Phenanthrene: Establishing lower and upper bounds to the binding energy of a very weakly bound anion

Elisabeth Gruber,‡a Siegfried Kollotzek,‡a Stefan Bergmeister, Fabio Zappa,a Milan Ončák,a Paul Scheier,a Olof Echt*ab

a Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck (Austria)
b Department of Physics, University of New Hampshire, Durham, NH 03824 (USA)
† Both authors contributed equally
* Corresponding Authors: Milan Ončák <Milan.Onca@uibk.ac.at>; Paul Scheier <Paul.Scheier@uibk.ac.at>; Olof Echt <olof.echt@unh.edu>

• Fig. S1: Negative ion mass spectrum of HNDs doped with Ph.
• Fig. S2: CID spectrum of (H₂O)₃Ph⁻ and Ph⁻ ions.
• Fig. S3: CID spectrum of mass 218 ions, including CaPh⁻ (HNDs doped with Ca and Ph).
• Fig. S4: CID spectrum of mass 218 ions, excluding CaPh⁻ (HNDs doped with Ca but no Ph).
• Fig. S5: Electron affinities and binding energies for phenanthrene complexed with Heₙ, n = 1-3, and He₂.
• Fig. S6: Electron affinities and binding energies for phenanthrene complexed with (H₂)ₙ and (H₂O)ₙ, n = 1-3.
• Fig. S7: Optimized structure of Ph⁻.
• Table S1: Method benchmark for electron affinities.
• Table S2: Method benchmark for vertical detachment energies.
• Table S3: The effect of zero point energies for neutral and anionic Ph and HePh.
• Cartesian coordinates of optimized structures

Fig. S1
Sections of a negative ion mass spectrum of HNDs doped with phenanthrene. Panels a, b, c show the regions where Ph⁻, Ph₂⁻ and Ph₃⁻ complexed with a few He atoms appear. The x-axis is chosen such that members of the homologous HeₙPh⁻ ion series (m = 1, 2, 3) with identical n are horizontally aligned. Ph₂⁻ and Ph₃⁻ are observed, but Ph⁻ is not.
**Fig. S2**
Mass spectra of ions produced by collisions of (H$_2$O)$_3$Ph$^-$ and Ph$_2^-$ with argon atoms at 5 eV ion energy (in the lab system) (panels a and b, respectively).

**Fig. S3**
Mass spectra of ions produced by collision of CaPh$^-$ with argon atoms at $E = 5$ eV ion energy (in the lab system) at two different argon pressures (panels a and b). The main product ion is Ca'. A contamination of the parent ion mass peak at 218 u by H$_2$OCa$^+$ gives rise to a weak series of H$_2$OCa$_n^-$ product ions. He$_8$Ph$^-$ and He$_9$Ph$^-$ arise from a contamination by He$_{10}$Ph$^-$, and H$_2$OPh$^-$ from a contamination by He(H$_2$O)$_2$Ph$^-$. Vertical bars indicate the expected position of ions; question marks flag ion peaks that are not positively identified.
Fig. S4
Panel a: Negative ion mass spectrum of HNDs doped with Ca but no Ph. Panels b and c: CID spectra of mass 218 u anions (mostly H$_2$OCa$_5^-$ ions) with argon atoms at 2 and 10 eV, respectively. The main dissociation channels are loss of H$_2$O, H$_2$, and one or two Ca, but Ca$^+$ is not detected.

Fig. S5
Electron affinities, EA, and binding energies, $E_{\text{bind}}$ (both in meV) for phenanthrene complexed with He$_n$, $n = 1-3$, and He$_2$. Binding energies are given for both neutral ("n") and anionic ("a") form. Energies are given as calculated at the $\omega$B97XD/aug-cc-pVDZ level; B3LYP-D3/aug-cc-pVDZ results are shown in parenthesis. Optimized structures of neutral molecules at the B3LYP-D3/aug-cc-pVDZ level are displayed.
Fig. S6
Electron affinities, EA, and binding energies, $E_{\text{bind}}$ (both in meV) for phenanthrene complexed with $(\text{H}_2)_n$ and $(\text{H}_2\text{O})_n$, $n = 1$-3. Binding energies are given for both neutral (“n”) and anionic (“a”) form. Energies are given as calculated at the $\omega$B97XD/aug-cc-pVDZ level, B3LYP-D3/aug-cc-pVDZ results are shown in parenthesis. Optimized structures of neutral molecules at the B3LYP-D3/aug-cc-pVDZ level are displayed. For the most stable isomers with water molecules, the vertical detachment energy, VDE, is also given (in meV). Experimental vertical detachment energies of $(\text{H}_2\text{O})_n$Ph are 270 ± 20, 510 ± 20, and 740 ± 20 meV for $n = 1, 2,$ and 3, respectively.¹

¹ Tschurl, M.; Boesl, U.; Gilb, S. The Electron Affinity of Phenanthrene. J. Chem. Phys. 2006, 125, 194310.

| Complex          | EA (meV) (d) | $E_{\text{bind},n}$ (meV) (d) | $E_{\text{bind},a}$ (meV) (d) |
|------------------|-------------|-------------------------------|-------------------------------|
| Ph.                 | 41 (190)    | 28.0 (41.9)                   | 57.8 (62.9)                   |
| Ph.$\cdot\text{H}_2$, I | 70 (211)    | 22.2 (40.4)                   | 49.4 (60.7)                   |
| Ph.$\cdot\text{H}_2$, II | 68 (210)    | 53.9 (87.0)                   | 104.1 (121.4)                 |
| Ph.$\cdot\text{H}_2$, III | 91 (224)    | 59.5 (65.8)                   | 102.1 (113.3)                 |
| Ph.$\cdot\text{H}_2\cdot\text{O}$, I | 83 (237)    | 78.3 (133.1)                  | 156 (185)                     |
| Ph.$\cdot\text{H}_2\cdot\text{O}$, II | 118 (242)   | 67.0 (97.9)                   | 148 (172)                     |
| Ph.$\cdot\text{H}_2\cdot\text{O}$, III | 122 (264)   | 64.0 (82.4)                   | 143 (164)                     |
| Ph.$\cdot\text{H}_2\cdot\text{O}$, IV | 119 (271)   | 62.3 (89.7)                   | 128 (157)                     |

Fig. S7
Structure of Ph$_2^-$ shown in top and side view as optimized at the B3LYP/aug-cc-pVDZ and $\omega$B97XD/aug-cc-pVDZ levels.
**Table S1**
Benchmark of electron affinities (in meV) calculated using various DFT functionals. Both results for aug-cc-pVDZ (“aug-cc-pVDZ”) and for optimization using aug-cc-pVDZ and single-point recalculation using aug-cc-pVTZ (“aug-cc-pVTZ//aug-cc-pVDZ”) are given. In the latter case, the zero-point energy correction calculated using the aug-cc-pVDZ basis set was employed.

| System (M)  | aug-cc-pVDZ | aug-cc-pVTZ//aug-cc-pVDZ |
|-------------|-------------|--------------------------|
|             | Ph          | Ph.He                    | Ph.H₂ | Ph.H₂O | Ph          | Ph.He | Ph.H₂ | Ph.H₂O |
| B3LYP-D3    | 190         | 191                      | 211   | 430     | 161         | 162   | 180   | 400    |
| wB97XD      | 41          | 43                       | 70    | 281     | -15         | -11   | 18    | 230    |
| M062X-D3    | 99          | 103                      | 119   | 339     | 101         | 106   | 125   | 348    |
| M06-D3      | 250         | 255                      | 254   | 494     | 120         | 126   | 141   | 370    |
| M06L-D3     | 167         | 170                      | 183   | 395     | 64          | 68    | 94    | 307    |
| CAMB3LYP-D3 | 81          | 84                       | 102   | 328     | 49          | 53    | 72    | 301    |

**Table S2**
Benchmark of vertical detachment energies (in meV) calculated using various DFT functionals. Both results for aug-cc-pVDZ (“aug-cc-pVDZ”) and for optimization using aug-cc-pVDZ and single-point recalculation using aug-cc-pVTZ (“aug-cc-pVTZ//aug-cc-pVDZ”) are given.

| System (M)  | aug-cc-pVDZ | aug-cc-pVTZ//aug-cc-pVDZ |
|-------------|-------------|--------------------------|
|             | Ph          | Ph.He                    | Ph.H₂ | Ph.H₂O | Ph          | Ph.He | Ph.H₂ | Ph.H₂O |
| B3LYP-D3    | 180         | 182                      | 216   | 482     | 200         | 202   | 236   | 503    |
| wB97XD      | 78          | 80                       | 110   | 377     | 75          | 77    | 111   | 375    |
| M062X-D3    | 136         | 140                      | 168   | 419     | 180         | 185   | 216   | 471    |
| M06-D3      | 246         | 252                      | 279   | 531     | 175         | 180   | 216   | 458    |
| M06L-D3     | 140         | 146                      | 166   | 405     | 87          | 93    | 120   | 357    |
| CAMB3LYP-D3 | 118         | 120                      | 155   | 430     | 139         | 142   | 177   | 452    |

**Table S3**
Electron affinity (EA<sub>noZPE</sub>) and vertical detachment energy (VDE<sub>noZPE</sub>) without accounting for zero-point energy, electron affinity with included zero-point energy (EA<sub>ZPE</sub>), and zero point energies for neutral and anionic complex (ZPE), all given for Ph and HePh in meV. Calculated at the wB97XD/aug-cc-pVDZ level, B3LYP/aug-cc-pVDZ values are shown in parenthesis.

| System (M) | EA<sub>noZPE</sub> | VDE<sub>noZPE</sub> | EA<sub>ZPE</sub> | ZPE(M<sup>-</sup>) | ZPE(M<sup>-</sup>) |
|------------|---------------------|---------------------|------------------|-------------------|-------------------|
| Ph         | -113 (30)           | 78 (180)            | 41 (190)         | 5333 (5283)       | 5180 (5123)       |
| HePh       | -111 (32)           | 80 (182)            | 43 (191)         | 5341 (5289)       | 5186 (5131)       |
Cartesian coordinates of optimized molecules and ions (in Ångstrom) along with electronic energies including zero-point correction (in Hartree)

B3LYP minima

Ph2

E = -1078.853707

C -3.062367 2.187821 0.143857
C -1.648507 2.282815 0.125258
C -0.900922 1.502140 -0.807081
C -1.615820 0.646713 -1.680847
C -2.997123 0.570846 -1.646568
C -3.731304 1.349265 -0.728540
C 0.552116 1.610066 -0.818724
C 1.190817 2.495947 0.100296
C 0.397331 3.257272 1.024602
C -0.961390 3.154605 1.037213
C 2.603137 2.611708 0.095190
C 3.374583 1.877274 -0.783411
C 2.749425 0.994501 -1.690380
C 1.371627 0.865521 -1.702158
H -3.618680 2.792403 0.861627
H -4.819008 1.282354 -0.702350
H -3.517171 -0.107960 -2.321410
H -1.078734 0.020168 -2.388320
H -1.553515 3.739494 1.742372
H 0.907673 3.925423 1.719641
H 3.075355 3.294448 -0.803031
H 4.460524 1.970938 -0.777040
H 3.535156 0.359703 -2.370804
H 0.921627 0.163253 0.291988
C -0.587603 -0.447795 2.089013
C 0.769436 -0.344579 2.074129
C 1.569233 -1.121106 1.167437
C 0.935915 -2.002818 -0.240281
C -0.518807 -2.113830 -0.247786
C -1.269338 -1.337276 1.181631
C -1.231231 -2.964688 -0.632200
C -2.613618 -3.054018 -0.589341
C -3.347654 -2.289727 0.339736
C -2.680411 -1.444064 1.206796
C 1.760084 -2.735225 -0.648610
C 3.140262 -2.612484 -0.621076
C 3.759483 -1.746058 0.302059
C 2.980366 -1.012334 1.178829
H 1.312799 -3.415021 -1.370678
H 3.748876 -3.191382 -1.316167
H 4.845155 -1.649388 0.317836
H 3.445932 -0.325078 1.884327
H 1.274432 0.345100 2.750171
H -1.184512 0.158020 2.762318
H -3.237929 -0.833005 1.916535
H -4.435199 -2.358275 0.366174
H -3.134223 -3.720291 -1.277620

Ph2-

E = -1078.871127

C 3.154094 2.857557 0.105475
C 3.166529 1.429181 0.097929
C 2.089688 0.732908 -0.554551
C 1.069229 1.497758 -1.158351
C 1.086458 2.892569 -1.154811
C 2.140619 3.571909 -0.509367
C 2.089687 -0.732909 -0.554552
C 3.166528 -1.429184 0.097929
C 4.209133 -0.692886 0.725745
C 4.209134 0.692883 -0.725745
C 3.154091 -2.857559 0.105475
C 2.140615 -3.571910 -0.509366
C 1.086454 -2.892569 -1.154810
C 1.069228 -1.497758 -1.158351
H 3.969988 3.381951 0.607618
H 2.154348 4.663883 -0.489772
H 0.269110 3.446638 -1.613606
H 0.227341 0.996630 -1.629343
H 5.015549 1.243201 1.214861
H 5.015548 -1.243205 1.214861
H 3.969984 -3.381954 0.607618
H 2.154343 -4.663884 -0.489771
H 0.269105 -3.446637 -1.613606
H 0.227340 -0.996629 -1.629343
C -0.600180 0.691735 1.418409
C -0.600181 -0.691735 1.418409
C -1.654945 -1.426849 0.808900
C -2.747050 -0.734300 0.179188
C -2.747049 0.734302 0.179188
C -1.654944 1.426850 0.808900
C -3.765908 1.502712 -0.422077
C -3.763214 2.898908 -0.424165
C -2.657972 3.573569 0.181766
C -1.638419 2.852530 0.781300
C -3.765909 -1.502710 -0.422077
C -3.763216 -2.898905 -0.424166
C -2.657974 -3.573567 0.181766
C -1.638421 -2.852530 0.781299
H -4.605581 -1.003737 -0.904818
H -4.541959 -3.461675 -0.897781
H -2.621170 -4.664945 0.171099
H -0.790750 -3.367951 1.232982
H 0.232812 -1.240868 1.855787
H 0.232812 1.240867 1.855788
H -0.790748 3.367951 1.232983
H -2.621166 4.664947 0.171010
H -4.541956 3.461678 -0.897781
H -4.605580 1.003740 -0.904818

H2

E = -1.164101
H2HePh-, I
E = -543.501010
C -3.585151 -0.351990 -0.003522
C -2.871878 0.835802 0.011362
C -1.435189 0.857568 0.009590
C -0.740049 -0.415499 -0.009123
C -1.502722 -1.593037 -0.023527
C -2.910001 -1.588791 -0.021080
C -0.705586 2.063946 0.024884
C 0.705585 2.063945 0.024884
C 1.435188 0.857567 0.009590
C 0.740048 -0.415500 -0.009123
C 2.871877 0.835802 0.011363
C 3.585151 -0.351991 -0.003521
C 2.910000 -1.588791 -0.021079
C 0.996394 -2.558313 -0.037616
He 0.000000 0.658464 2.998185
HePh-, I
E = -542.327715
C 0.394267 -0.053985 0.740050
C 0.394267 -0.053985 -0.740050
C -1.463162 -1.559317 -0.111076
C -0.689285 -0.372656 -0.084112
C -1.380752 0.876927 -0.088949
C -2.797226 0.894292 -0.119543
C -3.524923 -0.281808 -0.144858
C -2.847732 -1.518779 -0.146694
C -0.634174 2.104990 -0.061011
C 0.727756 2.101071 -0.029274
C 1.467686 0.868628 -0.022574
C 0.769257 -0.376998 -0.050006
C 1.536783 -1.568198 -0.042245
C 2.921563 -1.535791 -0.009321
C 3.605550 -0.302773 0.017449
C 2.884307 0.877621 0.018024
H 3.401688 1.837947 0.031346
H 4.695341 -0.282298 0.043263
H 3.484739 -2.469363 -0.004158
He -0.692893 2.959817 -0.000000
HeHePh-, II
E = -542.327611
C -1.463162 -1.559317 -0.111076
C -0.689285 -0.372656 -0.084112
C -1.380752 0.876927 -0.088949
C -2.797226 0.894292 -0.119543
C -3.524923 -0.281808 -0.144858
C -2.847732 -1.518779 -0.146694
C -0.634174 2.104990 -0.061011
C 0.727756 2.101071 -0.029274
C 1.467686 0.868628 -0.022574
C 0.769257 -0.376998 -0.050006
C 1.536783 -1.568198 -0.042245
C 2.921563 -1.535791 -0.009321
C 3.605550 -0.302773 0.017449
C 2.884307 0.877621 0.018024
H 3.401688 1.837947 0.031346
H 4.695341 -0.282298 0.043263
H 3.484739 -2.469363 -0.004158
He -0.757020 2.943410 -0.000000
HePh, I
E = -542.327715
C 0.394917 -0.055331 0.729421
C 0.394917 -0.055331 -0.729421
C -1.463162 -1.559317 -0.111076
C -0.689285 -0.372656 -0.084112
C -1.380752 0.876927 -0.088949
C -2.797226 0.894292 -0.119543
C -3.524923 -0.281808 -0.144858
C -2.847732 -1.518779 -0.146694
C -0.634174 2.104990 -0.061011
C 0.727756 2.101071 -0.029274
C 1.467686 0.868628 -0.022574
C 0.769257 -0.376998 -0.050006
C 1.536783 -1.568198 -0.042245
C 2.921563 -1.535791 -0.009321
C 3.605550 -0.302773 0.017449
C 2.884307 0.877621 0.018024
H 3.401688 1.837947 0.031346
H 4.695341 -0.282298 0.043263
H 3.484739 -2.469363 -0.004158
He -0.757020 2.943410 -0.000000
HePh, II
E = -542.327611
C -1.463162 -1.559317 -0.111076
C -0.689285 -0.372656 -0.084112
C -1.380752 0.876927 -0.088949
C -2.797226 0.894292 -0.119543
C -3.524923 -0.281808 -0.144858
C -2.847732 -1.518779 -0.146694
C -0.634174 2.104990 -0.061011
C 0.727756 2.101071 -0.029274
C 1.467686 0.868628 -0.022574
C 0.769257 -0.376998 -0.050006
C 1.536783 -1.568198 -0.042245
C 2.921563 -1.535791 -0.009321
C 3.605550 -0.302773 0.017449
C 2.884307 0.877621 0.018024
H 3.401688 1.837947 0.031346
H 4.695341 -0.282298 0.043263
H 3.484739 -2.469363 -0.004158
He -0.757020 2.943410 -0.000000
C -0.729026 -0.412184 -0.000004
C -2.841047 0.848656 -0.000004
C -3.565698 -0.329377 -0.000003
C -2.884649 -1.564439 -0.000004
C -1.499796 -1.601017 -0.000004
H -1.005630 -2.570229 -0.000004
H 1.005629 -2.570230 0.000004
H 1.233999 3.005100 -0.000001
H -1.233996 3.005100 -0.000003
H -3.450624 -2.496285 -0.000004
H 3.355736 1.810568 0.000003
H -3.355732 1.810571 -0.000004
H 3.450622 -2.496289 0.000010
H -4.655670 -0.305799 -0.000003
H 4.655671 -0.305804 0.000010
C 1.499459 1.251419 -0.000001
C 0.729561 0.059436 0.000000
C 1.424539 -1.188351 0.000002
C 2.841120 -1.200111 0.000001
C 3.565531 -0.212897 -0.000001
C 2.885735 1.214066 -0.000002
C 0.681029 -2.418657 0.000005
C -0.681030 -2.418657 0.000006
C -1.424540 -1.188351 0.000003
C -0.729561 0.059436 0.000000
C -1.499459 1.251420 -0.000003
C -2.841121 -1.200110 0.000004
O 0.000000 1.568628 -3.053042
O -3.356847 -2.161184 0.000006
H -3.356846 -2.161185 -0.000007
H 4.655225 -0.444948 0.000001
H -3.450568 2.146057 -0.000006
H -1.005312 2.220011 -0.000002
O 0.000003 1.568646 3.053034
O -0.760317 1.235341 2.559862

(H2)2Ph-, I
E = -541.757926
C -3.584781 -0.359360 0.000033
C -2.871596 0.828520 0.000009
C -1.435391 0.850110 0.000002
C -0.740118 -0.422565 0.000010
C -1.502502 -1.600339 0.000036
C -2.909413 -1.596019 0.000051
C -0.705971 2.057136 -0.000012
C 0.705975 2.057138 0.000010
C 1.435397 0.850114 -0.000003
C 0.740127 -0.422562 -0.000011
C 2.871603 0.828527 -0.000007
C 3.584791 -0.359350 -0.000030
C 2.909425 -1.596012 -0.000050
C 1.502515 -1.600335 -0.000037
H 0.996093 -2.565546 0.000051
H -0.996078 -2.565549 0.000048
H -1.253843 3.001743 -0.000010
H 1.253844 3.001746 0.000007
H 3.464598 -2.535083 -0.000071
H -3.401939 1.784081 -0.000003
H 3.401943 1.784089 0.000006
H -3.464584 -2.535091 0.000072
H 4.678157 -0.334872 -0.000035
H -4.678148 -0.334884 0.000041
H -0.000768 1.210258 -2.575690
H -0.000339 0.894412 -3.269902
H 0.000517 1.210254 2.575689
H 0.000180 0.894422 3.269907

(H2O)2Ph-, II
E = -692.300300
C 1.502774 -1.247607 0.000005
C 0.739096 -0.65894 0.000001
C 1.433696 1.207549 -0.000003
C 2.871176 1.184249 -0.000002
C 3.583752 -0.002523 0.000002
C 2.910800 -1.241569 0.000006
C 0.704457 2.411965 -0.000006
C -0.704457 2.411965 0.000005
C -1.433696 1.207549 0.000002
C -0.739096 0.658940 0.000000
C -1.502774 -1.247607 0.000001
C -2.910800 1.241569 0.000002
C -3.583752 0.002523 0.000001
C -2.871176 1.184249 0.000002
O 0.000001 -1.510327 2.974967
H -3.401539 2.139272 -0.000003
H -3.465424 -2.179784 0.000003
H -0.997461 -2.212837 0.000002
H 1.251852 3.356751 0.000007
H 1.251852 3.356751 -0.000007
H 3.401539 2.139272 -0.000005
H 4.676534 0.022419 0.000003
H 3.465424 -2.179784 0.000010
H \(0.997461\) -2.212837 0.000008
H \(0.753026\) -1.260069 2.419735
H -0.753025 -1.260086 -2.419735
O -0.000001 -1.510345 -2.974966
H -0.753026 -1.260085 -2.419735

\((H_2O)_{2}Ph, I\)

\[ E = -692.280877 \]

C -1.412925 -1.322728 0.965258
C -0.576287 -0.214185 0.685194
C -1.192573 1.061957 0.511712
C -2.600315 1.182592 0.613011
C -3.391554 0.081091 0.883595
C -2.788637 -1.181480 1.063572
C -0.378705 2.214005 0.230596
C 0.977878 2.112718 0.130179
C 1.641733 0.845604 0.28463
C 0.872290 -0.328005 0.554258
C 1.561174 -1.561424 0.664389
C 2.937620 -1.635042 0.883595
C 3.692035 0.081091 0.883595
C 4.774478 -0.535801 0.150646
C 3.439117 -2.598914 0.608361
C 1.043734 -0.143071 -0.863363
C 0.490996 -0.300307 -0.663269
C 1.109606 1.009524 -0.639268
C 2.529248 -2.311804 1.100088
C -2.256275 -1.233910 -1.554264
O -2.074768 -1.314568 -2.498003
H -1.282405 -0.766854 -2.638744
H 0.251324 1.061979 -2.160567
O 0.099553 0.701374 2.526837

\((H_2O)_{2}Ph, II\)

\[ E = -692.305067 \]

C 1.306739 -1.422426 -0.863363
C 0.490996 -0.300307 -0.658326
C 1.109606 1.009524 -0.639268
C 2.529248 1.083891 -0.827904
C 3.301096 -0.051112 -1.013865
C 2.70349 -1.325582 -1.032735
C 0.320364 2.164659 -0.431206
C -1.084537 2.075122 -0.298989
C -1.736093 0.825403 -0.288116
C -0.969295 -0.398794 -0.433916
C -1.646545 -1.625859 -0.352674
C -3.036669 -1.714511 -0.165431
C -3.784030 -0.525291 -0.044252

C -3.155349 0.707158 -0.100414
H -3.739643 1.624192 0.004896
H -4.866221 -0.574392 0.102329
H -3.524286 -2.688138 -0.107789
H -1.083235 -2.554273 -0.442695
H -1.680087 2.980116 -0.165656
H 0.809184 3.140728 -0.434002
H 3.002310 2.068800 -0.804550
H 4.382241 0.043495 -1.140356
H 3.300450 -2.222901 -1.184984
H 0.859429 -2.415611 -0.879178
H 2.581339 -1.093564 1.511805
O -0.998238 2.467714 2.541783
H 0.270748 1.341201 1.812792
O 0.099553 0.701374 2.526837
H -0.571928 0.130075 2.127107

\((H_2O)_{2}Ph, II\)

\[ E = -545.236907 \]

C -2.841413 0.893094 -0.105087
C -1.424573 0.879981 -0.107791
C -0.729450 -0.367315 -0.133950
C -1.500236 -1.556050 -0.156676
C -2.885235 -1.519690 -0.153462
C -3.566020 -0.284985 -0.127276
C 0.729450 -0.367315 -0.133950
C 1.424573 -0.879981 -0.107791
C 0.681150 2.110024 -0.082930
C -0.681150 2.110024 -0.082930
C -2.841413 0.893094 -0.105088
C 3.566019 -0.284985 -0.127276
C 2.885234 -1.519690 -0.153462
C 1.500236 -1.556050 -0.156676
He 1.922556 -0.298722 2.911908
H -3.356279 1.854723 -0.084587
H -4.656015 -0.261400 -0.124515
H -3.451076 -2.451483 -0.170947
H -1.085876 -2.524994 -0.176941
H -1.233793 3.050252 -0.063786
H 1.233794 3.050252 -0.063786
H 3.356280 1.854723 -0.084587
H 4.656015 -0.261400 -0.124515
H 3.451076 -2.451483 -0.170947
H 1.085876 -2.524994 -0.176941
H -1.922555 -0.298722 2.911904

\((H_2O)_{2}Ph, II\)

\[ E = -545.244018 \]

C -2.872167 0.888600 -0.102533
C -1.435104 0.910798 -0.102872
C -0.740074 -0.362600 -0.134570
C -1.502827 -1.539776 -0.161896
C -2.910416 -1.535728 -0.159239
C -3.585362 -0.299028 -0.129400
| Element | X | Y | Z |
|---------|---|---|---|
| C       | 0.740074 | -0.362600 | -0.134570 |
| C       | 1.435104  | 0.910798  | -0.102872  |
| C       | 0.705298  | 2.116559  | -0.072894  |
| C       | -0.705298 | 2.116559  | -0.072894  |
| C       | 2.872167  | 0.888600  | -0.102534  |
| C       | 3.585362  | -0.299028 | -0.129400  |
| C       | 1.502827  | -1.539776 | -0.161895  |
| He      | 2.019917  | -0.362210 | 2.901031   |
| H       | -3.402666 | 1.843930  | -0.078935  |
| H       | -4.678831 | -0.274421 | -0.127122  |
| H       | 3.465690  | -2.474566 | -0.180375  |
| He      | 2.019917  | -0.362210 | 2.901031   |
| H       | -3.402666 | 1.843930  | -0.078935  |
| H       | -4.678831 | -0.274421 | -0.127122  |
| H       | 3.465690  | -2.474566 | -0.180375  |
| He      | 2.019917  | -0.362210 | 2.901031   |
| H       | -3.402666 | 1.843930  | -0.078935  |
| H       | -4.678831 | -0.274421 | -0.127122  |
| H       | 3.465690  | -2.474566 | -0.180375  |
| He      | 2.019917  | -0.362210 | 2.901031   |

He2Ph, I

\[ E = -545.237029 \]

| Element | X | Y | Z |
|---------|---|---|---|
| C       | 0.000000  | 1.500242 | -1.595728 |
| C       | 0.000000  | 0.729325  | -0.406860 |
| C       | 0.000000  | 1.434956  | 0.866671  |
| C       | 0.000000  | 2.872167  | 0.847074  |
| C       | 0.000000  | 3.585362  | -0.300317 |
| C       | 0.000000  | 2.910416  | -0.072894 |
| C       | 0.000000  | 0.705298  | 2.116559  |

He2Ph-, I

\[ E = -545.244095 \]
H -0.386324 -2.416374 -2.459516

(H2)3Ph-, II
E = -542.92388
C 3.608344 -0.394004 -0.000608
C 2.909151 0.801736 -0.004427
C 1.474042 -0.389244 -0.026599
C 0.764188 0.874002 -0.039592
C 2.918502 -1.622949 -0.017752
C 0.758639 2.055821 -0.025442
C -0.652491 2.072097 -0.046534
C -1.395400 0.874002 -0.069662
C -0.715197 -0.406653 -0.076628
C -2.831745 0.868188 -0.089759
C -3.558158 -0.311016 -0.130678
C -2.897538 -1.554955 -0.148514
C -1.490844 -1.575613 -0.117066
C 0.152085 1.257781 -2.619862
C 0.465620 1.137193 3.294828
C -2.075522 -0.564544 3.232524
C -0.995181 -2.546258 -0.123998
C 0.994900 -2.570103 -0.052538
C 1.317533 2.939702 -0.010997
C -1.189457 3.022905 -0.042673
C -3.462880 -2.487216 -0.177857
C 3.450322 1.751004 0.010516
C 3.351323 1.829348 -0.075616
C 3.462701 -2.583312 -0.012535
C -4.650828 -0.273698 0.146253
C 4.701697 -0.382549 0.016703
C 0.142718 0.941680 -3.13894
C 0.557858 1.391716 2.581374
H -1.945370 -0.601625 2.482397

(H2)3Ph-, IV
E = -542.923330
C 3.579257 -0.231370 -0.204852
C 2.862812 0.948836 -0.076106
C 1.425332 0.967561 -0.076707
C 0.734072 -0.301969 -0.203644
C 1.499961 -1.478562 -0.332394
C 2.908560 -1.462063 -0.337602
C 0.692332 2.165638 0.040791
C -0.717674 2.163676 0.035931
C -1.443448 0.961291 -0.080892
C -0.745122 -0.305337 -0.197458
C -2.880058 0.934909 -0.082515
C -3.589743 -0.249570 -0.191841
C -2.911012 -1.480235 -0.301940
C -1.504921 -1.480727 -0.299034
H -2.052914 -0.588246 3.128464
H 2.121083 -0.510647 3.092150
H 0.413975 -2.350074 2.088177
H -0.995679 -2.441819 -0.375835
H 0.996464 -2.431415 -0.435783
H 1.238140 3.107281 0.134415
H -1.267742 3.103158 0.125141
H -3.463617 -2.417312 -0.380885
C 3.390825 1.899872 0.026677
H -3.413057 1.884546 0.088341
H 3.465957 -2.394141 -0.437496
H -4.682978 -0.228356 -0.187328
H 4.672400 -0.204039 -0.199714
H 2.257345 -0.258407 2.386407
H -0.082067 -2.846981 2.487501
H -2.140215 -0.365047 2.385542

(H2)3Ph, I
E = -542.915490
C 2.840150 0.881466 -0.013653
C 1.423520 0.869144 -0.022980
C 0.728295 -0.376308 -0.083242
C 1.497903 -1.564151 -0.136203
C 2.882754 -1.529452 -0.125854
C 3.564333 -0.296274 -0.063188
C -0.729228 -0.375825 -0.083887
(H2)3Ph-, I
E = -542.924374

(H2)3Ph-, III
E = -542.913627
He3Ph-, II
E = -548.153378
C -0.739880 -0.362549 -0.090436
C 0.739883 -0.362551 -0.090434
H -0.996661 -2.498399 -0.263953
C 0.705223 2.109005 0.110777
C -0.705216 2.109006 0.110777
H 0.996661 -2.498401 -0.263944
C -1.502888 -1.536019 -0.186423
C 1.434890 -0.970013 0.013219
C -1.434885 0.970015 0.013218
C 1.502889 -1.536023 -0.186426
C -2.910441 -1.531845 -0.186422
C 2.872062 0.885117 0.011781
C -2.872057 0.885122 0.011779
C 2.910442 -1.531850 -0.186422
C -3.585404 -0.298806 -0.085290
C 3.585407 -0.298805 -0.085291
H 1.253261 3.050961 0.187454
H -1.253252 3.050963 0.187458
H -3.465781 -2.467711 -0.262877
H 3.402529 1.837608 0.089763
H -3.402522 1.837614 0.089763
H 3.465781 -2.467718 -0.262863
H -4.678906 -0.274200 -0.083281
H 4.678910 -0.274209 -0.083273
H -0.000075 -2.186236 2.807998
H -0.000014 0.546443 3.01900
H 0.000004 0.960025 -3.010308

He3Ph, IV
E = -548.146061
C -0.766723 -0.338470 -0.184837
C 0.691654 -0.328359 -0.218505
H -1.031125 -2.493887 -0.320895
C 0.650925 2.144372 -0.063059
C -0.759232 2.135084 -0.032709
H 0.966976 -2.467347 -0.357167
C -1.537059 -1.520604 -0.239506
C 1.387028 0.945602 -0.154850
C -1.482248 0.926556 -0.091168
C 1.467951 -1.500308 -0.309716
C -2.944128 -1.529578 -0.207880
C 2.823827 0.933381 -0.190385
C -2.918885 0.894886 -0.060034
C 2.875164 -1.486477 -0.342836
C -3.625591 0.295602 -0.116999
C 3.543168 -0.247363 -0.282048
C 1.193764 3.091389 -0.017063
C -1.312061 3.074724 0.038248
C -3.494295 -2.467800 -0.252576
C 3.349001 1.890773 -0.143342
C -3.454353 1.845084 0.010570
C 3.435136 -2.419906 -0.413487
C -4.718922 -0.278365 -0.090755
H 4.636165 -0.215245 -0.306555
H -0.034425 -2.149595 2.705556
C 2.249366 -0.490004 2.783377
H -0.200868 0.654504 2.915153

He3Ph, I
E = -548.146294
C -1.500131 -1.565823 -0.147831
C -0.729355 -0.378675 -0.082879
C -1.424449 0.866898 -0.013946
C -2.841281 0.879994 -0.011852
C -3.565922 -0.296507 -0.075779
C -2.885107 -1.529582 -0.144499
C -0.681133 2.095252 0.053242
C -0.681132 2.095252 0.053244
C 1.424449 0.866898 -0.013943
C 0.729355 -0.378675 -0.082879
C 1.500131 -1.565822 -0.147836
C 2.885107 -1.529582 -0.144500
C 3.565922 -0.296507 -0.075777
He3Ph-, I
E = -548.153471
C -1.502739 -1.550623 -0.156943
C -0.739988 -0.375337 -0.085262
C -1.434978 0.895910 -0.006615
C -2.872022 0.873808 -0.007371
C -3.585245 -0.311913 -0.087905
C -2.910280 -1.546657 -0.154718
C -0.705251 2.099693 0.067542
C 0.705267 2.099692 0.067542
C 1.434991 0.895907 -0.006616
C 0.739999 -0.375339 -0.085262
C 1.502746 -1.550627 -0.156942
C 2.910288 -1.546663 -0.154715
C 3.585256 -0.311921 -0.078902
C 2.872036 0.873801 -0.007370
C 3.405207 1.827599 0.051766
C 4.678717 -0.287394 -0.076067
C 3.465551 -2.484029 -0.211210
H 0.996478 -2.514277 -0.216182
H 1.253242 3.043087 0.125126
H -1.253224 3.043089 0.125126
H -3.404291 1.827607 0.051765
H -4.678706 -0.287384 -0.076070
H -3.465545 -2.484021 -0.211213
H -0.996472 -2.514274 -0.216185
He -0.000094 0.884679 -3.040399
He 2.020411 -0.489390 2.950326
He -2.020581 -0.489484 2.950251

He3Ph-, III
E = -548.153158
C 1.502942 -1.559169 -0.173193
C 0.740087 -0.381679 -0.178803
C 1.435051 0.892133 -0.187310
C 2.872180 0.869845 -0.188613
C 3.585374 -0.318066 -0.183594
C 2.910469 -1.555041 -0.175710
C 0.705221 2.098120 -0.195507
C -0.705220 2.098120 -0.195507
C -1.435051 0.892133 -0.187310
C -0.740087 -0.381679 -0.178803
C -1.502942 -1.559169 -0.173193
C -2.910469 -1.555041 -0.175710
C -3.585374 -0.318066 -0.183594
C -2.872180 0.869845 -0.188613
He -2.233448 -0.430553 2.865922
He -0.000000 1.027651 2.885665
He 2.233447 -0.430552 2.865921
H -3.402696 1.825444 -0.194938
H -4.678833 -0.293382 -0.185207
H -3.465735 -2.494100 -0.171197
H -0.996598 -2.524589 -0.167211
H -1.253216 3.043227 -0.202576
H 1.253216 3.043227 -0.202575
H 3.402696 1.825443 -0.194937
H 4.678833 -0.293383 -0.185207
H 3.465735 -2.494100 -0.171197
H 0.996598 -2.524589 -0.167210

Ph
E = -539.418297
C 0.000000 1.500498 -1.569244
C 0.000000 0.729518 -0.380311
C 0.000000 1.424622 0.867497
Ph-  
E = -539.425261
C 0.000000  1.503121 -1.555822
C 0.000000  0.740127 -0.378316
C 0.000000  1.435201  0.895679
C 0.000000  2.872405  0.873575
C 0.000000  3.585728 -0.314412
C 0.000000  2.910858 -1.551582
C 0.000000  0.705316  2.101781
C 0.000000 -0.705316  2.101781
C 0.000000 -1.435201  0.895679
C 0.000000 -0.740127 -0.378316
C 0.000000 -1.503121 -1.555822
C 0.000000 -2.910858 -1.551582
C 0.000000 -3.585728 -0.314412
C 0.000000 -2.872405  0.873575
H 0.000000 -3.402912  1.829258
H 0.000000 -4.679248 -0.289695
H 0.000000 -3.465345  0.297334
H 0.000000 -3.451485 -2.464681
H 0.000000  1.233864  3.038173
H 0.000000 -1.233864  3.038173
H 0.000000  3.402912  1.829258
H 0.000000  4.679248 -0.289695
H 0.000000  3.465345  0.297334
H 0.000000  3.451485 -2.464681

Ph2  
E = -1078.438423
C -1.849983  2.952948 -0.010816
C -0.494091  2.559286  0.041708
H0.000000 0.981317 3.198716
H2Ph, II
E = -540.370473
C -3.513507 -0.281462 -0.139911
C -2.788468 0.890796 -0.118409
C -1.375646 -1.554182 -0.137122
C -0.630078 2.102057 -0.062106
C 0.724067 2.097849 -0.029085
C 1.463026 0.863148 -0.022584
C 0.769372 -0.372752 -0.051897
C 2.875840 0.837402 -0.062888
C 3.593929 -0.303113 0.19351
C 2.910884 -1.532530 -0.009104
C 1.531339 -1.563422 -0.043946
H 1.033621 -2.530646 -0.065530
H -0.965243 -2.524238 -0.113648
H -1.200384 3.052471 -0.056306
H 1.280500 3.035474 -0.006180
H 3.472903 -2.466287 -0.003812
H -3.302211 1.854020 -0.118526
H 3.392946 1.833614 0.034969
H -3.404773 -2.445429 -0.153068
H 4.683229 -0.283107 0.046785
H -4.602785 -0.254877 -0.158023
H -3.094428 -0.360887 2.579485
H -1.773863 -0.206212 3.259322
H2Ph-, II
E = -540.373046
C -3.532136 -0.294775 -0.142533
C -2.819023 0.887549 -0.065966
C -1.461425 -1.537075 -0.006180
C -2.863658 -1.530314 -0.145305
C -0.654917 2.106191 -0.055583
C 0.754018 2.108086 -0.024718
C 1.475331 0.894544 -0.020372
C 0.780281 -0.371818 -0.049355
C 2.908196 0.856344 -0.012426
C 3.612723 -0.322217 0.016759
C 2.934517 -1.552530 -0.018523
C 1.533155 -1.548558 -0.042839
H 1.021956 -2.511479 -0.063727
H -0.957078 -2.503700 -0.113648
H -1.200384 3.052471 -0.056306
H 1.306200 3.043168 -0.01785
H 3.484587 -2.494237 -0.006437
H -3.347130 1.844039 -0.108444
H 3.442959 1.818073 0.034219
H -3.420642 -2.467559 -0.165549
H 4.705581 -0.302461 0.042252
H -4.624830 -0.266229 -0.161007
H -1.910334 -0.310729 2.506341
H -1.992363 -0.334062 3.262103

H2OPh, I
E = -615.611730
C -2.623211 0.905759 -0.564795
C -1.215963 0.882953 -0.430991
C -0.534223 -0.359857 -0.385364
C -1.301224 -1.544183 -0.480350
C -2.674977 -1.501444 -0.608551
C -3.346843 -0.265887 -0.650116
C 0.916264 -0.369367 -0.224989
C 1.606132 0.864731 -0.119451
C 0.872338 2.101427 -0.173500
C -0.473998 2.110788 -0.322662
C 3.010460 0.870983 0.040265
C 3.722722 -0.307567 0.095386
C 3.043086 -1.534996 -0.007534
C 1.672140 -1.562597 -0.163878
C -0.131872 1.869903 -0.591984
H -4.431606 -0.235508 -0.748594
H -3.241339 -2.429841 -0.673493
H -0.812933 -2.515388 -0.444494
H -1.021499 3.052884 -0.357788
H 1.426093 3.036929 -0.088870
H 3.525113 1.829322 0.119792
H 4.805278 -0.290969 0.219119
H 3.601125 -2.469955 0.036627
H 1.177101 -2.528355 -0.239483
H -0.950066 0.044253 2.423496
H -1.825247 -0.111358 2.789244
H -2.380713 -0.221669 2.010905

H2OPh-, I
E = -615.622056
C -2.691954 0.264477 -0.704495
C -1.275740 0.459389 -0.596257
C -0.475028 -0.663047 -0.169706
C -1.115089 -1.869321 0.123173
C -2.504710 -2.036891 0.014636
C -3.284403 -0.950034 -0.405167
C 0.989872 -0.480828 -0.053479
C 1.551422 0.819147 -0.330421
C 0.728015 1.884615 -0.720323
C -0.673003 1.705401 -0.855808
C 2.968986 0.973834 -0.198387
C 3.784171 -0.075833 0.172715
C 3.235946 -1.343712 0.434454
C 1.852722 -1.517535 0.315850
H -3.305880 1.107902 -1.028159
H -4.367995 -1.059147 -0.498085
H -2.965611 -2.995040 0.256320
H -0.523802 -2.723294 0.454001
H -1.303737 2.533651 -1.185850
H 1.171536 2.856917 -0.927130
H 3.401456 1.956280 -0.401956
H 4.862101 0.081373 0.262305
H 3.874296 -2.178461 0.725718
H -1.444179 -2.506823 0.523106
H -1.409114 2.163435 1.397330
O -2.103541 2.059978 2.064008
HeH2Ph, II
E = -543.274154
C 3.556370 -0.285190 -0.129261
C 2.834943 0.889045 -0.106382
C 1.421813 0.874771 -0.112104
C 0.731318 -0.362756 -0.141824
C 1.496597 -1.550979 -0.165152
C 2.876419 -1.516265 -0.158856
C 0.679386 2.107033 -0.085384
C -0.675173 2.187341 -0.086125
C -1.417604 0.875276 -0.113631
C -0.727514 -0.362440 -0.142939
C -2.830685 0.889807 -0.104734
C -3.552542 -0.284479 -0.123487
C -2.872857 -1.515825 -0.154189
C -1.492924 -1.550583 -0.164192
He 1.793730 -0.311436 3.098399
H -0.997635 -2.518966 -0.185345
H 1.001277 -2.519373 -0.188099
H 1.233459 3.046082 -0.063584
H -1.229024 3.046479 -0.064675
H -3.437697 -2.447711 -0.186494
H 3.349598 1.850523 -0.083902
H -3.345160 1.851245 -0.079421
H 3.441103 -2.448249 -0.176769
H -4.642007 -0.261236 -0.113924
H 4.645928 -0.261240 -0.124013
H -2.066583 -0.347804 2.559889
H -1.706005 -0.254513 3.220194
HeH2Ph-, II
E = -543.274154
C 3.556370 -0.285190 -0.129261
C 2.834943 0.889045 -0.106382
C 1.421813 0.874771 -0.112104
C 0.731318 -0.362756 -0.141824
C 1.496597 -1.550979 -0.165152
C 2.876419 -1.516265 -0.158856
C 0.679386 2.107033 -0.085384
C -0.675173 2.187341 -0.086125
C -1.417604 0.875276 -0.113631
C -0.727514 -0.362440 -0.142939
C -2.830685 0.889807 -0.104734
C -3.552542 -0.284479 -0.123487
C -2.872857 -1.515825 -0.154189
C -1.492924 -1.550583 -0.164192
He 1.793730 -0.311436 3.098399
H -0.997635 -2.518966 -0.185345
H 1.001277 -2.519373 -0.188099
H 1.233459 3.046082 -0.063584
H -1.229024 3.046479 -0.064675
H -3.437697 -2.447711 -0.186494
H 3.349598 1.850523 -0.083902
H -3.345160 1.851245 -0.079421
H 3.441103 -2.448249 -0.176769
H -4.642007 -0.261236 -0.113924
H 4.645928 -0.261240 -0.124013
H -2.066583 -0.347804 2.559889
H -1.706005 -0.254513 3.220194
C -1.374727 0.890601 -0.181432
C -0.696775 -0.383666 -0.137265
C -2.807616 0.880216 -0.221749
C -3.527780 -0.298122 -0.224002
C -2.866297 -1.536695 -0.183819
C -1.465064 -1.551008 -0.140196
H -0.966802 -2.520273 -0.108536
H 1.011855 -2.538243 -0.035246
H 1.330227 3.013098 -0.157245
H -1.176796 3.031908 -0.003076
H -2.468999 -0.478339 3.131317

HeH2Ph, I
E = -543.274025
C -3.554614 -0.325762 -0.004578
C -2.833066 0.848409 -0.003898
C -1.419827 0.833597 -0.001800
C -0.729316 -0.404262 -0.001244
C -1.494956 -1.592594 -0.001934
C -2.874656 -1.557408 -0.003253
C -0.677505 2.065894 -0.003215
C 0.677507 2.065894 -0.003215
C 1.419827 0.833597 -0.001800
C 0.729316 0.404262 0.001244
C 2.833066 0.848409 0.003898
C 3.554614 -0.325762 0.004578
C 2.874656 -1.557408 0.003253
C 1.419827 -0.325762 0.001800
C 0.729316 0.404262 0.001244
C 2.833066 0.848409 0.003898
C 3.554614 -0.325762 0.004578
C 2.874656 -1.557408 0.003253
C 1.419827 -0.325762 0.001800
C 0.729316 0.404262 0.001244
C 2.833066 0.848409 0.003898
He -2.468999 -0.478339 3.131317

HeH2Ph-, I
E = -543.274025
C -3.573382 -0.349947 0.007161
C -2.864238 0.834915 0.007374
C -1.430993 0.858182 0.006508
C -0.740391 -0.409819 -0.011193
C -1.497721 -1.584199 -0.025445
C -2.899637 -1.582645 -0.023558
C 1.497720 -1.584199 -0.025445
H 0.990083 -2.548987 -0.038845
H -0.990083 -2.548987 -0.038845
H -1.253948 3.005959 0.031767
H 1.253948 3.005959 0.031767
H 3.453291 -2.522160 -0.035356
H -3.395569 1.789671 0.019411
H 3.395568 1.789671 0.019409
H -3.453292 -2.522160 -0.035356
H 4.666434 -0.325725 -0.005975
H -4.666435 -0.325724 -0.005975
H 0.000005 1.177397 -2.588448
H 0.000000 0.907469 -3.300004
He 0.000004 0.588136 3.168802

HePh, I
E = -542.111470
C -0.389102 -0.059990 -0.729532
C -0.389102 -0.059990 0.729532
H -2.545730 -0.012179 -1.000005
C 2.080845 -0.113757 0.677318
C 2.080845 -0.113757 -0.677318
H -2.545730 -0.012179 1.000005
C -1.577171 -0.033215 -1.495246
C 0.848709 -0.086808 1.419911
C 0.848709 -0.086808 -1.419911
C -1.577171 -0.033215 1.495246
C -1.542013 -0.033194 -2.875105
C 0.863302 -0.086215 2.833171
C 0.863302 -0.086215 -2.833171
C -1.542013 -0.033194 2.875105
C -0.310680 -0.059900 3.554862
C -0.310680 -0.059900 -3.554862
H 3.020009 -0.133970 1.231253
H 3.020009 -0.133970 -1.231253
H -2.473835 -0.012340 -3.440002
H 1.824942 -0.107081 3.347706
H 1.824942 -0.107081 -3.347706
H -2.473835 -0.012340 3.440002
H -0.287329 -0.059700 -4.644446
H -0.287329 -0.059700 4.644446
He 0.618597 3.163736 -0.000000

HePh-, I
E = -542.113058
He -0.636133 3.173851 0.000000

HePh, II
E = -542.111421
C -1.459902 -1.540580 -0.117214
C -0.699822 -0.368344 -0.089548
C -1.386920 0.902142 -0.095209
C -2.820154 0.882395 -0.129955
C -3.532070 -0.300672 -0.155799
C -2.861850 -1.534543 -0.149641
C -0.657976 2.103506 -0.066276
C 0.751020 2.099774 -0.031958
C 1.474027 0.894475 -0.024494
C 0.780545 -0.372357 -0.052628
C 1.534890 -1.548725 -0.043777
C 2.936796 -1.551052 -0.009118
C 3.613177 -0.319939 0.017962
C 2.907187 0.866991 0.010640
H 3.440889 1.820364 0.031857
H 4.706018 -0.298583 0.045147
H 3.487990 -2.492141 -0.003441
H 1.024985 -2.512281 -0.064758
H 1.302147 3.042597 -0.108094
H -1.284439 3.049290 -0.071532
H -3.349080 1.838624 -0.134457
H -4.624803 -0.273401 -0.181203
H -3.417754 -2.473536 -0.169932
H -0.954750 -2.506847 -0.113015
H -1.942429 -0.233586 3.146756

HePh-, II

(H2)2Ph, II
E = -541.533942
C 3.554708 -0.284821 -0.118287
C 2.833028 0.889600 -0.099878
C 1.420033 0.875252 -0.109713
C 0.729788 -0.362254 -0.139506
C 1.494876 -1.550493 -0.156965
C 2.874836 -1.516047 -0.148901
C 0.677745 2.107433 -0.082600
C -0.676740 2.107471 -0.082677
C -1.419041 0.875300 -0.109961
C -0.728883 -0.362241 -0.139688
C -2.832070 0.889598 -0.100257
C -3.553692 -0.284949 -0.119199
C -2.873796 -1.516118 -0.150238
C -1.493923 -1.550445 -0.160440
H -0.998506 -2.518716 -0.181044
H 0.999522 -2.518809 -0.180425
H 1.231756 3.046460 -0.060674
H -1.230717 3.046519 -0.060744
H -3.438407 -2.448116 -0.164293
H 3.347623 1.850954 -0.074348
H -3.346752 1.850917 -0.074810
H 3.439466 -2.448052 -0.162690
H -4.643156 -0.261851 -0.109337
H 4.644168 -0.261720 -0.108188
H 2.103026 -0.377653 2.563676
H 1.717744 -0.241761 3.202095
H -2.146752 -0.318087 2.555222  
H -1.720231 -0.303851 3.181586  
(H2)2Ph-, II  
E = -541.536999  
C 3.572818 -0.299145 -0.124560  
C 2.863963 0.885527 -0.095777  
C 1.430374 0.909902 -0.102078  
C 0.740196 -0.358386 -0.136103  
C 1.497427 -1.532838 -0.164958  
C 2.899402 -1.531671 -0.160398  
C 0.704554 2.112846 -0.071549  
C -0.704554 2.112845 -0.071549  
C -1.430374 0.909902 -0.102078  
C -0.740196 -0.358386 -0.136103  
C -2.863963 0.885526 -0.095777  
C -3.572818 -0.299145 -0.124560  
C 2.899402 -1.531671 -0.160398  
C -1.253549 3.056612 -0.045389  
H 1.253549 3.056612 -0.045389  
H -3.452912 -2.470942 -0.179852  
H 3.395513 -2.470941 -0.179852  
H -4.665682 -0.275174 -0.116238  
H 4.665682 -0.275174 -0.116238  
H 1.892227 -0.367804 2.483392  
H 1.946060 -0.402489 3.240908  
H -1.892227 -0.367793 2.483392  
H -1.946061 -0.402489 3.240907  
(H2)2Ph, I  
E = -541.533736  
C -3.591206 -0.324198 0.074851  
C -2.874115 0.852364 0.106132  
C -1.461337 0.844046 0.071806  
C -0.766584 -0.389506 0.003865  
C -1.527526 -1.580338 -0.026703  
C -2.906999 -1.551587 0.008366  
C -0.723799 2.078966 1.00788  
C 0.630676 2.085506 0.064116  
C 1.377023 0.857630 -0.03976  
C 0.691404 -0.382371 -0.034750  
C 2.789617 0.879022 -0.037818  
C 3.515447 -0.291145 -0.099375  
C 2.840246 -1.525035 -0.130322  
C 1.460899 -1.566280 -0.099214  
H 0.969367 -2.536505 -0.122157  
H -1.029103 -2.545986 -0.078871  
H -1.280904 3.014990 0.151977  
H 1.180801 3.026753 0.085538  
H 3.408361 -2.453805 -0.177928  
(H2)2Ph-, II  
E = -541.537071  
C -3.609773 -0.350408 0.068222  
C -2.906162 0.836704 0.114138  
C -1.473795 0.868115 0.081116  
C -0.777763 -0.393878 -0.003375  
C -1.529590 -1.571309 -0.047344  
C -2.930844 -1.577668 -0.012904  
C -0.753701 2.075003 0.125563  
C 0.655745 2.082677 0.091437  
C 1.386860 0.885023 0.010954  
C 0.702358 -0.385622 -0.040216  
C 2.820154 0.869210 -0.020853  
C 3.534110 -0.310154 -0.100665  
C 2.866434 -1.544960 -0.152582  
C 1.464653 -1.554269 -0.128018  
C 0.961101 -2.520505 -0.157893  
C -1.017751 -2.531915 -0.11109  
C -1.306616 3.014649 0.187334  
C 1.208351 3.028525 0.126990  
C 3.424049 -2.480855 -0.212782  
C -3.441443 1.787230 0.176884  
C 3.347285 1.825219 0.021450  
C -3.479813 -2.519065 -0.049330  
C 4.626666 -0.279961 -0.120725  
C -4.702553 -0.332715 0.095642  
C -0.106830 1.321905 -2.527159  
C -0.126222 1.057685 -3.240324  
C 1.924378 -0.445121 2.549600  
C 2.003120 -0.496658 3.304214  
(H2O)2Ph, II  
E = -692.015455  
C -1.564424 -0.853901 -1.398806  
C -0.786716 -0.215134 -0.398311  
C -1.462016 0.511441 0.615171  
C -2.873762 0.579802 0.607194  
C -3.606877 -0.053047 -0.373089  
C -2.942138 -0.776081 -1.388120  
C -0.706312 1.170365 1.648702  
C 0.646789 1.100234 1.679491  
C 1.374602 0.370673 0.674167  
C 0.671489 -0.282511 -0.371405  
C 1.424371 -0.976318 -1.347174  
C 2.802856 -1.022166 -1.289251
C 3.49375 -0.37554 -0.248310
C 2.78623 0.309131 0.715959
O 0.627650 3.014672 -1.304480
H 3.309559 0.818722 1.525314
H 4.581878 -0.415732 -0.207341
H 3.357575 -1.564275 -2.054370
H 0.920570 -1.489313 -2.163032
H 1.209529 1.596697 2.469855
H -1.248973 1.722302 2.416311
H -3.376560 1.143051 1.393950
H -4.694873 0.004622 -0.930544
H -3.517510 -1.278809 -2.156809
H -1.081662 -1.422578 -2.182297
H 0.189625 2.803986 -0.474051
H 1.117251 2.241612 -1.513322
H -0.867617 -2.120957 1.569746
O -0.139127 -2.611330 1.962018

(H2O)2Ph-, II
E = -692.034960
C -1.497929 -1.725063 0.021063
C -0.740051 -0.550753 -0.026432
C -1.426504 0.712850 -0.136035
C -2.853207 0.687647 -0.238693
C -3.562533 -0.496573 -0.209748
C -2.894276 -1.724047 -0.070263
C -0.699558 1.920263 -0.103960
C 0.699559 1.920263 0.103953
C 1.426506 0.712852 0.136033
C 0.740054 -0.550753 0.026435
C 1.497933 -1.725062 -0.021057
C 2.894280 -1.724044 0.070268
C 3.562536 -0.496573 0.209750
C 2.853209 0.687650 0.238691
O 0.462797 0.852662 -3.095922
H 3.308937 1.639848 0.332362
H 4.652199 -0.474933 0.286450
C 3.450455 -2.660736 0.029849
H 0.992301 -2.684383 -0.131411
H 1.246266 2.863093 0.152017
H -1.246266 2.863092 -0.152026
H -3.380936 1.639891 -0.332366
H -4.652196 -0.474937 -0.286448
H -3.450450 -2.660739 -0.029841
H -0.992296 -2.684384 0.131420
H -0.017598 1.330171 -2.405096
H 0.975263 0.220485 -2.580698
H -0.975276 0.220497 2.580692
O -0.462810 0.852673 3.095918
H 0.017589 1.330180 2.405093

(H2O)2Ph-, I
E = -692.019569
C 1.378861 -1.452736 -0.800680
C 0.555903 -0.313029 -0.654334
C 1.176264 0.961361 -0.648572
C 2.579627 1.060877 -0.777824
C 3.359281 -0.067060 -0.916535
C 2.748889 -1.334880 -0.930544
C 0.372075 2.147292 -0.508406
C -0.976382 2.068983 -0.386162
C -1.647593 0.794809 -0.373462
C -0.892634 -0.399653 -0.498214
C -1.584785 -1.631352 -0.445273
C -2.954940 -1.677326 -0.281082
C -3.698687 -0.489674 -0.164269
C -3.049735 0.726252 -0.210443
C -3.613333 1.655076 -0.115707
C -4.779753 -0.531100 -0.035161
C -3.461854 -2.641029 -0.240747
C -1.039643 -2.568751 -0.529025
C -1.577309 2.973714 -0.289637
C 0.871858 3.116381 -0.510932
C 3.040122 2.049663 -0.760866
C 4.441171 0.019327 -1.009273
C 3.360143 -2.230366 -1.036795
C 0.948036 -2.448055 -0.805699
C 2.367520 -0.896117 1.662990
O 2.196813 -0.852770 2.607738
H 1.373648 -0.345983 2.681857
C -0.233910 1.321669 2.017429
O -0.311315 0.619477 2.672668
H -0.970333 0.025742 2.299875

(H2O)2Ph-, I
E = -692.038275
C -1.306076 -1.477830 0.774672
C -0.499444 -0.345396 0.635300
C -1.118895 0.955589 0.687805
C -2.536746 1.011931 0.867910
C -3.300235 -0.131987 0.990891
C -2.694829 -1.399807 0.946053
C -0.336794 2.121828 0.555628
C 1.067510 2.044591 0.422395
C 1.728665 0.82409 0.342685
C 0.963269 -0.425896 0.414300
C 1.640382 -1.640527 0.266122
C 3.025908 -1.715283 0.078128
C 3.767534 -0.522343 0.029915
C 3.137839 0.699291 0.155503
C 3.719950 1.622165 0.106536
H 4.850023 -0.559309 -0.115112
C 3.515932 -2.682583 -0.033822
H 1.078882 -2.574032 0.298605
H 1.661731 2.958684 0.346659
H -0.830839 3.093617 0.612759
H -3.014971 1.993137 0.896312
H -4.382022 -0.049145 1.116782
H -3.290297 -2.306151 1.045735
C -0.000000 -2.864443 0.845935
H -0.000000 -3.395899 1.800795
H -0.000000 -4.666795 -0.314712
H -0.000000 -3.453833 -2.511644
H -0.000000 -0.990274 -2.538497
H -0.000000 -1.253680 3.017050
H 0.000000 1.253680 3.017050
H 0.000000 3.395899 1.800795
H 0.000000 4.666795 -0.314712
H 0.000000 3.453833 -2.511644
H 0.000000 0.990274 -2.538497
He 3.244537 -0.000000 0.560448
He -3.244537 0.000000 0.560448

(H2)3Ph, II
E = -542.696046
C 3.552550 -0.269225 -0.079277
C 2.831522 0.901451 0.015969
C 1.418202 0.886872 0.018258
C 0.727603 -0.347311 -0.078875
C 1.492764 -1.532013 -0.173921
C 2.872364 -1.497063 -0.175115
C 0.676939 2.115104 0.117928
C -0.677633 2.115031 0.123203
C -1.419803 0.886967 0.024260
C -0.729953 -0.346894 -0.079964
C -2.833060 0.902699 0.024856
C -3.555160 -0.267431 -0.077813
C -2.875837 -1.494453 -0.186720
C -1.496028 -1.529979 -0.187826
H -0.317017 0.954280 -2.787420
H 0.367849 0.386543 2.730222
H 0.274344 -2.839378 2.588327
H -1.008622 -2.494618 -0.275154
H 0.996479 -2.497308 -0.244193
H 1.231217 3.051205 0.191047
H -1.231418 3.051030 0.201510
H -3.440954 -2.422359 -0.271829
C 3.346290 1.860120 0.091322
H -3.347030 1.860518 0.106918
H 3.437129 -2.426999 -0.249958
H -4.644706 -0.243861 -0.077874
H 4.642110 -0.246308 -0.080432
H 0.371293 0.793559 -3.020294
H -0.233254 0.592117 3.143072
H -0.358011 -2.464197 2.324339

(H2)3Ph, IV
E = -542.695874
C 3.552550 -0.269225 -0.079277
C 2.831522 0.901451 0.015969
C 1.418202 0.886872 0.018258
C 0.727603 -0.347311 -0.078875
C 1.492764 -1.532013 -0.173921
C 2.872364 -1.497063 -0.175115
C 0.676939 2.115104 0.117928
C -0.677633 2.115031 0.123203
C -1.419803 0.886967 0.024260
C -0.729953 -0.346894 -0.079964
C -2.833060 0.902699 0.024856
C -3.555160 -0.267431 -0.077813
C -2.875837 -1.494453 -0.186720
C -1.496028 -1.529979 -0.187826
H -0.317017 0.954280 -2.787420
H 0.367849 0.386543 2.730222
H 0.274344 -2.839378 2.588327
H -1.008622 -2.494618 -0.275154
H 0.996479 -2.497308 -0.244193
H 1.231217 3.051205 0.191047
H -1.231418 3.051030 0.201510
H -3.440954 -2.422359 -0.271829
C 3.346290 1.860120 0.091322
H -3.347030 1.860518 0.106918
H 3.437129 -2.426999 -0.249958
H -4.644706 -0.243861 -0.077874
H 4.642110 -0.246308 -0.080432
H 0.371293 0.793559 -3.020294
H -0.233254 0.592117 3.143072
H -0.358011 -2.464197 2.324339

(H2)3Ph-, II
E = -542.700516
C 0.765186 2.053566 -0.019886
C -0.644868 2.070114 -0.048547
C -1.384917 0.875261 -0.069517
C -0.709654 -0.400919 -0.079112
C -2.818057 0.869029 -0.097365
C -3.540682 -0.307013 -0.145680
C -2.881828 -1.547167 -0.163425
C -1.479955 -1.565864 -0.127381
H 0.149798 1.204293 -2.638400
H 0.478097 1.321042 2.588167
H -2.254040 -0.591214 3.261207
H -0.983421 -2.536300 -0.137394
H 0.993784 -2.561170 -0.050172
H 1.325326 2.990456 -0.001284
H -1.182445 3.020423 -0.035896
H -3.445953 -2.479525 -0.199085
H 3.450532 1.747744 0.020755
H -3.338120 1.829678 -0.083587
H 3.455718 -2.564251 -0.003372
H -4.632876 -0.269475 -0.167147
H 4.695490 -0.383857 0.029855
H 0.142091 0.912836 -3.340832
H 0.435633 1.073740 3.306440
H -2.226854 -0.635668 2.502744

(H2)3Ph, IV
(H2)3Ph-, IV
E = -542.699781
C 3.568359 -0.228429 -0.201095
C 2.856400 0.948738 -0.073632
C 1.422474 0.969371 -0.075077
C 0.735480 -0.294697 -0.207330
C 1.495666 -1.459803 -0.338915
C 2.898807 -1.454950 -0.337866
C 0.693263 2.164056 0.047890
C -0.715664 2.162109 0.042422
C -1.438171 0.962914 -0.079311
C -0.744698 -0.298138 -0.201181
C -2.871380 0.935302 -0.080656
C -3.577201 -0.246097 -0.191045
C -2.900374 -1.472288 -0.305314
C -1.499304 -1.470192 -0.306507
H -1.998956 -0.466894 3.167011
H 2.118800 -0.274257 2.415505
H 0.323108 -2.543211 2.019616
H -0.989100 -2.429815 -0.389472
H 0.990652 -2.419619 -0.44883
H 1.240015 3.104350 0.146348
H -1.266678 3.100300 -0.016022
H -3.451546 -2.409560 -0.384611
H 3.385527 1.898575 0.03266
H -3.405114 1.883967 -0.01377
H 3.454523 -2.387435 -0.439642
H -4.670088 -0.225174 -0.184899
H 4.661154 -0.201930 -0.193352
H 2.047386 -0.472975 3.145607
H 0.014682 -3.127540 2.393634
H -1.996301 -0.336162 2.418460

(H2)3Ph-, I
E = -542.699781
C 3.568359 -0.228429 -0.201095
C 2.856400 0.948738 -0.073632
C 1.422474 0.969371 -0.075077
C 0.735480 -0.294697 -0.207330
C 1.495666 -1.459803 -0.338915
C 2.898807 -1.454950 -0.337866
C 0.693263 2.164056 0.047890
C -0.715664 2.162109 0.042422
C -1.438171 0.962914 -0.079311
C -0.744698 -0.298138 -0.201181
C -2.871380 0.935302 -0.080656
C -3.577201 -0.246097 -0.191045
C -2.900374 -1.472288 -0.305314
C -1.499304 -1.470192 -0.306507
H -1.998956 -0.466894 3.167011
H 2.118800 -0.274257 2.415505
H 0.323108 -2.543211 2.019616
H -0.989100 -2.429815 -0.389472
H 0.990652 -2.419619 -0.44883
H 1.240015 3.104350 0.146348
H -1.266678 3.100300 -0.016022
H -3.451546 -2.409560 -0.384611
H 3.385527 1.898575 0.03266
H -3.405114 1.883967 -0.01377
H 3.454523 -2.387435 -0.439642
H -4.670088 -0.225174 -0.184899
H 4.661154 -0.201930 -0.193352
H 2.047386 -0.472975 3.145607
H 0.014682 -3.127540 2.393634
H -1.996301 -0.336162 2.418460

(H2)3Ph, I
E = -542.696460
C 2.833774 0.874311 -0.016114
C 1.420668 0.862203 -0.020726
C 0.730222 -0.373762 -0.085666
C 1.495304 -1.560549 -0.193352
C 2.875063 -1.526413 -0.139719
C 3.553512 -0.296669 -0.073956
C -0.727774 -0.373568 -0.084870
C -1.417614 0.862461 -0.018633
C -0.675760 2.092893 0.045000
C 0.678757 2.093056 0.043914
C -2.830589 0.877444 -0.012513
C -3.552518 -0.295984 -0.070697
C -2.872753 -1.525810 -0.138293
C -1.492872 -1.560184 -0.145539
H 2.122526 -0.491447 2.611161
H -2.150671 -0.419981 2.608197
H 0.279796 0.904893 -2.792265

(H2)3Ph, III
E = -542.696460
C 2.833774 0.874311 -0.016114
C 1.420668 0.862203 -0.020726
C 0.730222 -0.373762 -0.085666
C 1.495304 -1.560549 -0.193352
C 2.875063 -1.526413 -0.139719
C 3.553512 -0.296669 -0.073956
C -0.727774 -0.373568 -0.084870
C -1.417614 0.862461 -0.018633
C -0.675760 2.092893 0.045000
C 0.678757 2.093056 0.043914
C -2.830589 0.877444 -0.012513
C -3.552518 -0.295984 -0.070697
C -2.872753 -1.525810 -0.138293
C -1.492872 -1.560184 -0.145539
H 2.122526 -0.491447 2.611161
H -2.150671 -0.419981 2.608197
H 0.279796 0.904893 -2.792265
|   | He3Ph-, IV |   | He3Ph-, I |   | He3Ph, III |
|---|---|---|---|---|---|
| E | -547.919342 | E | -547.919799 | E | -547.917584 |
| C | -0.771569 -0.325185 -0.209689 | C | -1.497756 -1.545288 -0.155710 | C | 1.495217 -1.595248 -0.100657 |
| C | 0.708939 -0.314671 -0.236316 | C | -0.740313 -0.372881 -0.088967 | C | 0.729545 -0.409156 -0.173893 |
| H | -1.009577 -2.458616 -0.384989 | H | -1.430827 0.893512 -0.015037 | H | 1.419856 0.826597 -0.250491 |
| C | 0.659341 2.148252 -0.026197 | C | -2.864388 0.869949 -0.015269 | C | 2.833066 0.841193 -0.250005 |
| C | -0.749828 2.138337 -0.002237 | C | -3.573538 -0.313108 -0.081750 | C | 3.554710 -0.330823 -0.177289 |
| H | -1.009577 -2.458616 -0.384989 | C | -2.899998 -1.544051 -0.152999 | C | 2.875018 -1.560123 -0.102415 |
| C | 0.659341 2.148252 -0.026197 | C | -0.704725 2.094884 0.054759 | C | 0.677277 2.056526 -0.328967 |
| C | -0.749828 2.138337 -0.002237 | C | 0.704725 2.094884 0.054757 | C | -0.677277 2.056526 -0.328967 |
| C | 0.659341 2.148252 -0.026197 | C | 1.430827 0.893512 -0.015039 | C | -1.419856 0.826597 -0.250491 |
| C | -0.749828 2.138337 -0.002237 | C | 0.740313 -0.372881 -0.088967 | C | -0.729545 -0.409156 -0.173893 |
| C | 1.392181 0.954533 -0.141620 | C | 1.497756 -1.545288 -0.155706 | C | 1.495217 -1.595248 -0.100657 |
| C | 0.708939 -0.314671 -0.236316 | C | 2.899998 -1.544052 -0.152996 | C | 2.833066 0.841193 -0.250005 |
| H | -1.009577 -2.458616 -0.384989 | C | 3.573538 -0.313108 -0.081751 | C | 3.554710 -0.330823 -0.177289 |
| C | 0.659341 2.148252 -0.026197 | C | 2.864388 0.869949 -0.015272 | C | 2.875018 -1.560123 -0.102415 |
| C | -0.749828 2.138337 -0.002237 | C | -0.990033 -2.508674 -0.211596 | C | 0.677277 2.056526 -0.328967 |
| C | 0.659341 2.148252 -0.026197 | C | 1.253624 3.037641 0.109285 | C | -0.677277 2.056526 -0.328967 |
| C | -0.749828 2.138337 -0.002237 | C | -1.253623 3.037641 0.109288 | C | -1.419856 0.826597 -0.250491 |
| C | 0.659341 2.148252 -0.026197 | C | -3.395758 1.823204 0.040349 | C | -0.729545 -0.409156 -0.173893 |
| C | -0.749828 2.138337 -0.002237 | C | 4.666626 -0.289092 -0.078622 | C | -3.347521 1.801253 -0.309065 |
| C | 0.659341 2.148252 -0.026197 | C | 3.453729 -2.482131 -0.205761 | C | -3.347521 1.801253 -0.309065 |
| C | -0.749828 2.138337 -0.002237 | C | 0.990033 -2.508674 -0.211596 | C | -3.347521 1.801253 -0.309065 |
| C | 0.659341 2.148252 -0.026197 | C | 1.253624 3.037641 0.109285 | C | -3.347521 1.801253 -0.309065 |
| C | -0.749828 2.138337 -0.002237 | C | -1.859409 -0.424111 3.172182 | C | -3.347521 1.801253 -0.309065 |
| C | 0.659341 2.148252 -0.026197 | C | -1.859410 -0.424116 3.172179 | C | -3.347521 1.801253 -0.309065 |
| X   | Y   | Z   |
|-----|-----|-----|
| -4.644268 | -0.307454 | -0.177779 |
| -3.439920 | -2.490380 | -0.045024 |
| -0.999983 | -2.562172 | -0.041332 |
| 1.231228 | 2.993992 | -0.388379 |
| 3.347521 | 1.801253 | -0.309065 |
| 4.644268 | -0.307454 | -0.177779 |
| 3.439920 | -2.490380 | -0.045024 |
| 0.999983 | -2.562172 | -0.041332 |

He3Ph-, III

E = -547.919366

| X   | Y   | Z   |
|-----|-----|-----|
| 1.497931 | -1.573233 | -0.126190 |
| 0.740402 | -0.400132 | -0.180146 |
| 1.430869 | 0.867162 | -0.240210 |
| 2.864514 | 0.843538 | -0.238890 |
| 3.573626 | -0.340171 | -0.184383 |
| 2.900158 | -1.571814 | -0.127159 |
| 0.704669 | 2.069117 | -0.298501 |
| -0.704669 | 2.069117 | -0.298501 |
| -1.430868 | 0.867162 | -0.240210 |
| -0.740402 | -0.400132 | -0.180146 |
| -1.497930 | -1.573233 | -0.126190 |
| -2.900157 | 2.069117 | -0.298501 |
| -3.573626 | -0.340171 | -0.184383 |

Ph-

E = -539.209593

| X   | Y   | Z   |
|-----|-----|-----|
| 0.000000 | 1.497981 | -1.549739 |
| 0.000000 | 0.740450 | -0.375398 |
| 0.000000 | 1.430956 | 0.893382 |
| 0.000000 | 2.864633 | 0.869796 |
| 0.000000 | 3.573821 | -0.315252 |
| 0.000000 | 2.900344 | -1.548256 |
| 0.000000 | 0.704713 | 2.096757 |
| -0.000000 | -0.704713 | 2.096757 |
| -1.497981 | -1.549739 |
| 0.000000 | 0.740450 | -0.375398 |
| 0.000000 | 1.430956 | 0.893382 |
| 0.000000 | 2.900344 | -1.548256 |
| -0.000000 | -2.864633 | 0.869796 |
| -0.000000 | -3.396101 | 1.824661 |
| -0.000000 | -4.666944 | -0.290900 |
| -0.000000 | -3.454085 | -2.487882 |
| -0.000000 | -0.990331 | -2.514722 |
| -0.000000 | -1.253682 | 3.041109 |
| 0.000000 | 1.253682 | 3.041109 |
| 0.000000 | 3.396101 | 1.824661 |
| 0.000000 | 4.666944 | -0.290900 |
| 0.000000 | 3.454085 | -2.487882 |
| 0.000000 | 0.990331 | -2.514722 |