7] | 0.938 | 1.550 | 1.7 (2.4)[9.7] | 1.299 | 1.314 | 1.9 (2.6)[9.6] | 0.989 | 1.374 |
| DSD-BLYP/pdz/apdz/aptz | 1.8 (2.4)[17.1] | 0.920 | 1.218 | 2.1 (3.4)[17.9] | 1.168 | 1.179 | 2.1 (3.3)[17.6] | 0.955 | 1.232 |
| B98/pdz/apdz/aptz | 2.6 (3.2)[17.7] | 0.843 | 1.357 | 2.4 (3.7)[17.8] | 1.257 | 1.494 | 2.6 (3.6)[17.4] | 0.861 | 1.506 |
| B3LYP/pdz/apdz/aptz | 2.7 (3.3)[22.4] | 0.810 | 2.173 | 3.8 (6.0)[24.9] | 0.891 | 1.441 | 3.5 (5.4)[25.3] | 0.902 | 1.451 |

Table S3. The performance (MUE in kcal/mol) and optimized coefficients of doubly hybrid methods on the NGBE59 database, MGAE109 database, and all 168 energies. The root-mean-square deviations and maximum absolute errors are shown in parentheses and brackets.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | NGBE59 |  | MGAE109 | Total 168 |
| Method | MUE | c1 | c2 | MUE | c1 | c2 | MUE | c1 | c2 |
| MPW1B95/aptz + MP2/apdz | 2.1 (2.6)[7.5] | 0.991 | 0.006 | 2.9 (4.4)[20.0] | 0.992 | 0.005 | 2.6 (3.9)[20.1] | 1.000 | 0.005 |
| MPW1PW91/aptz + MP2/apdz | 2.4 (3.0)[31.3] | 0.890 | 0.132 | 3.9 (6.0)[28.7] | 0.920 | 0.119 | 3.4 (5.2)[29.0] | 0.935 | 0.101 |
| B2GP-PLYP/aptz + MP2/apdz | 1.5 (2.0)[12.1] | 1.176 |  | 2.2 (3.5)[13.9] | 1.031 | 0.006 | 2.0 (3.2)[14.1] | 1.072 |  |
| DSD-BLYP /aptz + MP2/apdz | 1.4 (1.9)[25.7] | 1.252 |  | 2.4 (4.1)[19.1] | 1.104 | 0.099 | 2.1 (3.6)[19.6] | 1.118 |  |
| B98 /aptz + MP2/apdz | 2.8 (3.6)[29.2] | 0.918 | 0.059 | 3.0 (4.9)[21.8] | 1.105 | 0.096 | 3.1 (4.7)[21.8] | 1.101 | 0.093 |
| B3YP /aptz + MP2/apdz | 3.2 (4.1)[32.9] | 0.880 | 0.110 | 3.8 (6.2)[27.2] | 0.880 | 0.168 | 3.9 (5.9)[28.2] | 0.929 | 0.108 |
| M06-2X /aptz + MP2/apdz | 3.1 (3.9)[32.0] | 1.019 | 0.048 | 2.3 (3.9)[19.4] | 1.041 | 0.038 | 2.9 (4.1)[19.0] | 0.902 | 0.132 |
| BMK /aptz + MP2/apdz | 2.2 (3.0)[7.8] | 1.096 | 0.069 | 3.0 (4.6)[22.1] | 1.081 |  | 2.8 (4.1)[22.1] | 1.009 | 0.002 |
| MPW1B95/apdz + MP2/apdz | 2.4 (3.3)[10.6] | 0.983 | 0.033 | 4.4 (8.3)[49.1] | 1.100 | 0.074 | 3.7 (6.9[48.1]) | 1.064 |  |
| MPW1PW91/apdz + MP2/apdz | 2.7 (3.5)[10.1] | 0.934 | 0.116 | 5.2 (9.1)[53.2] | 0.939 | 0.146 | 4.4 (7.9)[56.0] | 0.986 | 0.089 |
| B2GP-PLYP/apdz + MP2/apdz | 2.1 (2.8)[7.2] | 1.187 |  | 4.2 (7.6)[42.6] | 1.220 | 0.079 | 3.5 (6.6)[44.3] | 1.268 | 0.132 |
| DSD-BLYP/ apdz + MP2/apdz | 2.1 (2.9)[10.0]  | 1.243 |  | 4.6 (8.0)[40.4] | 1.280 | 0.143 | 3.8 (7.0)[43.3] | 1.365 | 0.238 |
| B98/apdz + MP2/apdz | 3.2 (4.1)[56.2] | 0.856 | 0.143 | 4.8 (8.5)[49.6] | 1.115 | 0.038 | 4.7 (7.9)[53.4] | 1.186 |  |
| B3YP/ apdz + MP2/apdz | 3.6 (4.6)[59.6] | 0.857 | 0.156 | 5.3 (8.8)[46.4] | 0.881 | 0.225 | 5.3 (8.4)[50.8] | 0.955 | 0.135 |
| M06-2X/apdz + MP2/apdz | 3.2 (4.0)[9.7] | 1.063 | 0.069 | 4.1 (7.8)[41.9] | 1.220 | 0.184 | 4.2 (6.2)[33.1] | 0.910 | 0.172 |
| BMK/apdz + MP2/apdz | 2.2 (3.0)[31.3] | 1.099 | -0.071 | 5.0 (8.1)[46.7] | 1.072 |  | 4.5 (6.8)[10.6] | 1.052 | 0.010 |

Table S4. Calculated %TAE*e*[(T)] at CCSD(T)/CBS level.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | He | Ne | Ar | Kr | Xe |
| HNgF | 3.6 |  | 3.7 | 24.6 | 12.5 |
| HNgH |  |  |  |  | 86.6 |
| HNgCl |  |  |  | 73.2 | 19.3 |
| HNgCCH |  |  |  | 5.6 | 4.8 |
| FNgCCH |  |  | 6.7 | 6.1 | 5.1 |
| FNgBO |  |  | 4.0 | 4.1 | 3.6 |
| FNgCN |  |  | 13.0 | 9.8 | 7.6 |
| HNgCN |  |  |  | 7.6 | 6.6 |
| HNgNC |  |  |  | 7.0 | 6.3 |
| FNgCH3 |  |  | 3.7 | 3.6 | 3.2 |
| FNgBNH |  |  | 9.8 | 13.0 | 5.3 |
| FNgNBH |  |  |  | 2.7 | 2.5 |
| HNgNBH |  |  |  | 7.5 | 5.8 |
| NgBeO | 5.8 | 5.3 | 2.4 | 2.4 | 1.6 |
| NgAuF | 4.4 | 4.6 | 3.9 | 5.1 | 5.3 |
| FNgCC | 7.0 |  | 7.4 | 7.4 | 6.7 |
| FNgO | 1.9 |  | 6.6 | 7.8 | 5.7 |
| HBNNgO |  |  |  | 6.2 | 5.9 |
| FNgBN | 7.6 | 9.9 | 7.4 | 8.1 | 7.7 |

Table S5. Cartesian coordinates of the molecules in NGBE59 database

HHeF

H 0.00000000 0.00000000 -1.80466700

He 0.00000000 0.00000000 -0.99366700

F 0.00000000 0.00000000 0.42133300

HArF

F 0.00000000 0.00000000 -1.39967700

Ar 0.00000000 0.00000000 0.59260300

H 0.00000000 0.00000000 1.93023600

HKrF

F 0.00000000 0.00000000 -1.67458700

Kr 0.00000000 0.00000000 0.36741300

H 0.00000000 0.00000000 1.84441300

HXeF

F 0.00000000 0.00000000 -1.84469100

Xe 0.00000000 0.00000000 0.27162700

H 0.00000000 0.00000000 1.93434900

HXeH

H 0.00000000 0.00000000 1.92194900

Xe 0.00000000 0.00000000 0.00000000

H 0.00000000 0.00000000 -1.92194900

HKrCl

H 0.00000000 0.00000000 2.28975000

Kr 0.00000000 0.00000000 0.76669000

Cl 0.00000000 0.00000000 -1.75827000

HXeCl

H 0.00000000 0.00000000 2.28747700

Xe 0.00000000 0.00000000 0.59565700

Cl 0.00000000 0.00000000 -2.02664300

HKrCCH

H 0.00000000 0.00000000 2.36515300

Kr 0.00000000 0.00000000 0.75118900

C 0.00000000 0.00000000 -1.52022400

C 0.00000000 0.00000000 -2.74581900

H 0.00000000 0.00000000 -3.81170100

HXeCCH

H 0.00000000 0.00000000 2.32007600

Xe 0.00000000 0.00000000 0.56603500

C 0.00000000 0.00000000 -1.78746600

C 0.00000000 0.00000000 -3.01360100

H 0.00000000 0.00000000 -4.07954800

FArCCH

F 0.00000000 0.00000000 2.32237700

Ar 0.00000000 0.00000000 0.39907300

C 0.00000000 0.00000000 -1.42659700

C 0.00000000 0.00000000 -2.63711800

H 0.00000000 0.00000000 -3.70241800

FKrCCH

F 0.00000000 0.00000000 2.26679400

Kr 0.00000000 0.00000000 0.28882300

C 0.00000000 0.00000000 -1.63461500

C 0.00000000 0.00000000 -2.84660900

H 0.00000000 0.00000000 -3.91145500

FXeCCH

F 0.00000000 0.00000000 2.30200200

Xe 0.00000000 0.00000000 0.23787000

C 0.00000000 0.00000000 -1.84579200

C 0.00000000 0.00000000 -3.06044000

H 0.00000000 0.00000000 -4.12558700

FArBO

F 0.00000000 0.00000000 2.37543000

Ar 0.00000000 0.00000000 0.38813700

B 0.00000000 0.00000000 -1.43906300

O 0.00000000 0.00000000 -2.64625500

FKrBO

F 0.00000000 0.00000000 2.32431400

Kr 0.00000000 0.00000000 0.29349000

B 0.00000000 0.00000000 -1.67784400

O 0.00000000 0.00000000 -2.88690800

FXeBO

F 0.00000000 0.00000000 2.34647600

Xe 0.00000000 0.00000000 0.24896300

B 0.00000000 0.00000000 -1.91327600

O 0.00000000 0.00000000 -3.12448500

FArCN

F 0.00000000 0.00000000 2.32410700

Ar 0.00000000 0.00000000 0.40926400

C 0.00000000 0.00000000 -1.54624200

N 0.00000000 0.00000000 -2.71518200

FKrCN

F 0.00000000 0.00000000 2.22257200

Kr 0.00000000 0.00000000 0.28240200

C 0.00000000 0.00000000 -1.69247200

N 0.00000000 0.00000000 -2.85925700

FXeCN

F 0.00000000 0.00000000 2.26100700

Xe 0.00000000 0.00000000 0.23011700

C 0.00000000 0.00000000 -1.89286000

N 0.00000000 0.00000000 -3.05974500

HArCN

H 0.00000000 0.00000000 2.55684400

Ar 0.00000000 0.00000000 1.13496900

C 0.00000000 0.00000000 -1.13630300

N 0.00000000 0.00000000 -2.30978000

HKrCN

H 0.00000000 0.00000000 2.28278800

Kr 0.00000000 0.00000000 0.74010000

C 0.00000000 0.00000000 -1.59362300

N 0.00000000 0.00000000 -2.76637900

HXeCN

H 0.00000000 0.00000000 2.27407200

Xe 0.00000000 0.00000000 0.55837200

C 0.00000000 0.00000000 -1.86302800

N 0.00000000 0.00000000 -3.03542800

HArNC

H 0.00000000 0.00000000 2.39965600

Ar 0.00000000 0.00000000 1.08510200

N 0.00000000 0.00000000 -1.14009300

C 0.00000000 0.00000000 -2.32513900

HKrNC

H 0.00000000 0.00000000 2.17164500

Kr 0.00000000 0.00000000 0.70397400

N 0.00000000 0.00000000 -1.56965900

C 0.00000000 0.00000000 -2.75451300

HXeNC

H 0.00000000 0.00000000 2.19129300

Xe 0.00000000 0.00000000 0.52761600

N 0.00000000 0.00000000 -1.81330900

C 0.00000000 0.00000000 -2.99823300

FArCH3

F 0.00000000 0.00000000 2.04371600

Ar 0.00000000 0.00000000 0.00487000

C 0.00000000 0.00000000 -1.97157300

H 0.00000000 1.05538000 -2.21722500

H -0.91398600 -0.52769000 -2.21722500

H 0.91398600 -0.52769000 -2.21722500

FKrCH3

F 0.00000000 0.00000000 2.08750000

Kr 0.00000000 0.00000000 0.01106000

C 0.00000000 0.00000000 -2.03637000

H 0.00000000 1.04662000 -2.32247300

H -0.90640000 -0.52331000 -2.32247300

H 0.90640000 -0.52331000 -2.32247300

FXeCH3

F 0.00000000 0.00000000 2.15608500

Xe 0.00000000 0.00000000 0.02062400

C 0.00000000 0.00000000 -2.17436100

H 0.00000000 1.03918800 -2.49076400

H -0.89996300 -0.51959400 -2.49076400

H 0.89996300 -0.51959400 -2.49076400

FArBNH

F 0.00000000 0.00000000 2.43177200

Ar 0.00000000 0.00000000 0.39885900

B 0.00000000 0.00000000 -1.40017500

N 0.00000000 0.00000000 -2.63367500

H 0.00000000 0.00000000 -3.62880600

FKrBNH

F 0.00000000 0.00000000 2.36977500

Kr 0.00000000 0.00000000 0.30537800

B 0.00000000 0.00000000 -1.64810600

N 0.00000000 0.00000000 -2.88578200

H 0.00000000 0.00000000 -3.88057700

FXeBNH

F 0.00000000 0.00000000 2.38691200

Xe 0.00000000 0.00000000 0.25928900

B 0.00000000 0.00000000 -1.88897500

N 0.00000000 0.00000000 -3.13057200

H 0.00000000 0.00000000 -4.12495300

FKrNBH

F 0.00000000 0.00000000 0.00000000

Kr 0.00000000 0.00000000 1.93184000

X 1.00000000 0.00000000 1.93184000

N 0.00000000 -0.00000000 3.82942700

X -1.00000000 -0.00000000 3.82942700

B 0.00000000 -0.00000000 5.08255200

X 1.00000000 -0.00000000 5.08255200

H 0.00000000 -0.00000000 6.25304300

FXeNBH

F 0.00000000 0.00000000 2.25282000

Xe 0.00000000 0.00000000 0.22204100

N 0.00000000 0.00000000 -1.81255300

B 0.00000000 0.00000000 -3.06771600

H 0.00000000 0.00000000 -4.23911700

HKrNBH

H 0.00000000 0.00000000 2.69943200

Kr 0.00000000 0.00000000 0.63503500

N 0.00000000 0.00000000 -1.31844900

B 0.00000000 0.00000000 -2.55612500

H 0.00000000 0.00000000 -3.55092000

HXeNBH

H 0.00000000 0.00000000 2.63120800

Xe 0.00000000 0.00000000 0.50358500

N 0.00000000 0.00000000 -1.64467900

B 0.00000000 0.00000000 -2.88627600

H 0.00000000 0.00000000 -3.88065700

HeBeO

He 0.00000000 0.00000000 -2.07066700

Be 0.00000000 0.00000000 -0.54675000

O 0.00000000 0.00000000 0.79104100

NeBeO

Ne 0.00000000 0.00000000 1.46825000

Be 0.00000000 0.00000000 -0.33059300

O 0.00000000 0.00000000 -1.67001700

ArBeO

Ar 0.00000000 0.00000000 1.18698300

Be 0.00000000 0.00000000 -0.88632600

O 0.00000000 0.00000000 -2.22754800

KrBeO

Kr 0.00000000 0.00000000 0.77402300

Be 0.00000000 0.00000000 -1.42726800

O 0.00000000 0.00000000 -2.76947200

XeBeO

Xe 0.00000000 0.00000000 0.59382200

Be 0.00000000 0.00000000 -1.77617000

O 0.00000000 0.00000000 -3.12021400

HeAuF

He 0.00000000 0.00000000 1.99158900

Au 0.00000000 0.00000000 0.14989600

F 0.00000000 0.00000000 -1.75832800

NeAuF

Ne 0.00000000 0.00000000 -2.37779700

Au 0.00000000 0.00000000 0.07368900

F 0.00000000 0.00000000 1.99517000

ArAuF

Ar 0.00000000 0.00000000 -2.15563800

Au 0.00000000 0.00000000 0.24473200

F 0.00000000 0.00000000 2.16307500

KrAuF

Kr 0.00000000 0.00000000 -1.89475100

Au 0.00000000 0.00000000 0.57837400

F 0.00000000 0.00000000 2.50216700

XeAuF

Xe 0.00000000 0.00000000 -1.71223400

Au 0.00000000 0.00000000 0.85325700

F 0.00000000 0.00000000 2.78370400

FHeCC

F 0.00000000 0.00000000 1.88597700

He 0.00000000 0.00000000 0.29204100

C 0.00000000 0.00000000 -0.83438900

C 0.00000000 0.00000000 -2.09192200

FArCC

F 0.00000000 0.00000000 2.41634400

Ar 0.00000000 0.00000000 0.24062000

C 0.00000000 0.00000000 -1.54173600

C 0.00000000 0.00000000 -2.80463700

FKrCC

F 0.00000000 0.00000000 2.38739500

Kr 0.00000000 0.00000000 0.18603200

C 0.00000000 0.00000000 -1.71807900

C 0.00000000 0.00000000 -2.97920400

FXeCC

F 0.00000000 0.00000000 2.41188100

Xe 0.00000000 0.00000000 0.16022200

C 0.00000000 0.00000000 -1.89939900

C 0.00000000 0.00000000 -3.16041500

FHeO

F 0.00000000 0.00000000 0.00000000

He 0.00000000 0.00000000 1.62468600

O 0.00000000 0.00000000 2.73423900

FArO

F 0.00000000 0.00000000 -2.05713200

Ar 0.00000000 0.00000000 0.16872000

O 0.00000000 0.00000000 1.93465200

FKrO

F 0.00000000 0.00000000 -2.15570600

Kr 0.00000000 0.00000000 0.10378400

O 0.00000000 0.00000000 1.95813800

FXeO

F 0.00000000 0.00000000 -2.23625000

Xe 0.00000000 0.00000000 0.07224000

O 0.00000000 0.00000000 2.02816200

HBNKrO

O 0.00000000 0.00000000 2.30472100

Kr 0.00000000 0.00000000 0.45532100

N 0.00000000 0.00000000 -2.00159000

B 0.00000000 0.00000000 -3.27258000

H 0.00000000 0.00000000 -4.45527400

HBNXeO

O 0.00000000 0.00000000 2.29285400

Xe 0.00000000 0.00000000 0.34202600

N 0.00000000 0.00000000 -2.15503400

B 0.00000000 0.00000000 -3.42411000

H 0.00000000 0.00000000 -4.60643900

FHeBN

F 0.00000000 0.00000000 2.06167800

He 0.00000000 0.00000000 0.33807800

B 0.00000000 0.00000000 -0.86422200

N 0.00000000 0.00000000 -2.13002200

FArBN

F 0.00000000 0.00000000 2.53833100

Ar 0.00000000 0.00000000 0.25993100

B 0.00000000 0.00000000 -1.55286900

N 0.00000000 0.00000000 -2.82276900

FNeBN

F 0.00000000 0.00000000 2.53833100

Ar 0.00000000 0.00000000 0.25993100

B 0.00000000 0.00000000 -1.55286900

N 0.00000000 0.00000000 -2.82276900

FKrBN

F 0.00000000 0.00000000 2.50798600

Kr 0.00000000 0.00000000 0.20468600

B 0.00000000 0.00000000 -1.75351400

N 0.00000000 0.00000000 -3.02471400

FXeBN

F 0.00000000 0.00000000 2.51892500

Xe 0.00000000 0.00000000 0.18142500

B 0.00000000 0.00000000 -1.96267500

N 0.00000000 0.00000000 -3.23627500