# Supporting Information

**"The Metal Ion Decorated Hexasilaprismane and Its Derivative as Molecular Container for the Separation of $CO_2$ from Flue Gas Molecules: A Computational Study"**

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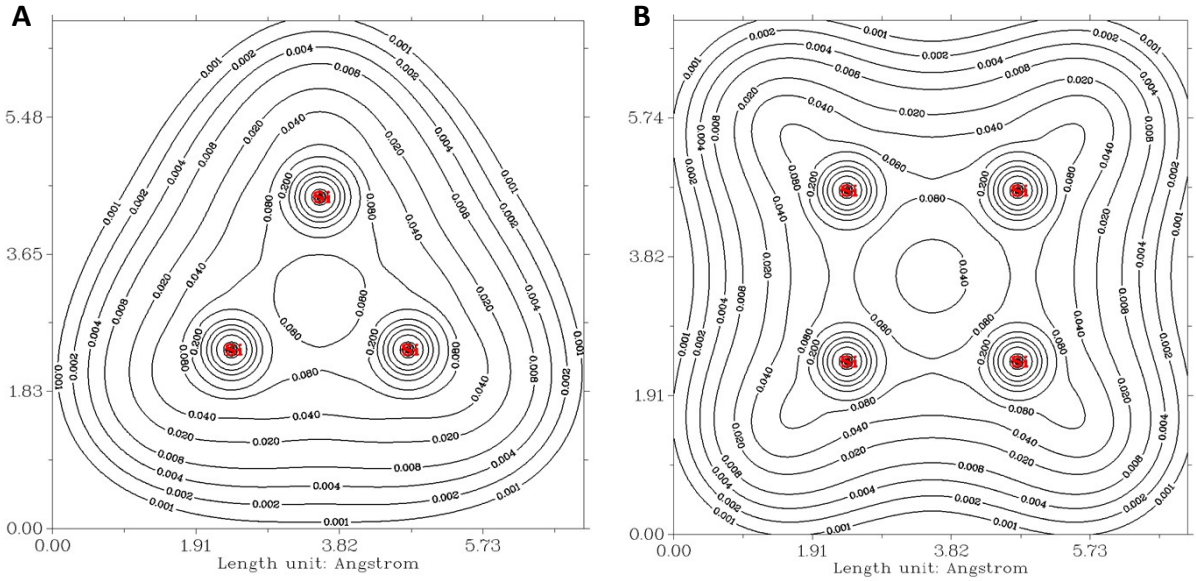


**Figure S1:** Electron density contour maps generated at m06-2x/6-311+g(d) level of theory. (A) Triangular face of the silaprismane molecule (B) Rectangular face of the silaprismane molecule.

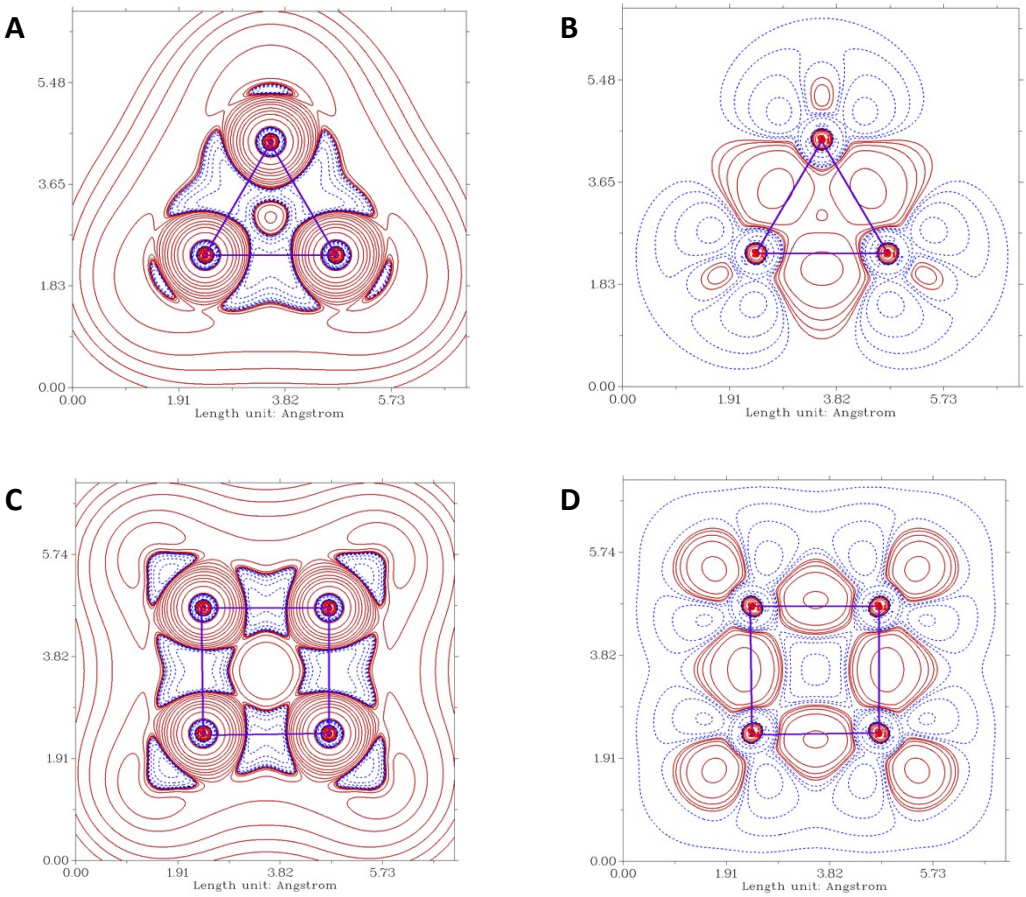


**Figure S2:** A) Laplacian of electron density ($\nabla^2\rho$) map for the triangular face of the silaprismane, B) Deformation density ($\rho_{def}$) map for the triangular face of the silaprismane C) $\nabla^2\rho$ map for the rectangular face of the silaprismane, D) $\rho_{def}$ map for the rectangular face of the silaprismane

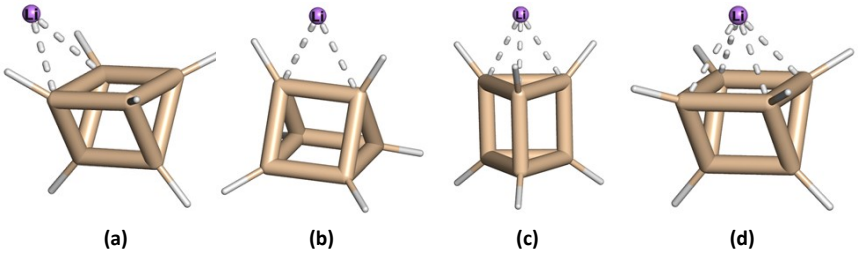


**Figure S3:** $Li^+$ ion binding with multiple sites on silaprismane (a) edge of the triangular face (b) edge of rectangular face (c) triangular face (d) rectangular face.

**Table S1:** $Li^+$ ion binding energy (ΔE) at different sites on silaprismane molecule calculated at M06-2X- 6-311+g(d) in eV/molecule.

| Complex | ΔE |
|---|---|
| HSP-$Li^+$-triangle-edge | -1.340 |
| HSP-$Li^+$-rectangle-edge | -1.049 |
| HSP-$Li^+$-triangle-face | -0.963 |
| HSP-$Li^+$-rectangle-face | -1.678 |

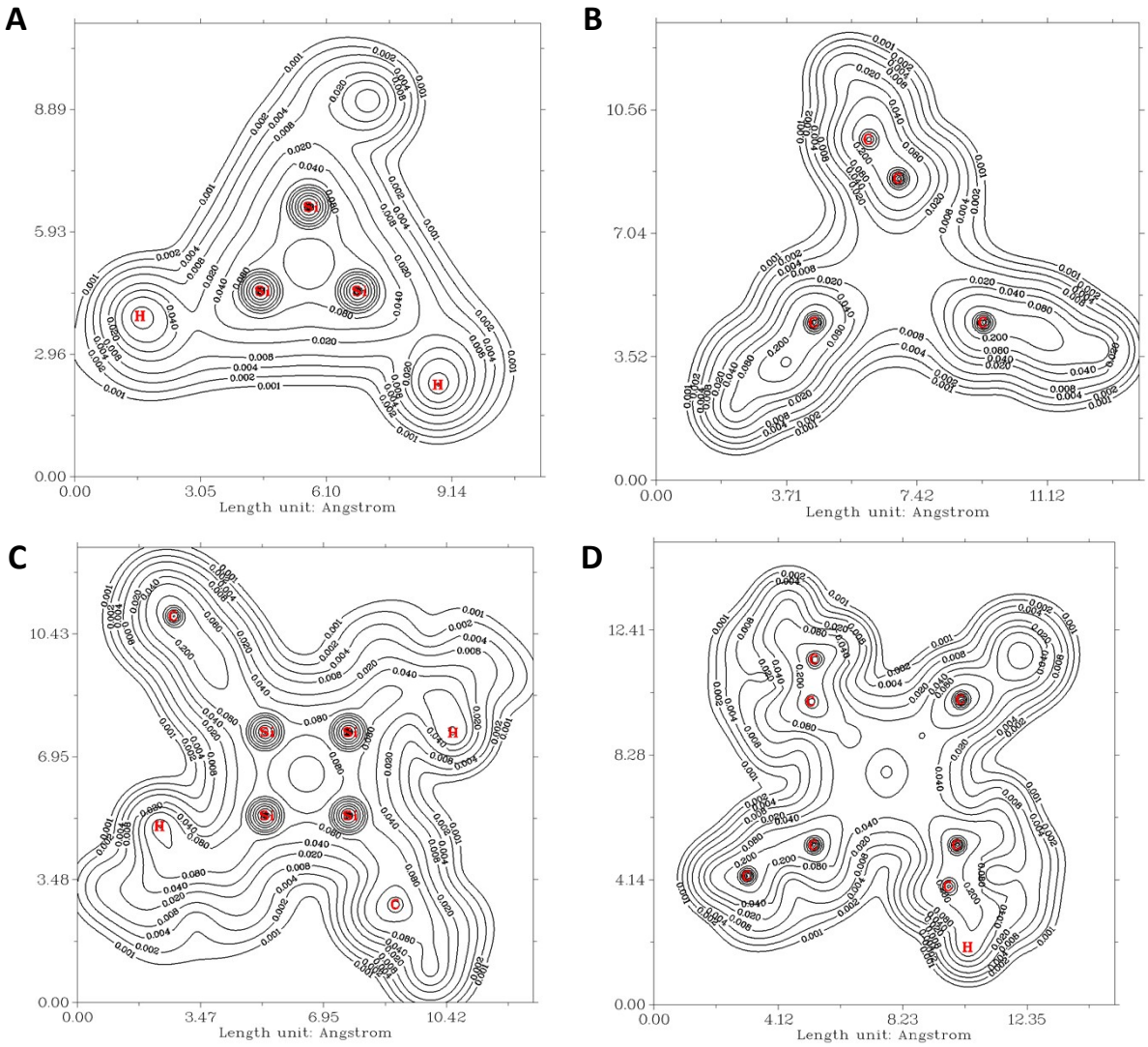


**Figure S4:** Electron density contour maps for HSP molecule generated at m06-2x/6-31g(d) level of theory A) Plane passing through three silaprismane atoms on the triangular face is plotted B) Plane passing through the three carbon atoms of phenyl ring directly attached to the silaprismane ring on the triangular face is plotted. C) Plane passing through four silaprismane atoms on the rectangular face is plotted D) Plane passing through the four carbon atoms of phenyl ring directly attached to the silaprismane ring on the rectangular face is plotted.

**Table S2:** The binding energies of one $CO_2$ gas molecule with metal ion bound to HSP or the HPPS molecule, calculated at M06-2X- 6-31g(d) level of theory (eV/molecule). The radius and the charge of each metal ion are given.

| Metal ion | Radius | Charge on metal ion | The binding energy of one $CO_2$ gas molecule on each metal ion |
|---|---|---|---|
| HSP-1$Li^{+}$-1$CO_2$ | 0.76 | +1 | -0.733 |
| HSP-1$K^{+}$-1$CO_2$ | 1.38 | +1 | -0.403 |
| HSP-1$Ca^{2+}$-1$CO_2$ | 1.00 | +2 | -1.240 |

| | | | |
|---|---|---|---|
| HPPS-2$Ca^{2+}$-1$CO_2$ | 1.00 | +2 | -1.010 |
| HPPS-3$Mg^{2+}$-1$CO_2$ | 0.72 | +2 | -1.366 |
| HPPS-3$Li^{+}$-1$CO_2$ | 0.76 | +1 | -0.525 |

**Table S3:** Gravimetric densities reported in experimental and computational studies.

| System | Gravimetric density (wt%) | Pressure | Temperature | Type of Study |
|---|---|---|---|---|
| MC-60ox-K | 4.52 | 1atm | 313K | Experimental[1] |
| MC-80ox-K | 5.76 | 1atm | 313K | Experimental[1] |
| Li-doped COF-105 | ~25 | 1atm | 298 K | Experimental[2,3] |
| 2-Li | ~15 | 1atm | 298 K | Experimental[3,4] |
| Ca-embedded $C_2N$ | 23 | 1atm | 298 K | Experimental[5] |
| MOF-5 | 48 | 14 bar | 298 K | Experimental[6] |
| MOF-177 | 39.7 | 14 bar | 298 K | Experimental[6] |
| zeolite 5A | 22.3 | 14 bar | 298 K | Experimental[6] |
| Graphene derivatives | 37.9 | 1atm | 195K | Experimental[7] |
| MIL-101Cr-$NH_2$ | 22.2 | 1 bar | 273K | Experimental[1] |
| $Si_2B_2N_2$ | 22.7 | 1atm | 298 K | Computational[8] |
| d-6$CO_2$ | 69.1 | 1atm | 298 K | Computational[9] |
| HPPS-3$Mg^{2+}$-15$CO_2$ | 48.4 | 1atm | 298 K | This work |
| HPPS-2$Ca^{2+}$-12$CO_2$ | 42.6 | 1atm | 298 K | This work |

**Table S4:** Average adsorption energies (ΔE) of water and $CO_2$ with HSP-metal complexes (eV/molecule) calculated at M06-2X- 6-311+g(d) level of theory.

| Complex | ΔE | |
|---|---|---|
| | 1$CO_2$ | 1$H_2O$ |
| HSP-$Li^{+}$ | -0.620 | -1.331 |
| HSP-$K^{+}$ | -0.338 | -0.824 |
| HSP-$Ca^{2+}$ | -1.114 | -1.951 |

$$\Delta E = E_{nGAS\_complex} - \left(E_{(n-1)GAS\_complex} + E_{1GAS}\right) \qquad \text{S1}$$

Where the $E_{nGAS\_complex}$ electronic energy of the n number of gas adsorbed complex and $E_{(n-1)GAS\_complex}$ is electronic energy of the (n-1) number of gas adsorbed complex and $E_{1GAS}$ is the electronic energy of the one gas molecule.

$$\Delta G = G_{nGAS\_complex} - \left(G_{(n-1)GAS\_complex} + G_{1GAS}\right) \qquad \text{S2}$$

Where the $E_{nGAS\_complex}$ free energy of the n number of gas adsorbed complex and $E_{(n-1)GAS\_complex}$ is free energy of the (n-1) number of gas adsorbed complex and $E_{1GAS}$ is the free energy of the one gas molecule.

**Table S5:** Adsorption energies (ΔE) and free energies (ΔG) calculated for addition of the last gas molecule in the metal ion bound HSP complex (eV/molecule). The adsorption energies and free energies was calculated with formula given equation S1 and equation S2.

| Complex | ΔE (ΔG) CBS-QB3 | ΔE (ΔG) m06-2x/6-311+g(d) |
|---|---|---|
| HSP-1$Ca^{2+}$-4$CO_2$ | -0.66 (-0.27) | -0.70 (-0.70) |
| HSP-1$Ca^{2+}$-6$N_2$ | -0.39 (0.08) | -0.41 (0.06) |
| HSP-1$Ca^{2+}$-4$CH_4$ | -0.33 (0.04) | -0.38 (0.03) |

**Table S6:** Adsorption energies (ΔE) and free energies (ΔG) calculated for addition of the last gas molecule in the metal ion bound HPPS complex calculated at m06-2x/6-31g(d) level of theory (eV/molecule). Single point energies calculated at m06-2x/6-311+g(d) level of theory (ΔE1). The adsorption energies and free energies was calculated with formula given equation S1 and equation S2.

| Complex | ΔE | ΔG | ΔE1 |
|---|---|---|---|
| HPPS-2$Ca^{2+}$-12$CO_2$ | -0.54 | -0.24 | -0.54 |
| HPPS-2$Ca^{2+}$-9$N_2$ | -0.40 | 0.04 | -0.33 |
| HPPS-2$Ca^{2+}$-4$CH_4$ | -0.52 | -0.09 | -0.54 |
| HPPS-3$Mg^{2+}$-15$CO_2$ | -0.76 | -0.25 | -0.67 |
| HPPS-3$Mg^{2+}$-18$N_2$ | -0.34 | 0.004 | -0.27 |
| HPPS-3$Mg^{2+}$-9$CH_4$ | -0.36 | 0.14 | -0.34 |
| HPPS-3$Li^{+}$-9$CO_2$ | -0.51 | -0.19 | -0.21 |
| HPPS-3$Li^{+}$-1$N_2$ | -0.29 | 0.11 | -0.43 |
| HPPS-3$Li^{+}$-1$CH_4$ | -0.20 | 0.17 | -0.24 |

**Table S7:** Adsorption energies (ΔE) of gas molecules with Au(111) surface calculated at M06-2X method and 6-31g(d) basis set for the gas molecules and the lanl2dz for Au surface (eV/molecule). The Au surface was kept frozen during optimization.

| Complex | ΔE |
|---|---|
| Au-1$CO_2$ | -0.221 |
| Au-1$N_2$ | -0.156 |
| Au-1$CH_4$ | 0.477 |

**Table S8:** Coordinates of the optimized geometries at the CBS-QB3 method.

| **Hexasilaprismane (HSP)** | | | | **HSP-1$Li^{+}$** | | | |
|---|---|---|---|---|---|---|---|
| 0 1 | | | | 1 1 | | | |
| H | 2.16326100 | 0.78888500 | 2.36429900 | Si | -1.20509500 | -0.58116900 | -1.22744600 |
| H | 2.16257000 | 1.65297000 | -1.86593400 | Si | -1.20515100 | -0.58104500 | 1.22745100 |
| H | 2.16266500 | -2.44214500 | -0.49993300 | Si | -1.18625400 | 1.42543200 | -0.00009800 |
| H | -2.16240700 | 0.78867200 | 2.36493400 | Si | 1.20509500 | -0.58104600 | 1.22750400 |
| H | -2.16322600 | 1.65321000 | -1.86521600 | Si | 1.20515100 | -0.58116800 | -1.22739200 |
| H | -2.16264500 | -2.44245500 | -0.49870600 | Si | 1.18625500 | 1.42543200 | -0.00004500 |
| Si | 1.18852600 | -1.33998600 | -0.27402900 | Li | -0.00000100 | -2.61598700 | 0.00013100 |

| | | | |
|---|---|---|---|
| Si | 1.18830100 | 0.90725000 | -1.02355900 |
| Si | 1.18885200 | 0.43278500 | 1.29719600 |
| Si | -1.18874200 | 0.90727100 | -1.02327500 |
| Si | -1.18861600 | -1.33999900 | -0.27376500 |
| Si | -1.18833600 | 0.43274000 | 1.29747100 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| H | 2.18613700 | -1.13473100 | 2.19305700 |
| H | -2.18623700 | -1.13473300 | 2.19295800 |
| H | 2.18623600 | -1.13495400 | -2.19284400 |
| H | -2.18613800 | -1.13494900 | -2.19294400 |
| H | 2.19283200 | 2.50861500 | -0.00007400 |
| H | -2.19283100 | 2.50861600 | -0.00017700 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1K$^{+}$**

1 1

| | | | |
|---|---|---|---|
| Si | 0.00605300 | -1.19425200 | -1.20535500 |
| Si | 0.00593600 | -1.19430700 | 1.20530000 |
| Si | -2.02093100 | -1.18991500 | -0.00012600 |
| Si | 0.00593600 | 1.19425200 | 1.20535400 |
| Si | 0.00605300 | 1.19430700 | -1.20530100 |
| Si | -2.02093100 | 1.18991500 | -0.00007200 |
| H | 0.57342300 | 2.16245700 | 2.18140100 |
| H | 0.57342400 | -2.16255600 | 2.18130300 |
| H | 0.57363500 | 2.16255600 | -2.18124900 |
| H | 0.57363300 | -2.16245800 | -2.18134700 |
| H | -3.11396400 | 2.18941900 | -0.00010200 |
| H | -3.11396500 | -2.18941900 | -0.00020300 |
| K | 3.16758900 | 0.00000000 | 0.00015800 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1Ca$^{2+}$**

2 1

| | | | |
|---|---|---|---|
| Si | 0.08840000 | -1.21087700 | -1.24952900 |
| Si | 0.08813600 | -1.21093400 | 1.24949600 |
| Si | -1.90471100 | -1.19275600 | -0.00022600 |
| Si | 0.08816000 | 1.21090000 | 1.24955400 |
| Si | 0.08841800 | 1.21095800 | -1.24948400 |
| Si | -1.90468400 | 1.19274100 | -0.00017300 |
| H | 0.68551700 | 2.18445800 | 2.19799700 |
| H | 0.68562800 | -2.18452100 | 2.19782800 |
| H | 0.68598400 | 2.18456000 | -2.19775200 |
| H | 0.68608000 | -2.18442400 | -2.19778300 |
| H | -2.96883300 | 2.21468200 | -0.00025700 |
| H | -2.96887100 | -2.21468600 | -0.00036700 |
| Ca | 2.57912200 | -0.00002600 | 0.00027000 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1Ca$^{2+}$-1$CO_2$**

2 1

| | | | |
|---|---|---|---|
| Si | -0.94106800 | -1.20964500 | -1.24376100 |
| Si | -0.94111100 | -1.20936800 | 1.24391600 |
| Si | -2.93754700 | -1.19136400 | 0.00002900 |
| Si | -0.94090700 | 1.20982500 | 1.24374800 |
| Si | -0.94080900 | 1.20954700 | -1.24403600 |
| Si | -2.93726700 | 1.19132300 | -0.00022000 |
| H | -0.35345400 | 2.18275500 | 2.19915900 |
| H | -0.35280900 | -2.18205300 | 2.19907300 |
| H | -0.35330100 | 2.18225800 | -2.19963500 |
| H | -0.35250000 | -2.18247800 | -2.19860800 |
| H | -4.00283800 | 2.21215700 | -0.00042500 |
| H | -4.00328700 | -2.21202700 | 0.00014700 |
| Ca | 1.59581700 | -0.00027500 | 0.00003400 |
| C | 5.12875800 | 0.00006000 | 0.00022700 |
| O | 3.94254900 | 0.00001200 | 0.00022200 |
| O | 6.26635300 | -0.00000200 | 0.00012500 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1Ca$^{2+}$-$N_2$**

2 1

| | | | |
|---|---|---|---|
| Si | 0.57137400 | -1.21016300 | 1.24630900 |
| Si | 0.56814700 | -1.21072200 | -1.24512000 |
| Si | 2.56505300 | -1.18813300 | -0.00200400 |
| Si | 0.56292300 | 1.20907600 | -1.24557300 |
| Si | 0.56629600 | 1.20963200 | 1.24594900 |
| Si | 2.55994000 | 1.19556400 | -0.00248700 |
| H | -0.03352700 | 2.18076400 | -2.19667300 |
| H | -0.02452300 | -2.18526400 | -2.19566000 |
| H | -0.02785600 | 2.18165700 | 2.19814200 |
| H | -0.01844600 | -2.18434300 | 2.19898000 |
| H | 3.62262600 | 2.21920000 | -0.00427500 |
| H | 3.63225000 | -2.20706700 | -0.00309500 |
| Ca | -1.95262500 | -0.00573000 | 0.00368100 |
| N | -5.66277300 | 0.00406200 | -0.00313600 |
| N | -4.56726800 | 0.00109500 | -0.00116200 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1Ca$^{2+}$-1$CH_4$**

2 1

| | | | |
|---|---|---|---|
| Si | 0.34877300 | -1.21624600 | 1.21765700 |
| Si | 0.40981400 | -1.20394700 | -1.27129800 |
| Si | 2.37431000 | -1.16996300 | 0.02165200 |
| Si | 0.38186900 | 1.21540300 | -1.25965800 |
| Si | 0.32178900 | 1.20306000 | 1.22941200 |

**HSP-1Ca$^{2+}$-4$CO_2$**

2 1

| | | | |
|---|---|---|---|
| Si | -1.82651400 | 0.98390600 | -1.40648000 |
| Si | -1.82871600 | -1.42762800 | -0.95301700 |
| Si | -3.83592500 | -0.21915600 | -1.16792800 |
| Si | -1.82612400 | -0.98375300 | 1.40720000 |
| Si | -1.82830400 | 1.42781600 | 0.95374000 |

| | | | |
|---|---|---|---|
| Si | 2.34719800 | 1.21355700 | 0.03258200 |
| H | -0.19921000 | 2.18602200 | -2.22132900 |
| H | -0.15120300 | -2.17835400 | -2.24103200 |
| H | -0.30265200 | 2.16597000 | 2.17145200 |
| H | -0.25410700 | -2.20149000 | 2.15058000 |
| H | 3.40088200 | 2.24602300 | 0.06347000 |
| H | 3.45157200 | -2.17806100 | 0.04349000 |
| Ca | -2.15473200 | -0.02942300 | -0.08069700 |
| C | -4.85345600 | -0.01476400 | 0.26815800 |
| H | -4.66927400 | 0.52918400 | -0.66885000 |
| H | -4.44025900 | 0.49736300 | 1.14817500 |
| H | -5.93643800 | -0.00947900 | 0.40397400 |
| H | -4.56567900 | -1.07384400 | 0.21329700 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| Si | -3.83551800 | 0.21948800 | 1.16939900 |
| H | -1.25106900 | -1.74857900 | 2.54304200 |
| H | -1.25696700 | -2.55184600 | -1.73695300 |
| H | -1.25606500 | 2.55191500 | 1.73749500 |
| H | -1.25188200 | 1.74873100 | -2.54253300 |
| H | -4.90343100 | 0.40506300 | 2.17214200 |
| H | -4.90425200 | -0.40464200 | -2.17024700 |
| Ca | 0.88204700 | 0.00003400 | 0.00007900 |
| C | 2.72031900 | -0.21709100 | -3.09198400 |
| O | 2.16439900 | -0.13814200 | -2.05537700 |
| O | 3.26008200 | -0.29341600 | -4.09579700 |
| C | 1.99104700 | 3.43238900 | -0.24909600 |
| O | 1.62164200 | 2.31584800 | -0.17000800 |
| O | 2.34916400 | 4.51456100 | -0.32572100 |
| C | 1.99059400 | -3.43247700 | 0.24866100 |
| O | 1.62137200 | -2.31585900 | 0.16978900 |
| O | 2.34851300 | -4.51472700 | 0.32510000 |
| C | 2.72338200 | 0.21672500 | 3.09034300 |
| O | 2.16634800 | 0.13800800 | 2.05431500 |
| O | 3.26424000 | 0.29272300 | 4.09359000 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1Ca$^{2+}$-6N$_2$**

2 1

| | | | |
|---|---|---|---|
| Si | -1.69503200 | -1.23088600 | -1.24055600 |
| Si | -1.71566500 | -1.21377900 | 1.22029900 |
| Si | -3.71171000 | -1.22322400 | -0.02583800 |
| Si | -1.74086200 | 1.18719400 | 1.20288200 |
| Si | -1.72008100 | 1.17244000 | -1.25366700 |
| Si | -3.73801100 | 1.15169500 | -0.04106400 |
| H | -1.17629400 | 2.17623200 | 2.15458200 |
| H | -1.15930000 | -2.17652000 | 2.20251000 |
| H | -1.16350800 | 2.16016100 | -2.21023600 |
| H | -1.14298500 | -2.21585500 | -2.20203200 |
| H | -4.81033400 | 2.16666500 | -0.05687600 |
| H | -4.76263800 | -2.26034900 | -0.02764800 |
| Ca | 1.01674800 | 0.00516800 | 0.00378800 |
| N | 1.85133600 | 0.59564500 | 3.68354000 |
| N | 1.61652200 | 0.42690400 | 2.62713900 |
| N | 2.09303800 | 1.61827300 | -3.29853700 |
| N | 1.78314600 | 1.15380600 | -2.35631900 |
| N | 1.72420400 | 2.61218900 | 0.38370700 |
| N | 1.95731200 | 3.67250000 | 0.52930500 |
| N | 1.90018000 | -1.84756300 | -1.82639800 |
| N | 2.24411800 | -2.59764300 | -2.54658100 |
| N | 2.17100400 | -3.24729400 | 1.66852800 |
| N | 1.86003700 | -2.30661400 | 1.20152700 |
| N | 4.83064200 | 0.13992400 | 0.12813200 |
| N | 3.73691100 | 0.09960800 | 0.09097900 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HSP-1Ca$^{2+}$-4CH$_4$**

2 1

| | | | |
|---|---|---|---|
| Si | 0.95727300 | -1.21031900 | 1.23286900 |
| Si | 0.95674500 | -1.20885200 | -1.23471600 |
| Si | 2.95966500 | -1.26946800 | -0.00144000 |
| Si | 1.04723400 | 1.19533300 | -1.23285900 |
| Si | 1.04793000 | 1.19372600 | 1.23491500 |
| Si | 3.04915400 | 1.10682100 | 0.00040800 |
| H | 0.50620100 | 2.19722500 | -2.18563900 |
| H | 0.34796300 | -2.16639400 | -2.19107900 |
| H | 0.50673600 | 2.19357700 | 2.18972200 |
| H | 0.35038400 | -2.16967900 | 2.18858900 |
| H | 4.14970600 | 2.09058900 | 0.00015000 |
| H | 3.98591200 | -2.33049300 | -0.00205500 |
| Ca | -1.64342700 | 0.10566800 | 0.00041000 |
| C | -3.25867500 | -2.53740600 | -0.00431700 |
| H | -2.16179500 | -2.45203200 | -0.00405800 |
| H | -3.78688600 | -1.57581500 | -0.00435300 |
| H | -3.55460200 | -3.08810200 | -0.89631200 |
| H | -3.55521300 | -3.08867000 | 0.88711400 |
| C | -2.76155700 | -0.04208700 | 2.64384600 |
| H | -3.62353000 | 0.15237400 | 1.99773100 |
| H | -2.28902000 | -1.00585200 | 2.42599400 |
| H | -2.04450400 | 0.78623200 | 2.63872300 |
| H | -3.14577500 | -0.10926900 | 3.66273100 |
| C | -2.76235700 | -0.03190300 | -2.64332700 |
| H | -2.29011500 | -0.99709200 | -2.43139600 |
| H | -2.04348300 | 0.79475700 | -2.64032700 |
| H | -3.15373300 | -0.09537900 | -3.65972200 |
| H | -3.61985900 | 0.16253400 | -1.99115600 |
| C | -2.91949900 | 2.68141400 | 0.00407200 |
| H | -3.41332200 | 3.65416600 | 0.00851300 |
| H | -2.31030600 | 2.64290100 | -0.90453200 |
| H | -2.30601400 | 2.63733300 | 0.90961000 |
| H | -3.71969700 | 1.93223800 | 0.00342600 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-

| | |
|---|---|
| | 06.<br>Requested convergence on energy=1.00D-06. |

**Table S9:** Coordinates of optimized geometry at m06-2x/6-31g(d)

| **HPPS** | | | |
|---|---|---|---|
| 0 1 | | | |
| Si | 1.14828900 | -1.10069400 | -0.79316500 |
| Si | 1.17536300 | 1.23011400 | -0.47706500 |
| Si | 1.12729200 | -0.20553800 | 1.38628500 |
| Si | -1.17950600 | 1.29145300 | -0.49243300 |
| Si | -1.20537100 | -1.03603700 | -0.87100200 |
| Si | -1.23936100 | -0.19585700 | 1.33003000 |
| C | 2.42341000 | 2.53340500 | -0.99462500 |
| C | 2.08603800 | 3.89404000 | -0.98383100 |
| C | 3.71800500 | 2.16461100 | -1.38889800 |
| C | 3.01827500 | 4.85986300 | -1.35250200 |
| H | 1.08526600 | 4.20193800 | -0.68709400 |
| C | 4.65225500 | 3.13068600 | -1.74893900 |
| H | 3.99382600 | 1.11205900 | -1.42136500 |
| C | 4.30324300 | 4.47968900 | -1.73212800 |
| H | 2.74168500 | 5.91009200 | -1.34273900 |
| H | 5.65117000 | 2.83065600 | -2.05146200 |
| H | 5.03082100 | 5.23309800 | -2.01917000 |
| C | 2.39713900 | -2.23491300 | -1.61718500 |
| C | 3.65115700 | -2.44289400 | -1.02317700 |
| C | 2.11389400 | -2.87743700 | -2.82997600 |
| C | 4.59825700 | -3.26020500 | -1.63197800 |
| H | 3.88393700 | -1.96674900 | -0.07202100 |
| C | 3.05826700 | -3.70291500 | -3.43432100 |
| H | 1.14757700 | -2.73047300 | -3.30833800 |
| C | 4.30250700 | -3.89274300 | -2.83775500 |
| H | 5.56533700 | -3.41086500 | -1.16141600 |
| H | 2.82364000 | -4.19678200 | -4.37267200 |
| H | 5.03932200 | -4.53607500 | -3.30935500 |
| C | -2.40907900 | -2.17457400 | -1.75482400 |
| C | -2.03771400 | -3.48858300 | -2.07386400 |
| C | -3.69696000 | -1.73895100 | -2.09777200 |
| C | -2.92966800 | -4.34368900 | -2.71476000 |
| H | -1.04234700 | -3.84738400 | -1.81814300 |
| C | -4.59129300 | -2.59610900 | -2.73132800 |
| H | -4.00010400 | -0.71842600 | -1.87205700 |
| C | -4.20842100 | -3.89937000 | -3.04179700 |
| H | -2.62724300 | -5.35809800 | -2.95772600 |
| H | -5.58583100 | -2.24501500 | -2.99023900 |
| H | -4.90508800 | -4.56640300 | -3.54072400 |
| C | -2.31099500 | 2.69766300 | -1.01448400 |
| C | -3.46822400 | 3.00998900 | -0.28750300 |
| C | -1.99855300 | 3.46687700 | -2.14490300 |
| C | -4.29601000 | 4.05578600 | -0.68767900 |
| H | -3.71945100 | 2.43406700 | 0.60067500 |
| C | -2.82073500 | 4.51731400 | -2.53960800 |
| H | -1.10280000 | 3.24241300 | -2.72056400 |
| C | -3.97229800 | 4.81121100 | -1.81237000 |
| H | -5.19040500 | 4.28670700 | -0.11666500 |
| H | -2.56417900 | 5.10589000 | -3.41540300 |
| H | -4.61449000 | 5.63098400 | -2.12009800 |
| C | -2.56347100 | -0.43406400 | 2.64512800 |
| C | -2.59219700 | 0.36593300 | 3.79707700 |
| C | -3.55866200 | -1.40754600 | 2.47820900 |
| C | -3.58600900 | 0.19607800 | 4.75566900 |
| H | -1.83097800 | 1.12866600 | 3.94456200 |
| C | -4.55898400 | -1.57155500 | 3.43340000 |
| H | -3.54952000 | -2.04024100 | 1.59341700 |
| C | -4.57184500 | -0.77224100 | 4.57334900 |
| H | -3.59359700 | 0.81992800 | 5.64453500 |

| **HPPS-2Ca$^{2+}$** | | | |
|---|---|---|---|
| 4 1 | | | |
| Si | -0.28666700 | 1.14560800 | -1.25653700 |
| Si | -0.31823800 | 1.20679400 | 1.16947800 |
| Si | 1.70049200 | 1.19417300 | -0.01819500 |
| Si | -0.28585000 | -1.14609500 | 1.25595900 |
| Si | -0.31875800 | -1.20729200 | -1.17006300 |
| Si | 1.70064800 | -1.19465700 | 0.01648100 |
| Ca | -3.10828100 | -0.00002300 | 0.00078500 |
| C | -1.69664000 | 2.12215200 | 2.06033400 |
| C | -1.77976600 | 2.13237500 | 3.45983300 |
| C | -2.82951700 | 2.53410200 | 1.31301300 |
| C | -2.95575600 | 2.53070600 | 4.09927400 |
| H | -0.92813100 | 1.82739100 | 4.06243000 |
| C | -4.00860400 | 2.91945700 | 1.95932000 |
| H | -2.74784700 | 2.69579100 | 0.23354700 |
| C | -4.07449800 | 2.90423800 | 3.35472200 |
| H | -2.99731800 | 2.55056400 | 5.18406800 |
| H | -4.85481500 | 3.28065400 | 1.38037900 |
| H | -4.98416600 | 3.21490500 | 3.85921900 |
| C | -1.67216400 | 2.11192800 | -2.07815700 |
| C | -1.78027300 | 3.50685900 | -2.04413100 |
| C | -2.79556000 | 1.35430900 | -2.49758400 |
| C | -2.97698900 | 4.13406200 | -2.39930300 |
| H | -0.93400300 | 4.11778900 | -1.74148000 |
| C | -3.99624700 | 1.98986300 | -2.83799100 |
| H | -2.69412400 | 0.28503900 | -2.71332300 |
| C | -4.09095600 | 3.38146000 | -2.77177200 |
| H | -3.03778400 | 5.21812200 | -2.38712200 |
| H | -4.83404500 | 1.40660800 | -3.21223700 |
| H | -5.01501600 | 3.87800800 | -3.05054200 |
| C | -1.69796100 | -2.12220200 | -2.06018400 |
| C | -1.78183600 | -2.13253600 | -3.45962400 |
| C | -2.83070700 | -2.53334300 | -1.31222300 |
| C | -2.95843500 | -2.53017400 | -4.09839700 |
| H | -0.93033700 | -1.82814200 | -4.06270600 |
| C | -4.01039200 | -2.91800200 | -1.95784300 |
| H | -2.74850400 | -2.69507800 | -0.23280100 |
| C | -4.07703300 | -2.90287200 | -3.35321700 |
| H | -3.00057600 | -2.55012500 | -5.18316700 |
| H | -4.85651600 | -3.27862000 | -1.37841100 |
| H | -4.98717400 | -3.21300800 | -3.85718900 |
| C | -1.67106300 | -2.11240000 | 2.07809400 |
| C | -1.77967200 | -3.50728200 | 2.04336800 |
| C | -2.79393900 | -1.35465000 | 2.49864900 |
| C | -2.97640500 | -4.13427900 | 2.39883400 |
| H | -0.93378100 | -4.11834100 | 1.73990700 |
| C | -3.99469600 | -1.98997300 | 2.83926400 |
| H | -2.69201400 | -0.28552700 | 2.71486400 |
| C | -4.08992700 | -3.38150500 | 2.77228400 |
| H | -3.03756800 | -5.21831200 | 2.38608100 |
| H | -4.83206600 | -1.40665000 | 3.21436900 |
| H | -5.01402500 | -3.87788300 | 3.05123400 |
| C | 3.47870200 | -1.90586500 | 0.05625900 |
| C | 4.15764000 | -2.08447100 | 1.28345900 |
| C | 4.18049600 | -2.18159300 | -1.13955900 |
| C | 5.48726600 | -2.53771700 | 1.31701400 |
| H | 3.63826600 | -1.91117600 | 2.22413400 |
| C | 5.51018600 | -2.63568100 | -1.11082800 |
| H | 3.67954700 | -2.08456800 | -2.10084200 |

| | | | |
|---|---|---|---|
| H | -5.32508200 | -2.32763900 | 3.28966100 |
| H | -5.34826900 | -0.90370400 | 5.32103700 |
| C | 2.39230300 | -0.39673000 | 2.76379500 |
| C | 2.24078300 | -1.37539900 | 3.75674800 |
| C | 3.52737800 | 0.42610900 | 2.79836100 |
| C | 3.19697100 | -1.52776500 | 4.75595700 |
| H | 1.36738600 | -2.02365800 | 3.74874900 |
| C | 4.48979600 | 0.26640200 | 3.79211000 |
| H | 3.65508100 | 1.20016500 | 2.04431000 |
| C | 4.32442100 | -0.70872900 | 4.77264200 |
| H | 3.06464000 | -2.28763100 | 5.52034200 |
| H | 5.36542200 | 0.90864700 | 3.80505800 |
| H | 5.07249300 | -0.82979400 | 5.55035300 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| C | 6.16671700 | -2.81623500 | 0.11858800 |
| H | 5.97445000 | -2.71755100 | 2.27279700 |
| H | 6.01576000 | -2.89218300 | -2.03923000 |
| H | 7.17804900 | -3.21579900 | 0.14453600 |
| C | 3.47844300 | 1.90564700 | -0.05734000 |
| C | 4.15784600 | 2.08463600 | -1.28422200 |
| C | 4.17969600 | 2.18127100 | 1.13882400 |
| C | 5.48740700 | 2.53813000 | -1.31712800 |
| H | 3.63890600 | 1.91144400 | -2.22515400 |
| C | 5.50930200 | 2.63562100 | 1.11073900 |
| H | 3.67835800 | 2.08395700 | 2.09987500 |
| C | 6.16630900 | 2.81654300 | -0.11837100 |
| H | 5.97494700 | 2.71825400 | -2.27267600 |
| H | 6.01444300 | 2.89203500 | 2.03940200 |
| H | 7.17757700 | 3.21630100 | -0.14381500 |
| Ca | 5.63632600 | 0.00008300 | -0.00027900 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-3Mg$^{2+}$**

6 1

| | | | |
|---|---|---|---|
| Si | 0.65124200 | 1.19912800 | 1.18186200 |
| Si | -1.42456000 | -0.00099000 | 1.18446600 |
| Si | 0.65223300 | -1.19900100 | 1.18155800 |
| Si | -1.42476900 | -0.00005300 | -1.18304700 |
| Si | 0.65139200 | 1.19924400 | -1.18168700 |
| Si | 0.65164700 | -1.19897000 | -1.18195700 |
| C | -3.24365500 | -0.00114800 | 1.80558900 |
| C | -3.96990000 | 1.21091200 | 1.91820700 |
| C | -3.96904000 | -1.21362600 | 1.91869600 |
| C | -5.36124300 | 1.21530700 | 2.14616000 |
| H | -3.45914700 | 2.16810900 | 1.84366900 |
| C | -5.36037400 | -1.21898800 | 2.14658200 |
| H | -3.45756500 | -2.17046800 | 1.84453400 |
| C | -6.06418000 | -0.00207700 | 2.26058400 |
| H | -5.89083900 | 2.15994100 | 2.25651700 |
| H | -5.88929100 | -2.16394600 | 2.25735300 |
| H | -7.13433600 | -0.00240300 | 2.46288700 |
| C | 1.59683800 | 2.75229500 | 1.80734300 |
| C | 3.00940100 | 2.73022100 | 1.92276700 |
| C | 0.94965200 | 4.00876900 | 1.91643700 |
| C | 3.74775700 | 3.90962400 | 2.14824000 |
| H | 3.55134200 | 1.79009300 | 1.85217700 |
| C | 1.67947300 | 5.19351000 | 2.14346900 |
| H | -0.13277100 | 4.07885000 | 1.84002400 |
| C | 3.08468600 | 5.14938200 | 2.25837600 |
| H | 4.82933300 | 3.86175200 | 2.26088500 |
| H | 1.15697100 | 6.14231000 | 2.25216100 |
| H | 3.64859800 | 6.05920100 | 2.45927300 |
| C | 1.59617100 | 2.75299400 | -1.80700500 |
| C | 3.00864600 | 2.73115700 | -1.92351500 |
| C | 0.94869400 | 4.00939900 | -1.91527300 |
| C | 3.74666000 | 3.91075300 | -2.14914500 |
| H | 3.55079600 | 1.79109700 | -1.85358800 |
| C | 1.67817100 | 5.19430300 | -2.14252900 |
| H | -0.13368200 | 4.07927200 | -1.83799500 |
| C | 3.08331500 | 5.15042100 | -2.25846700 |
| H | 4.82816500 | 3.86308900 | -2.26256100 |
| H | 1.15545200 | 6.14305700 | -2.25057800 |
| H | 3.64692800 | 6.06039400 | -2.45950200 |
| C | -3.24365200 | -0.00056900 | -1.80476900 |
| C | -3.96910400 | -1.21300100 | -1.91827500 |
| C | -3.96968800 | 1.21156200 | -1.91779800 |

**HPPS-3Li$^{+}$**

3 1

| | | | |
|---|---|---|---|
| Si | 1.33171700 | -0.31889400 | 1.17645000 |
| Si | -0.38774100 | 1.31062600 | 1.17626600 |
| Si | -0.93932500 | -0.99351600 | 1.17600700 |
| Si | -0.38745900 | 1.31096900 | -1.17598400 |
| Si | 1.33150800 | -0.31900900 | -1.17678400 |
| Si | -0.93969700 | -0.99305900 | -1.17646400 |
| C | -0.87297400 | 3.01340400 | 1.84357500 |
| C | 0.09759500 | 4.02956400 | 1.94647800 |
| C | -2.23065000 | 3.37718200 | 1.93928200 |
| C | -0.27506500 | 5.36518200 | 2.13372600 |
| H | 1.15401800 | 3.78312100 | 1.87395000 |
| C | -2.60700400 | 4.71193100 | 2.12600900 |
| H | -3.00485400 | 2.61807500 | 1.86042800 |
| C | -1.62942500 | 5.71028500 | 2.21712900 |
| H | 0.48712100 | 6.13363800 | 2.21976700 |
| H | -3.65818800 | 4.97247600 | 2.20511700 |
| H | -1.92021200 | 6.74553800 | 2.36700400 |
| C | 3.04834500 | -0.75077600 | 1.84349700 |
| C | 3.44304400 | -2.09932700 | 1.94634100 |
| C | 4.04224700 | 0.24315800 | 1.94029200 |
| C | 4.78631000 | -2.44467400 | 2.13219900 |
| H | 2.70081200 | -2.89033800 | 1.87431100 |
| C | 5.38636100 | -0.09843400 | 2.12617400 |
| H | 3.77137000 | 1.29327600 | 1.86438000 |
| C | 5.76237500 | -1.44416100 | 2.21527500 |
| H | 5.07109800 | -3.48909000 | 2.21648900 |
| H | 6.13782000 | 0.68119000 | 2.20679800 |
| H | 6.80439700 | -1.70990400 | 2.36442500 |
| C | 3.04800700 | -0.75115900 | -1.84395000 |
| C | 3.44260900 | -2.09974400 | -1.94678000 |
| C | 4.04196700 | 0.24270800 | -1.94093700 |
| C | 4.78583500 | -2.44520100 | -2.13263400 |
| H | 2.70032500 | -2.89068000 | -1.87459600 |
| C | 5.38610100 | -0.09898800 | -2.12679200 |
| H | 3.77113500 | 1.29286100 | -1.86539600 |
| C | 5.76200900 | -1.44477200 | -2.21568500 |
| H | 5.07060900 | -3.48965600 | -2.21652800 |
| H | 6.13762000 | 0.68056700 | -2.20744700 |
| H | 6.80401300 | -1.71065100 | -2.36472900 |
| C | -0.87274400 | 3.01398000 | -1.84293300 |
| C | -2.23043900 | 3.37775800 | -1.93836100 |

| | | | |
|---|---|---|---|
| C | -5.36035000 | -1.21816800 | -2.14675000 |
| H | -3.45775000 | -2.16988900 | -1.84389000 |
| C | -5.36094200 | 1.21614500 | -2.14617100 |
| H | -3.45875800 | 2.16865300 | -1.84316300 |
| C | -6.06396700 | -0.00113900 | -2.26082900 |
| H | -5.88934100 | -2.16305400 | -2.25778800 |
| H | -5.89041300 | 2.16083000 | -2.25665600 |
| H | -7.13407400 | -0.00135800 | -2.46338400 |
| C | 1.59763900 | -2.75191100 | -1.80733700 |
| C | 0.95117500 | -4.00881600 | -1.91597800 |
| C | 3.01011800 | -2.72891100 | -1.92350800 |
| C | 1.68166900 | -5.19310000 | -2.14321900 |
| H | -0.13115700 | -4.07961500 | -1.83894700 |
| C | 3.74913200 | -3.90788000 | -2.14913200 |
| H | 3.55144600 | -1.78841700 | -1.85310000 |
| C | 3.08680400 | -5.14806100 | -2.25877400 |
| H | 1.15975000 | -6.14225900 | -2.25152100 |
| H | 4.83062700 | -3.85930100 | -2.26221100 |
| H | 3.65118500 | -6.05755200 | -2.45981900 |
| C | 1.59834100 | -2.75186600 | 1.80691300 |
| C | 3.01088100 | -2.72882700 | 1.92242500 |
| C | 0.95196800 | -4.00877800 | 1.91603900 |
| C | 3.75003200 | -3.90773000 | 2.14796300 |
| H | 3.55217000 | -1.78833400 | 1.85164600 |
| C | 1.68259300 | -5.19299500 | 2.14313500 |
| H | -0.13039500 | -4.07960500 | 1.83948300 |
| C | 3.08777900 | -5.14790400 | 2.25810300 |
| H | 4.83156900 | -3.85909100 | 2.26060900 |
| H | 1.16075100 | -6.14215200 | 2.25182200 |
| H | 3.65226200 | -6.05734900 | 2.45907500 |
| Mg | -5.04488400 | -0.00186100 | -0.00008700 |
| Mg | 2.55372500 | -4.27676000 | -0.00037000 |
| Mg | 2.55137500 | 4.27858600 | 0.00000200 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| C | 0.09780300 | 4.03013900 | -1.94584700 |
| C | -2.60682200 | 4.71248800 | -2.12516600 |
| H | -3.00461700 | 2.61862500 | -1.85958500 |
| C | -0.27486700 | 5.36573000 | -2.13322500 |
| H | 1.15423600 | 3.78372600 | -1.87338700 |
| C | -1.62924100 | 5.71081100 | -2.21653800 |
| H | -3.65800200 | 4.97310000 | -2.20406100 |
| H | 0.48732100 | 6.13416800 | -2.21936900 |
| H | -1.92009700 | 6.74602800 | -2.36650100 |
| C | -2.17449600 | -2.26274100 | -1.84294200 |
| C | -3.54030500 | -1.92864700 | -1.93237700 |
| C | -1.81281900 | -3.61993800 | -1.95074400 |
| C | -4.51333800 | -2.91691200 | -2.11851500 |
| H | -3.85353000 | -0.89090200 | -1.84975700 |
| C | -2.78326700 | -4.61124900 | -2.13574700 |
| H | -0.76779900 | -3.91235400 | -1.88471900 |
| C | -4.13709000 | -4.26205100 | -2.21338300 |
| H | -5.56054200 | -2.63970800 | -2.19301300 |
| H | -2.48495400 | -5.65161000 | -2.22326600 |
| H | -4.89067400 | -5.02935200 | -2.36116500 |
| C | -2.17340300 | -2.26390200 | 1.84260200 |
| C | -1.81109400 | -3.62094000 | 1.95024100 |
| C | -3.53931700 | -1.93044000 | 1.93248600 |
| C | -2.78105500 | -4.61269600 | 2.13550000 |
| H | -0.76596800 | -3.91288700 | 1.88374000 |
| C | -4.51181900 | -2.91911300 | 2.11895900 |
| H | -3.85302700 | -0.89284000 | 1.84992700 |
| C | -4.13498100 | -4.26408000 | 2.21377700 |
| H | -2.48225100 | -5.65292200 | 2.22294700 |
| H | -5.55911200 | -2.64235500 | 2.19388800 |
| H | -4.88817700 | -5.03169900 | 2.36190000 |
| Li | -1.33691600 | 4.63652300 | 0.00002900 |
| Li | -3.35322900 | -3.47561100 | 0.00013800 |
| Li | 4.67804700 | -1.18268600 | -0.00029100 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-2Ca$^{2+}$-1CO$_2$**

4 1

| | | | |
|---|---|---|---|
| Si | 0.07265500 | -1.13932300 | 1.25731300 |
| Si | 0.04050400 | -1.20967000 | -1.16144400 |
| Si | 2.06243500 | -1.19328200 | 0.02244900 |
| Si | 0.07282000 | 1.13982100 | -1.25705600 |
| Si | 0.04068500 | 1.21018000 | 1.16167800 |
| Si | 2.06264000 | 1.19383800 | -0.02219500 |
| Ca | -2.81132700 | 0.00032100 | -0.00004200 |
| C | -1.31417400 | -2.15304300 | -2.05353600 |
| C | -1.38010000 | -2.19097200 | -3.45406900 |
| C | -2.43863500 | -2.58822700 | -1.31009000 |
| C | -2.53138300 | -2.64607400 | -4.09790400 |
| H | -0.53247300 | -1.86679400 | -4.05234500 |
| C | -3.59232900 | -3.03395100 | -1.96165500 |
| H | -2.36912500 | -2.71267400 | -0.22499900 |
| C | -3.64115500 | -3.05279800 | -3.35671100 |
| H | -2.56068700 | -2.68787300 | -5.18239200 |
| H | -4.43097600 | -3.41312000 | -1.38363000 |
| H | -4.53014800 | -3.41333200 | -3.86484200 |
| C | -1.29302400 | -2.10334900 | 2.10935200 |
| C | -1.39115400 | -3.49988400 | 2.09983100 |
| C | -2.40600300 | -1.34603300 | 2.55043800 |
| C | -2.56858300 | -4.12897100 | 2.50793900 |
| H | -0.55045900 | -4.10912900 | 1.77871200 |
| C | -3.58694800 | -1.98424200 | 2.94659300 |
| H | -2.30978800 | -0.27009100 | 2.73184800 |

**HPPS-2Ca$^{2+}$-N$_2$**

4 1

| | | | |
|---|---|---|---|
| Si | -0.06159900 | 1.15172500 | -1.24700300 |
| Si | -0.09330900 | 1.21194200 | 1.17581200 |
| Si | 1.92713100 | 1.19592600 | -0.01020000 |
| Si | -0.06599900 | -1.14012400 | 1.26149300 |
| Si | -0.09905500 | -1.19988800 | -1.16202000 |
| Si | 1.92115800 | -1.19241700 | 0.02331200 |
| Ca | -2.90669600 | 0.00840100 | 0.00541900 |
| C | -1.46283600 | 2.13493800 | 2.07040000 |
| C | -1.53988200 | 2.14987900 | 3.47049100 |
| C | -2.59445300 | 2.55324700 | 1.32634200 |
| C | -2.70923900 | 2.56048300 | 4.11319300 |
| H | -0.68813300 | 1.83971900 | 4.07028100 |
| C | -3.76716600 | 2.95055200 | 1.97594500 |
| H | -2.51877100 | 2.70376000 | 0.24489500 |
| C | -3.82719600 | 2.94220300 | 3.37131600 |
| H | -2.74656900 | 2.58420700 | 5.19802100 |
| H | -4.61285700 | 3.31463000 | 1.39809400 |
| H | -4.73146100 | 3.26375500 | 3.87867600 |
| C | -1.43731200 | 2.12328400 | -2.07674300 |
| C | -1.53978700 | 3.51907500 | -2.04375200 |
| C | -2.55755500 | 1.37013300 | -2.50904800 |
| C | -2.72846000 | 4.15086600 | -2.41497400 |
| H | -0.69465400 | 4.12629200 | -1.73055300 |
| C | -3.75031000 | 2.01041800 | -2.86574400 |
| H | -2.46085000 | 0.29858300 | -2.71486700 |

| | | | |
|---|---|---|---|
| C | -3.67191800 | -3.37667100 | 2.91230200 |
| H | -2.62237200 | -5.21335900 | 2.51589200 |
| H | -4.41542500 | -1.39849000 | 3.33655900 |
| H | -4.57943300 | -3.87528900 | 3.23783000 |
| C | -1.31405700 | 2.15338700 | 2.05386000 |
| C | -1.38003600 | 2.19107400 | 3.45438800 |
| C | -2.43862100 | 2.58838000 | 1.31045200 |
| C | -2.53147900 | 2.64573600 | 4.09826500 |
| H | -0.53234100 | 1.86703200 | 4.05264000 |
| C | -3.59248200 | 3.03363500 | 1.96205100 |
| H | -2.36906400 | 2.71313600 | 0.22539900 |
| C | -3.64136500 | 3.05221200 | 3.35711300 |
| H | -2.56082000 | 2.68735800 | 5.18275900 |
| H | -4.43122000 | 3.41267300 | 1.38407000 |
| H | -4.53048900 | 3.41237100 | 3.86528000 |
| C | -1.29288000 | 2.10395300 | -2.10896000 |
| C | -1.39114500 | 3.50047700 | -2.09924600 |
| C | -2.40576900 | 1.34659800 | -2.55022600 |
| C | -2.56861700 | 4.12951200 | -2.50731000 |
| H | -0.55052300 | 4.10975500 | -1.77799900 |
| C | -3.58676800 | 1.98475500 | -2.94631400 |
| H | -2.30944800 | 0.27069200 | -2.73180700 |
| C | -3.67187200 | 3.37717200 | -2.91181800 |
| H | -2.62250200 | 5.21389600 | -2.51510600 |
| H | -4.41517100 | 1.39898400 | -3.33641000 |
| H | -4.57942100 | 3.87575300 | -3.23730400 |
| C | 3.84050600 | 1.90734900 | -0.06643800 |
| C | 4.51964300 | 2.07843400 | -1.29466400 |
| C | 4.54346600 | 2.18924600 | 1.12732100 |
| C | 5.85016400 | 2.52871500 | -1.33136500 |
| H | 3.99934200 | 1.90029200 | -2.23391500 |
| C | 5.87407100 | 2.64042900 | 1.09568800 |
| H | 4.04238500 | 2.09810100 | 2.08910700 |
| C | 6.53089400 | 2.81196200 | -0.13482000 |
| H | 6.33744000 | 2.70191800 | -2.28826500 |
| H | 6.38061500 | 2.90090300 | 2.02240500 |
| H | 7.54329100 | 3.20844200 | -0.16330800 |
| C | 3.84001100 | -1.90746700 | 0.06637800 |
| C | 4.51928600 | -2.07896000 | 1.29447200 |
| C | 4.54271300 | -2.18935300 | -1.12753600 |
| C | 5.84968800 | -2.52961100 | 1.33088500 |
| H | 3.99918300 | -1.90082400 | 2.23383300 |
| C | 5.87319100 | -2.64091600 | -1.09618900 |
| H | 4.04151200 | -2.09789100 | -2.08922900 |
| C | 6.53016100 | -2.81282600 | 0.13418700 |
| H | 6.33707800 | -2.70308900 | 2.28767900 |
| H | 6.37952700 | -2.90134800 | -2.02303200 |
| H | 7.54246400 | -3.20956400 | 0.16245200 |
| Ca | 5.98942900 | -0.00032700 | -0.00004400 |
| C | -6.35190900 | -0.00083700 | -0.00120900 |
| O | -7.49303700 | -0.00122800 | -0.00158900 |
| O | -5.16641900 | -0.00043000 | -0.00082800 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| C | -3.83968700 | 3.40208000 | -2.80377400 |
| H | -2.78535800 | 5.23510300 | -2.40378200 |
| H | -4.58565200 | 1.42882100 | -3.24781200 |
| H | -4.75701400 | 3.90271400 | -3.09706700 |
| C | -1.46974200 | -2.12166100 | -2.05612900 |
| C | -1.54558100 | -2.13803700 | -3.45640900 |
| C | -2.60093100 | -2.54163200 | -1.31265100 |
| C | -2.71305500 | -2.55259600 | -4.09968200 |
| H | -0.69406300 | -1.82633100 | -4.05574100 |
| C | -3.77158000 | -2.94360700 | -1.96298400 |
| H | -2.52659400 | -2.68943100 | -0.23072800 |
| C | -3.83029900 | -2.93753800 | -3.35825500 |
| H | -2.74947800 | -2.57745800 | -5.18451100 |
| H | -4.61664600 | -3.30938400 | -1.38529700 |
| H | -4.73291500 | -3.26298200 | -3.86608500 |
| C | -1.44548400 | -2.10652900 | 2.09139600 |
| C | -1.55096800 | -3.50211700 | 2.06146100 |
| C | -2.56503500 | -1.34996400 | 2.51969000 |
| C | -2.74186600 | -4.13044200 | 2.43160400 |
| H | -0.70650100 | -4.11188000 | 1.75147300 |
| C | -3.76007300 | -1.98668000 | 2.87506800 |
| H | -2.46638800 | -0.27822700 | 2.72360800 |
| C | -3.85236000 | -3.37833800 | 2.81599500 |
| H | -2.80104400 | -5.21458100 | 2.42300000 |
| H | -4.59510000 | -1.40235200 | 3.25366100 |
| H | -4.77144100 | -3.87625700 | 3.10844700 |
| C | 3.69691800 | -1.91041300 | 0.05771400 |
| C | 4.37972300 | -2.09240100 | 1.28229000 |
| C | 4.39408200 | -2.18685700 | -1.14067800 |
| C | 5.70835000 | -2.54887100 | 1.31075500 |
| H | 3.86392900 | -1.91874500 | 2.22485500 |
| C | 5.72271400 | -2.64416300 | -1.11714900 |
| H | 3.88994400 | -2.08733000 | -2.10003600 |
| C | 6.38317300 | -2.82738300 | 0.10973700 |
| H | 6.19844200 | -2.73084100 | 2.26463200 |
| H | 6.22452000 | -2.90062900 | -2.04758700 |
| H | 7.39377900 | -3.22893800 | 0.13173700 |
| C | 3.70727700 | 1.90258300 | -0.05826300 |
| C | 4.38152300 | 2.07387400 | -1.28915600 |
| C | 4.41557700 | 2.18082100 | 1.13313600 |
| C | 5.71277200 | 2.52157700 | -1.33072600 |
| H | 3.85704300 | 1.89846300 | -2.22661400 |
| C | 5.74697900 | 2.62945800 | 1.09649900 |
| H | 3.91848500 | 2.08941200 | 2.09696000 |
| C | 6.39885200 | 2.80194800 | -0.13653200 |
| H | 6.19636900 | 2.69538700 | -2.28940000 |
| H | 6.25785700 | 2.88767700 | 2.02148200 |
| H | 7.41174900 | 3.19695900 | -0.16862700 |
| Ca | 5.85581000 | -0.01030700 | -0.00430900 |
| N | -5.49673800 | -0.04440600 | -0.06062100 |
| N | -6.59354600 | -0.07865700 | -0.10011300 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-2Ca$^{2+}$-1CH$_4$**

4 1

| | | | |
|---|---|---|---|
| Si | -0.14418400 | 1.15534700 | -1.25233600 |
| Si | -0.17533700 | 1.21344400 | 1.16982200 |
| Si | 1.84460000 | 1.19933300 | -0.01600900 |
| Si | -0.15217500 | -1.13837400 | 1.25312200 |
| Si | -0.18322400 | -1.19589600 | -1.17001300 |
| Si | 1.83614200 | -1.18820200 | 0.01658600 |
| Ca | -2.98716800 | 0.00119900 | 0.00857000 |
| C | -1.53801000 | 2.14536200 | 2.06404900 |

**HPPS-2Ca$^{2+}$-12CO$_2$**

4 1

| | | | |
|---|---|---|---|
| Si | -0.79026600 | 1.73008200 | 0.81760900 |
| Si | -0.57228400 | 1.50770800 | -1.46237200 |
| Si | -1.84254500 | -0.16146100 | -0.08952400 |
| Si | 1.08465300 | -0.10102900 | -1.44619000 |
| Si | 0.92931600 | 0.12978200 | 0.92457700 |
| Si | -0.05042800 | -1.67828200 | -0.15006500 |
| Ca | 6.28886200 | -0.18216100 | 0.01154000 |
| C | -1.68458200 | 2.14884100 | -2.80938000 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -1.60505500 | 2.17450500 | 3.46460500 | C | -2.09109200 | 1.31542900 | -3.86530200 |
| C | -2.66861800 | 2.57141900 | 1.32311500 | C | -2.20743200 | 3.44819300 | -2.72665800 |
| C | -2.76300300 | 2.60951800 | 4.11124800 | C | -3.00849200 | 1.76897700 | -4.80619700 |
| H | -0.75344200 | 1.85815300 | 4.06139200 | H | -1.68991200 | 0.30683500 | -3.95069500 |
| C | -3.82887100 | 2.99671900 | 1.97765500 | C | -3.13220500 | 3.89968600 | -3.66680600 |
| H | -2.59914600 | 2.70894400 | 0.23935500 | H | -1.87471500 | 4.12267000 | -1.94000000 |
| C | -3.87902800 | 3.00410900 | 3.37305400 | C | -3.53460900 | 3.05933600 | -4.70278900 |
| H | -2.79262400 | 2.64404900 | 5.19601600 | H | -3.30582100 | 1.12679200 | -5.62957800 |
| H | -4.67285700 | 3.36985700 | 1.40293500 | H | -3.51796400 | 4.91257600 | -3.60620700 |
| H | -4.77405900 | 3.34675000 | 3.88296200 | H | -4.23931100 | 3.41794400 | -5.44675200 |
| C | -1.51659500 | 2.12866900 | -2.08328200 | C | -1.53859600 | 2.96167200 | 1.99144200 |
| C | -1.61047400 | 3.52514500 | -2.05900700 | C | -2.33392600 | 4.00836700 | 1.49787100 |
| C | -2.64060300 | 1.37886800 | -2.51142000 | C | -1.34941700 | 2.83748500 | 3.37693100 |
| C | -2.79416500 | 4.16157100 | -2.43754900 | C | -2.93316500 | 4.90881700 | 2.37374300 |
| H | -0.76220200 | 4.12904300 | -1.74797400 | H | -2.46924500 | 4.13506400 | 0.42483600 |
| C | -3.82752300 | 2.02445700 | -2.87746200 | C | -1.94592400 | 3.74328600 | 4.24949100 |
| H | -2.55009100 | 0.30473300 | -2.70887000 | H | -0.73778200 | 2.03183900 | 3.77923200 |
| C | -3.90822800 | 3.41673500 | -2.82605900 | C | -2.73695900 | 4.77648900 | 3.74825300 |
| H | -2.84477600 | 5.24616600 | -2.43326400 | H | -3.53595600 | 5.72481700 | 1.98761600 |
| H | -4.66694900 | 1.44624900 | -3.25575200 | H | -1.78855300 | 3.64975900 | 5.31927400 |
| H | -4.82151900 | 3.92071200 | -3.12611200 | H | -3.19158000 | 5.48787800 | 4.43033400 |
| C | -1.54340200 | -2.12750000 | -2.06707000 | C | 2.59393600 | 0.23701600 | 1.79644300 |
| C | -1.61481800 | -2.14638200 | -3.46802200 | C | 2.94174200 | 1.36134400 | 2.56496700 |
| C | -2.66524900 | -2.57295200 | -1.32552600 | C | 3.51706700 | -0.82444700 | 1.72417500 |
| C | -2.76850400 | -2.59295500 | -4.11343400 | C | 4.15930200 | 1.43118600 | 3.24458400 |
| H | -0.76961300 | -1.81405700 | -4.06530900 | H | 2.23931400 | 2.18707400 | 2.66314200 |
| C | -3.82091900 | -3.01207400 | -1.97881600 | C | 4.73161200 | -0.76440200 | 2.41545500 |
| H | -2.59263000 | -2.71085100 | -0.24199300 | H | 3.25484400 | -1.73944900 | 1.19451800 |
| C | -3.87533900 | -3.01117800 | -3.37370000 | C | 5.05623500 | 0.36552700 | 3.17791500 |
| H | -2.80220500 | -2.61909100 | -5.19831000 | H | 4.38160000 | 2.29453100 | 3.86538800 |
| H | -4.65903300 | -3.39634100 | -1.40279000 | H | 5.37530400 | -1.64186500 | 2.44908900 |
| H | -4.76660900 | -3.36426200 | -3.88314800 | H | 5.96570300 | 0.37945000 | 3.77355600 |
| C | -1.52248100 | -2.10097800 | 2.10176100 | C | 2.84506900 | -0.01338400 | -2.13312200 |
| C | -1.62541600 | -3.49753400 | 2.08463600 | C | 3.77804600 | -1.03959800 | -1.89342500 |
| C | -2.62988000 | -1.34335300 | 2.55726900 | C | 3.23907500 | 1.05970200 | -2.95027100 |
| C | -2.80085500 | -4.12578200 | 2.49965500 | C | 5.05302500 | -0.99572800 | -2.46974000 |
| H | -0.78936800 | -4.10761400 | 1.75295700 | H | 3.48427600 | -1.92246500 | -1.32667100 |
| C | -3.80809200 | -1.98140800 | 2.96400600 | C | 4.51758500 | 1.12082600 | -3.50714200 |
| H | -2.53017400 | -0.26872300 | 2.74473400 | H | 2.52694300 | 1.84827000 | -3.18799800 |
| C | -3.89788800 | -3.37321900 | 2.92103000 | C | 5.42579800 | 0.08770600 | -3.27602200 |
| H | -2.85780300 | -5.21006300 | 2.50053000 | H | 5.71748400 | -1.85380700 | -2.38001400 |
| H | -4.63091100 | -1.39594200 | 3.36716700 | H | 4.78073900 | 1.94252100 | -4.16736400 |
| H | -4.80398900 | -3.87083800 | 3.25205600 | H | 6.38863200 | 0.08328300 | -3.78185200 |
| C | 3.61031400 | -1.90949700 | 0.05318900 | C | 0.06014800 | -3.50466400 | 0.15343900 |
| C | 4.29083100 | -2.09360100 | 1.27873900 | C | -0.07785900 | -4.41076900 | -0.91061400 |
| C | 4.30938900 | -2.18509600 | -1.14430200 | C | 0.21008700 | -3.99326100 | 1.46184300 |
| C | 5.61898200 | -2.55130100 | 1.30900700 | C | -0.07366000 | -5.78081700 | -0.66717800 |
| H | 3.77355700 | -1.92047200 | 2.22057700 | H | -0.18362400 | -4.04784900 | -1.93084400 |
| C | 5.63758600 | -2.64356600 | -1.11895300 | C | 0.21272200 | -5.36420400 | 1.69974900 |
| H | 3.80710400 | -2.08390400 | -2.10444000 | H | 0.32025200 | -3.30086700 | 2.29383700 |
| C | 6.29572200 | -2.82887600 | 0.10886000 | C | 0.06854300 | -6.25526000 | 0.63658200 |
| H | 6.10723400 | -2.73482300 | 2.26352800 | H | -0.17757300 | -6.47992100 | -1.49080700 |
| H | 6.14081700 | -2.89930200 | -2.04881600 | H | 0.32818500 | -5.74072200 | 2.71117100 |
| H | 7.30594600 | -3.23131500 | 0.13216800 | H | 0.07132500 | -7.32438200 | 0.82432300 |
| C | 3.62545400 | 1.90479000 | -0.05714900 | C | -3.42018600 | -0.12532000 | -1.14394100 |
| C | 4.30407300 | 2.07956800 | -1.28511400 | C | -4.15998600 | 1.07501500 | -1.26389700 |
| C | 4.33011400 | 2.17798500 | 1.13758800 | C | -3.88417300 | -1.24331300 | -1.86638000 |
| C | 5.63598400 | 2.52589800 | -1.32054800 | C | -5.26644600 | 1.16988500 | -2.11256000 |
| H | 3.78263200 | 1.90811000 | -2.22498900 | H | -3.83851700 | 1.96264900 | -0.72058300 |
| C | 5.66213100 | 2.62513500 | 1.10711600 | C | -5.00926100 | -1.16142100 | -2.69640600 |
| H | 3.82963100 | 2.08379200 | 2.09939500 | H | -3.33684600 | -2.18435100 | -1.81690500 |
| C | 6.31837500 | 2.80126000 | -0.12308200 | C | -5.70288100 | 0.04687800 | -2.82891600 |
| H | 6.12302700 | 2.70253100 | -2.27696900 | H | -5.77426600 | 2.12338900 | -2.23078300 |
| H | 6.17015100 | 2.87938000 | 2.03477400 | H | -5.32376900 | -2.03249100 | -3.26435600 |
| H | 7.33186900 | 3.19509000 | -0.15032200 | H | -6.54966700 | 0.11983300 | -3.50430600 |
| Ca | 5.77088400 | -0.01096700 | -0.00260500 | Ca | -6.06923100 | -0.61187800 | 0.03252300 |
| C | -5.68551500 | -0.10029800 | -0.15201500 | C | 6.39595000 | -3.70397200 | 0.20561100 |

| | | | |
|---|---|---|---|
| H | -5.40468100 | -0.72685700 | 0.70690500 |
| H | -5.42382800 | 0.95771100 | -0.00877100 |
| H | -5.31250500 | -0.50365700 | -1.10367500 |
| H | -6.77595800 | -0.13687200 | -0.20985900 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| O | 6.84857200 | -4.75208700 | 0.29756200 |
| O | 5.92540700 | -2.62458300 | 0.11157800 |
| C | -3.82506600 | 0.27823400 | 2.63227100 |
| O | -4.70401300 | 0.43984000 | 1.86267300 |
| O | -3.00151200 | 0.10982000 | 3.41522300 |
| C | -3.82294400 | -3.17402800 | 0.97773900 |
| O | -4.63665400 | -2.32935400 | 1.09271500 |
| O | -3.02785000 | -3.99395900 | 0.86099100 |
| C | 3.76522800 | 2.31332900 | -0.20793900 |
| O | 2.78864200 | 2.91402500 | -0.28361600 |
| O | 4.78665500 | 1.73252500 | -0.13099900 |
| C | 7.31107600 | 2.36306600 | -2.19333400 |
| O | 7.43963400 | 1.51470000 | -1.38524100 |
| O | 7.17713500 | 3.18418700 | -2.98325800 |
| C | -9.28993400 | 0.34217700 | -1.13839300 |
| O | -8.32294600 | -0.28694900 | -0.88547000 |
| O | -10.22637600 | 0.95208900 | -1.38822400 |
| C | 8.76549300 | -1.02056600 | 2.44209900 |
| C | -8.05422800 | -1.45350200 | 2.90297200 |
| O | 7.90088000 | -1.11851200 | 1.64237000 |
| O | 9.59822800 | -0.92507500 | 3.22196800 |
| O | -8.69520200 | -1.74534300 | 3.80523700 |
| O | -7.39098800 | -1.15161800 | 1.97457400 |
| C | -7.75308800 | -3.55076400 | -1.04840900 |
| C | 7.00884400 | 2.60662000 | 2.00738300 |
| O | -6.95067400 | -2.79660100 | -0.62306300 |
| O | -8.52746500 | -4.28568700 | -1.46296500 |
| O | 7.27764700 | 1.62702800 | 1.40988800 |
| O | 6.73541900 | 3.55597500 | 2.59127400 |
| C | -6.60162600 | 2.60409700 | 1.26515000 |
| O | -6.91132000 | 1.63472400 | 0.66948000 |
| O | -6.29123900 | 3.54701100 | 1.84036300 |
| C | 9.10522800 | -1.32117800 | -1.90240300 |
| O | 8.10357400 | -1.26083500 | -1.27800600 |
| O | 10.07259700 | -1.38069300 | -2.51151000 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-2Ca$^{2+}$-9N$_2$**

4 1

| | | | |
|---|---|---|---|
| Si | 1.11401500 | -0.57003000 | -1.21913000 |
| Si | 1.10572600 | -0.45682100 | 1.22432500 |
| Si | -0.72569600 | -1.24113600 | 0.02904300 |
| Si | 0.59821600 | 1.83859900 | 1.10242200 |
| Si | 0.58297300 | 1.73294400 | -1.27419400 |
| Si | -1.30210200 | 1.02805600 | -0.03259400 |
| Ca | 4.93101100 | -1.41123200 | 0.04333800 |
| C | 2.67902500 | -1.26502600 | 1.91348900 |
| C | 3.64798200 | -0.45596300 | 2.54920300 |
| C | 2.94584500 | -2.64692500 | 1.81810500 |
| C | 4.82926700 | -1.00531000 | 3.05700900 |
| H | 3.45565700 | 0.60673000 | 2.69397600 |
| C | 4.14813800 | -3.19355300 | 2.28586400 |
| H | 2.19367700 | -3.31738600 | 1.41250800 |
| C | 5.09937800 | -2.37137600 | 2.90253500 |
| H | 5.52892000 | -0.37204600 | 3.59486400 |
| H | 4.31891300 | -4.26495400 | 2.21722900 |
| H | 6.00999300 | -2.79925500 | 3.31261800 |
| C | 2.64210700 | -1.55016700 | -1.78420800 |
| C | 2.85036500 | -2.89273300 | -1.40279800 |
| C | 3.63006600 | -0.94109300 | -2.58890900 |
| C | 4.01296600 | -3.58523000 | -1.76179900 |
| H | 2.08040000 | -3.42081700 | -0.84669100 |

**HPPS-2Ca$^{2+}$-4CH$_4$**

4 1

| | | | |
|---|---|---|---|
| Si | -0.89798500 | -0.56972000 | 1.17859300 |
| Si | -0.92200300 | -0.51399900 | -1.26607900 |
| Si | 0.89699600 | -1.33055900 | -0.07930200 |
| Si | -0.33439700 | 1.78515300 | -1.20250800 |
| Si | -0.33097000 | 1.71766100 | 1.18762100 |
| Si | 1.52174300 | 0.92361100 | -0.04141000 |
| Ca | -4.69559300 | -1.62874700 | -0.01914100 |
| C | -2.51280700 | -1.37364000 | -1.87266900 |
| C | -3.54969000 | -0.60502900 | -2.44922600 |
| C | -2.71750700 | -2.76744700 | -1.76282400 |
| C | -4.73935400 | -1.20147600 | -2.89144600 |
| H | -3.41646000 | 0.46672400 | -2.59106700 |
| C | -3.90850300 | -3.36802700 | -2.19452500 |
| H | -1.92483900 | -3.40233100 | -1.37372100 |
| C | -4.92547300 | -2.58542600 | -2.76105900 |
| H | -5.50165800 | -0.59449800 | -3.37447400 |
| H | -4.02581700 | -4.44708500 | -2.13257700 |
| H | -5.82977300 | -3.05436000 | -3.13980800 |
| C | -2.47342800 | -1.44700400 | 1.79560400 |
| C | -2.68843800 | -2.83497500 | 1.64156100 |
| C | -3.49141300 | -0.69417200 | 2.42447200 |
| C | -3.87207000 | -3.44467700 | 2.08078200 |
| H | -1.90956400 | -3.45891600 | 1.20899200 |
| C | -4.67385500 | -1.29988400 | 2.87298900 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | 4.77189800 | -1.64461400 | -2.98887900 | H | -3.34778700 | 0.37148300 | 2.60045400 |
| H | 3.48393800 | 0.07584700 | -2.95016300 | C | -4.87090700 | -2.67744200 | 2.69831200 |
| C | 4.98348200 | -2.95905300 | -2.55467500 | H | -3.99717400 | -4.52031700 | 1.98373400 |
| H | 4.13854900 | -4.62455500 | -1.46866100 | H | -5.42166900 | -0.70706100 | 3.39462500 |
| H | 5.48469900 | -1.17653500 | -3.66154400 | H | -5.76911100 | -3.15485000 | 3.08098100 |
| H | 5.86170400 | -3.50930500 | -2.88079300 | C | -0.55157300 | 2.97744700 | 2.52049000 |
| C | 0.85421500 | 3.00669200 | -2.59026100 | C | -0.64692700 | 2.58619400 | 3.86645300 |
| C | 0.33474100 | 2.83624400 | -3.88511400 | C | -0.60916600 | 4.34122100 | 2.18819600 |
| C | 1.59843800 | 4.16073400 | -2.29276700 | C | -0.79272600 | 3.54633800 | 4.86165200 |
| C | 0.55334800 | 3.80370500 | -4.85816800 | H | -0.60314600 | 1.53366100 | 4.14188300 |
| H | -0.24135100 | 1.94774500 | -4.13524500 | C | -0.75000100 | 5.29605600 | 3.18959200 |
| C | 1.80890200 | 5.12964300 | -3.26984600 | H | -0.53986000 | 4.66318600 | 1.15107100 |
| H | 2.01397000 | 4.30609600 | -1.29781800 | C | -0.84313000 | 4.89881000 | 4.52271700 |
| C | 1.28690200 | 4.95068800 | -4.54924600 | H | -0.86601000 | 3.24400900 | 5.90128500 |
| H | 0.15061000 | 3.67049800 | -5.85694200 | H | -0.79024500 | 6.34930900 | 2.93195200 |
| H | 2.37819500 | 6.02282100 | -3.03435500 | H | -0.95758800 | 5.64610900 | 5.30125300 |
| H | 1.45069200 | 5.70684600 | -5.31023600 | C | -0.56878300 | 3.13234200 | -2.44306500 |
| C | 0.98109000 | 3.13749900 | 2.36330400 | C | 0.03361900 | 3.05720100 | -3.71108500 |
| C | 1.11269300 | 4.48400000 | 1.98698500 | C | -1.36170500 | 4.24658200 | -2.11764000 |
| C | 1.15118600 | 2.77698500 | 3.71096900 | C | -0.15323900 | 4.07953800 | -4.63248200 |
| C | 1.40161500 | 5.45109400 | 2.94413100 | H | 0.64858400 | 2.20104900 | -3.97990100 |
| H | 0.98205600 | 4.78276600 | 0.94895700 | C | -1.53919300 | 5.27033700 | -3.04341100 |
| C | 1.44338700 | 3.74812200 | 4.66262100 | H | -1.83806300 | 4.31891700 | -1.14222300 |
| H | 1.04633700 | 1.73873900 | 4.02288900 | C | -0.93619600 | 5.18598400 | -4.29695800 |
| C | 1.56762700 | 5.08323500 | 4.27881200 | H | 0.31136400 | 4.02036200 | -5.61131700 |
| H | 1.49774900 | 6.49151500 | 2.65122900 | H | -2.14453700 | 6.13376700 | -2.78803400 |
| H | 1.57127200 | 3.46820900 | 5.70334100 | H | -1.07536500 | 5.98496100 | -5.01810100 |
| H | 1.79327600 | 5.84015300 | 5.02323800 | C | 3.41570500 | 1.11260500 | 0.03949700 |
| C | -3.16219700 | 1.43926400 | -0.13701400 | C | 4.19888200 | 1.24700800 | -1.12859600 |
| C | -3.89944600 | 1.83265400 | 1.00081200 | C | 4.08202100 | 1.10670400 | 1.28602700 |
| C | -3.82313400 | 1.44993500 | -1.38450900 | C | 5.59107700 | 1.40693600 | -1.05302000 |
| C | -5.22864000 | 2.26806600 | 0.88986300 | H | 3.71473500 | 1.28491800 | -2.10212700 |
| H | -3.41442500 | 1.85880500 | 1.97450600 | C | 5.47349500 | 1.26560800 | 1.36469500 |
| C | -5.14906800 | 1.88715400 | -1.50131700 | H | 3.50513600 | 1.03671400 | 2.20574800 |
| H | -3.27713600 | 1.17442900 | -2.28399100 | C | 6.23102400 | 1.42069500 | 0.19442600 |
| C | -5.85164500 | 2.31041200 | -0.36455300 | H | 6.16760800 | 1.56213900 | -1.96186800 |
| H | -5.75753400 | 2.62113000 | 1.77215500 | H | 5.95895600 | 1.31300200 | 2.33657600 |
| H | -5.61413200 | 1.94820400 | -2.48196300 | H | 7.30227600 | 1.59726300 | 0.25664500 |
| H | -6.85986000 | 2.70502400 | -0.46165700 | C | 2.39132300 | -2.52325800 | -0.11032600 |
| C | -2.13902600 | -2.48862000 | 0.10553800 | C | 2.97623000 | -2.99429800 | 1.08419100 |
| C | -2.25687900 | -3.58300000 | -0.75706000 | C | 3.01525400 | -2.85024600 | -1.33369300 |
| C | -3.15370800 | -2.27111300 | 1.06333100 | C | 4.12093500 | -3.80553700 | 1.05559800 |
| C | -3.35314200 | -4.44727100 | -0.67732100 | H | 2.51285200 | -2.76787800 | 2.04258400 |
| H | -1.48581700 | -3.77543000 | -1.49897300 | C | 4.15900900 | -3.66197100 | -1.36571500 |
| C | -4.24552500 | -3.14285900 | 1.15069700 | H | 2.58225100 | -2.51013600 | -2.27265600 |
| H | -3.02298700 | -1.48625200 | 1.81309600 | C | 4.70967800 | -4.14765100 | -0.17021600 |
| C | -4.34927100 | -4.22789000 | 0.26969000 | H | 4.52763800 | -4.20071800 | 1.98332000 |
| H | -3.41654800 | -5.30373200 | -1.34191000 | H | 4.59457000 | -3.94735800 | -2.32046600 |
| H | -4.95938900 | -3.05061500 | 1.96873600 | H | 5.56519400 | -4.81855800 | -0.19627100 |
| H | -5.17543000 | -4.92721500 | 0.35980900 | Ca | 5.11428500 | -1.26537900 | -0.00480800 |
| Ca | -5.46462500 | -0.52429700 | 0.13136600 | C | 7.03194600 | -1.91066500 | 1.91360000 |
| N | 4.34594500 | 1.13609200 | -0.18154200 | H | 6.97382200 | -2.79229000 | 1.26375500 |
| N | 4.02654400 | 2.18332400 | -0.27321600 | H | 6.07375900 | -1.68295700 | 2.40411400 |
| N | -7.95664300 | -3.32502500 | 0.38120900 | H | 7.72934000 | -2.16526800 | 2.71564500 |
| N | -7.21504000 | -2.51790300 | 0.31005700 | H | 7.45641900 | -1.04025200 | 1.39945700 |
| N | 7.74526200 | 0.15411400 | -2.06688500 | C | -7.29297900 | -2.52515200 | -0.00265500 |
| N | 6.93203400 | -0.28969100 | -1.47640000 | H | -7.20869400 | -1.92249200 | -0.91597100 |
| N | -4.37875900 | -2.22029400 | -2.96726800 | H | -6.62434600 | -3.39839400 | -0.01043300 |
| N | -4.70073100 | -1.74675600 | -2.03063000 | H | -7.19032100 | -1.92429300 | 0.91015100 |
| N | -7.84470400 | 0.27699000 | 1.15505400 | H | -8.31016300 | -2.92446200 | 0.00758500 |
| N | -8.80505900 | 0.63246900 | 1.55287900 | C | 7.14859600 | -1.71179000 | -1.85648200 |
| N | -5.50738100 | -0.56839800 | 2.78418300 | H | 7.04459900 | -2.67301500 | -1.33929200 |
| N | -5.54982700 | -0.53250500 | 3.88121900 | H | 7.91414300 | -1.85536000 | -2.62297600 |
| N | 7.87597500 | 0.38647500 | 1.78167400 | H | 6.23291600 | -1.41962600 | -2.39161600 |
| N | 7.03041100 | -0.11184900 | 1.28812900 | H | 7.52062700 | -0.91926400 | -1.19572800 |
| N | 7.85190500 | -3.69658000 | 0.18552900 | C | -5.70915600 | 0.96445200 | 0.04362000 |
| N | 6.98514000 | -3.02348800 | 0.14251100 | H | -6.08209200 | 0.49290300 | 0.96091300 |

| | | | |
|---|---|---|---|
| N | -7.38661000 | -0.37021800 | -1.76201000 |
| N | -8.17781500 | -0.27753400 | -2.51843400 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| H | -4.61054300 | 1.01884800 | 0.01897300 |
| H | -6.12464300 | 0.50657100 | -0.86254800 |
| H | -6.07200100 | 1.99456600 | 0.05937500 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-3Mg$^{2+}$-1CO$_2$**

6 1

| | | | |
|---|---|---|---|
| Si | -0.96793700 | 0.92305900 | 1.19552900 |
| Si | -0.30721400 | -1.37487900 | 1.16891200 |
| Si | 1.35877700 | 0.34974400 | 1.17460400 |
| Si | -0.32072100 | -1.33888800 | -1.19404900 |
| Si | -0.99075900 | 0.95682000 | -1.16594900 |
| Si | 1.33962500 | 0.39007700 | -1.18541300 |
| C | -0.76161600 | -3.14501400 | 1.76954200 |
| C | -2.11623700 | -3.54819000 | 1.87611200 |
| C | 0.23001200 | -4.15405200 | 1.86345500 |
| C | -2.46944300 | -4.89841100 | 2.07200000 |
| H | -2.91323300 | -2.81084200 | 1.81690400 |
| C | -0.11311600 | -5.50700400 | 2.06035300 |
| H | 1.28396800 | -3.89508400 | 1.79533600 |
| C | -1.46734300 | -5.88653000 | 2.16132900 |
| H | -3.51635100 | -5.17786400 | 2.17444100 |
| H | 0.66817100 | -6.25854700 | 2.15530300 |
| H | -1.73494500 | -6.92732700 | 2.33626500 |
| C | -2.26851300 | 2.17430700 | 1.85946700 |
| C | -1.93962800 | 3.54694400 | 1.99146000 |
| C | -3.63409800 | 1.81411600 | 1.98136100 |
| C | -2.92932200 | 4.52009200 | 2.23762700 |
| H | -0.90468300 | 3.87248400 | 1.91600600 |
| C | -4.63073900 | 2.78003000 | 2.22841100 |
| H | -3.93636200 | 0.77301500 | 1.89655900 |
| C | -4.28233200 | 4.14076400 | 2.35244300 |
| H | -2.64751200 | 5.56432500 | 2.35889600 |
| H | -5.66899700 | 2.47387400 | 2.34212200 |
| H | -5.04670000 | 4.88690200 | 2.56297200 |
| C | -2.30736400 | 2.22881400 | -1.75815500 |
| C | -1.98452600 | 3.60644600 | -1.84624100 |
| C | -3.67494300 | 1.87088300 | -1.86160000 |
| C | -2.98060100 | 4.58591200 | -2.03570500 |
| H | -0.94936700 | 3.93280000 | -1.77867600 |
| C | -4.67837900 | 2.84285800 | -2.05056300 |
| H | -3.97439100 | 0.82693500 | -1.80798200 |
| C | -4.33531900 | 4.20801600 | -2.13447300 |
| H | -2.70292800 | 5.63450200 | -2.12422200 |
| H | -5.71851700 | 2.53844000 | -2.15080100 |
| H | -5.10511900 | 4.95927000 | -2.30193100 |
| C | -0.78232500 | -3.08801900 | -1.84793500 |
| C | 0.20922100 | -4.09147700 | -1.99103000 |
| C | -2.13811200 | -3.48814100 | -1.95266100 |
| C | -0.13617400 | -5.43714400 | -2.23034000 |
| H | 1.26386700 | -3.83324300 | -1.93056000 |
| C | -2.49308600 | -4.83089900 | -2.19225200 |
| H | -2.93424900 | -2.75372200 | -1.85819400 |
| C | -1.49137000 | -5.81424800 | -2.32753800 |
| H | 0.64415900 | -6.18412900 | -2.36130500 |
| H | -3.54094600 | -5.10753100 | -2.29253000 |
| H | -1.76034600 | -6.84858200 | -2.53512900 |
| C | 3.07250500 | 0.84496000 | -1.83933800 |
| C | 4.13714800 | 0.00442400 | -1.45702500 |
| C | 3.37353300 | 2.04189200 | -2.50883300 |
| C | 5.46683100 | 0.32251600 | -1.78919400 |
| H | 3.94659600 | -0.94027800 | -0.95157900 |
| C | 4.69619400 | 2.40043400 | -2.80113200 |

**HPPS-3Mg$^{2+}$-1N$_2$**

6 1

| | | | |
|---|---|---|---|
| Si | 0.83936900 | 1.28423900 | -1.18218900 |
| Si | 1.15710500 | -1.09279600 | -1.18202200 |
| Si | -1.05813000 | -0.17925600 | -1.17471800 |
| Si | 1.15715500 | -1.09279600 | 1.18202300 |
| Si | 0.83942900 | 1.28423900 | 1.18219900 |
| Si | -1.05807000 | -0.17925200 | 1.17482300 |
| C | 2.25390200 | -2.54210200 | -1.81037600 |
| C | 3.66058400 | -2.40306900 | -1.91808100 |
| C | 1.71389800 | -3.84787100 | -1.92454400 |
| C | 4.49443800 | -3.51796500 | -2.14004400 |
| H | 4.12248600 | -1.42167300 | -1.84206300 |
| C | 2.53965900 | -4.96871300 | -2.14465900 |
| H | 0.64017400 | -4.00585300 | -1.85614200 |
| C | 3.93655900 | -4.80869700 | -2.25124500 |
| H | 5.56901600 | -3.38105000 | -2.24684300 |
| H | 2.09775000 | -5.95707600 | -2.25509200 |
| H | 4.57547500 | -5.66855500 | -2.44704900 |
| C | 1.53822100 | 2.96319700 | -1.80910700 |
| C | 0.69927100 | 4.10135900 | -1.90948900 |
| C | 2.93577600 | 3.16684000 | -1.93127900 |
| C | 1.22937900 | 5.38869900 | -2.13109500 |
| H | -0.38010500 | 3.99701100 | -1.82729900 |
| C | 3.47529900 | 4.45056000 | -2.15286900 |
| H | 3.62141300 | 2.32513200 | -1.86916800 |
| C | 2.62272400 | 5.56971200 | -2.25091900 |
| H | 0.56145400 | 6.24240800 | -2.23006200 |
| H | 4.55015100 | 4.57648100 | -2.26969100 |
| H | 3.03448000 | 6.55897600 | -2.44520300 |
| C | 1.53829900 | 2.96319900 | 1.80909000 |
| C | 0.69934800 | 4.10135600 | 1.90951300 |
| C | 2.93585800 | 3.16684600 | 1.93121000 |
| C | 1.22945900 | 5.38869600 | 2.13111100 |
| H | -0.38003100 | 3.99700300 | 1.82736700 |
| C | 3.47538400 | 4.45056700 | 2.15279200 |
| H | 3.62149700 | 2.32514100 | 1.86906900 |
| C | 2.62280700 | 5.56971300 | 2.25088400 |
| H | 0.56153400 | 6.24240200 | 2.23010900 |
| H | 4.55024000 | 4.57649200 | 2.26957400 |
| H | 3.03456600 | 6.55897800 | 2.44515500 |
| C | 2.25397400 | -2.54209800 | 1.81034600 |
| C | 1.71397200 | -3.84786600 | 1.92453800 |
| C | 3.66066000 | -2.40306600 | 1.91800200 |
| C | 2.53973900 | -4.96870800 | 2.14462600 |
| H | 0.64024500 | -4.00584600 | 1.85617100 |
| C | 4.49452000 | -3.51796300 | 2.13993700 |
| H | 4.12256000 | -1.42167100 | 1.84196500 |
| C | 3.93664300 | -4.80869400 | 2.25116100 |
| H | 2.09783200 | -5.95707100 | 2.25507800 |
| H | 5.56910200 | -3.38104900 | 2.24669900 |
| H | 4.57556500 | -5.66855200 | 2.44694500 |
| C | -2.85724700 | -0.43249200 | 1.77286000 |
| C | -3.42144000 | -1.72559100 | 1.79348900 |
| C | -3.71468100 | 0.66532300 | 2.01647400 |
| C | -4.77729300 | -1.92954300 | 2.11466800 |
| H | -2.80516600 | -2.59940300 | 1.59503700 |
| C | -5.06712900 | 0.47348300 | 2.34845000 |

| | | | |
|---|---|---|---|
| H | 2.57733100 | 2.70645800 | -2.83342800 |
| C | 5.74795800 | 1.53531800 | -2.46800700 |
| H | 6.25586800 | -0.41964300 | -1.64510200 |
| H | 4.90310600 | 3.31689500 | -3.34802000 |
| H | 6.75921500 | 1.74826200 | -2.81547300 |
| C | 3.07034400 | 0.88969500 | 1.81938000 |
| C | 3.50367500 | 2.19019500 | 1.49236400 |
| C | 3.98652300 | 0.01043200 | 2.41857300 |
| C | 4.80476700 | 2.62046400 | 1.80904100 |
| H | 2.81939500 | 2.90775400 | 1.04410300 |
| C | 5.30126500 | 0.40630300 | 2.69738200 |
| H | 3.68265200 | -0.99458000 | 2.69898000 |
| C | 5.71262400 | 1.71750700 | 2.41887700 |
| H | 5.06855700 | 3.67597000 | 1.70764000 |
| H | 5.98351500 | -0.28092700 | 3.19161500 |
| H | 6.68769800 | 2.06648100 | 2.75964200 |
| Mg | -1.20942600 | -4.83923500 | -0.06752600 |
| Mg | 6.05138300 | 1.77153200 | -0.02107800 |
| Mg | -3.56097700 | 3.44170300 | 0.08800000 |
| C | 9.06008200 | 2.78010100 | -0.04196800 |
| O | 7.92247300 | 2.40319600 | -0.03145800 |
| O | 10.13541200 | 3.13596200 | -0.05164800 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| H | -3.32863000 | 1.68153100 | 1.99858300 |
| C | -5.59660600 | -0.83010500 | 2.42569700 |
| H | -5.17645200 | -2.94001300 | 2.17814000 |
| H | -5.69277600 | 1.32995400 | 2.59219600 |
| H | -6.62740400 | -0.98742200 | 2.73903400 |
| C | -2.85732200 | -0.43252100 | -1.77272600 |
| C | -3.71472300 | 0.66525300 | -2.01663000 |
| C | -3.42154500 | -1.72562000 | -1.79311900 |
| C | -5.06715200 | 0.47336700 | -2.34865400 |
| H | -3.32865900 | 1.68145900 | -1.99891800 |
| C | -4.77737500 | -1.92961500 | -2.11437900 |
| H | -2.80530500 | -2.59940200 | -1.59443100 |
| C | -5.59664300 | -0.83022100 | -2.42569600 |
| H | -5.69277100 | 1.32980300 | -2.59259000 |
| H | -5.17654200 | -2.94009400 | -2.17768700 |
| H | -6.62742000 | -0.98758200 | -2.73908200 |
| Mg | 3.32178800 | -3.97644900 | -0.00003500 |
| Mg | -5.07703700 | -0.51731500 | 0.00001300 |
| Mg | 2.24434900 | 4.60764800 | -0.00000800 |
| N | -8.36946500 | 0.22598900 | -0.00005800 |
| N | -7.29579100 | -0.00916700 | -0.00003900 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-3Mg$^{2+}$-1CH$_4$**

6 1

| | | | |
|---|---|---|---|
| Si | -0.51354200 | 1.23452300 | -1.18186300 |
| Si | 1.39231600 | -0.22086200 | -1.18109500 |
| Si | -0.81997700 | -1.14130800 | -1.17659800 |
| Si | 1.39228000 | -0.22082600 | 1.18126300 |
| Si | -0.51357800 | 1.23456100 | 1.18192500 |
| Si | -0.82001300 | -1.14127100 | 1.17672500 |
| C | 3.19718800 | -0.42962900 | -1.81125500 |
| C | 4.05935600 | 0.69109300 | -1.90986000 |
| C | 3.77912200 | -1.71659800 | -1.93521400 |
| C | 5.44305300 | 0.53808400 | -2.13003200 |
| H | 3.65925200 | 1.69877000 | -1.82752300 |
| C | 5.16208200 | -1.87968800 | -2.15541300 |
| H | 3.15893300 | -2.60790600 | -1.87730600 |
| C | 6.00226500 | -0.75095700 | -2.25001200 |
| H | 6.07934500 | 1.41585300 | -2.22704600 |
| H | 5.58061100 | -2.87733400 | -2.27390500 |
| H | 7.06702000 | -0.87304100 | -2.44291100 |
| C | -1.18902100 | 2.92294700 | -1.80907600 |
| C | -2.58415000 | 3.14372700 | -1.92927000 |
| C | -0.33643000 | 4.05065000 | -1.91154300 |
| C | -3.10807600 | 4.43384000 | -2.15084300 |
| H | -3.27989300 | 2.31048300 | -1.86497300 |
| C | -0.85083700 | 5.34432600 | -2.13314000 |
| H | 0.74170600 | 3.93290100 | -1.83141800 |
| C | -2.24204700 | 5.54235500 | -2.25085300 |
| H | -4.18146400 | 4.57287600 | -2.26599000 |
| H | -0.17253800 | 6.18958600 | -2.23394500 |
| H | -2.64197100 | 6.53644900 | -2.44513600 |
| C | -1.18908900 | 2.92300100 | 1.80906100 |
| C | -2.58422400 | 3.14377700 | 1.92919100 |
| C | -0.33650900 | 4.05071100 | 1.91153200 |
| C | -3.10816700 | 4.43389300 | 2.15070600 |
| H | -3.27996000 | 2.31052700 | 1.86488800 |
| C | -0.85093300 | 5.34439100 | 2.13307300 |
| H | 0.74163100 | 3.93296700 | 1.83145600 |
| C | -2.24214800 | 5.54241500 | 2.25072300 |
| H | -4.18156000 | 4.57292500 | 2.26580400 |
| H | -0.17264300 | 6.18965800 | 2.23388200 |

**HPPS-3Mg$^{2+}$-15CO$_2$**

6 1

| | | | |
|---|---|---|---|
| Si | 1.02331000 | -0.61731700 | 1.91990100 |
| Si | -0.07175600 | 1.47808700 | 1.94436300 |
| Si | -1.33440900 | -0.52462500 | 1.91545200 |
| Si | 0.01425200 | 1.44301700 | -0.41068000 |
| Si | 1.08847700 | -0.68877800 | -0.44842100 |
| Si | -1.29542000 | -0.56572400 | -0.43811400 |
| C | -0.01667600 | 3.03043000 | 2.99389400 |
| C | 1.03508600 | 3.95242600 | 2.84380000 |
| C | -1.00268600 | 3.28921500 | 3.95675100 |
| C | 1.10283500 | 5.09059000 | 3.64760500 |
| H | 1.84165200 | 3.74387900 | 2.14087700 |
| C | -0.93128900 | 4.42159000 | 4.76695500 |
| H | -1.82848900 | 2.59506700 | 4.08848400 |
| C | 0.12116200 | 5.32126000 | 4.61598800 |
| H | 1.94707300 | 5.76979100 | 3.56278700 |
| H | -1.68879600 | 4.59444500 | 5.52459700 |
| H | 0.19029200 | 6.18813100 | 5.26599900 |
| C | 2.32564100 | -1.47728200 | 2.95053600 |
| C | 2.61528000 | -2.82886500 | 2.69412400 |
| C | 3.02135300 | -0.81743400 | 3.97319300 |
| C | 3.57249300 | -3.50266400 | 3.45227200 |
| H | 2.06024400 | -3.36929700 | 1.92822200 |
| C | 3.97594600 | -1.49322400 | 4.73250100 |
| H | 2.81117700 | 0.22660000 | 4.19041400 |
| C | 4.25150100 | -2.83419900 | 4.47524700 |
| H | 3.75392800 | -4.56111700 | 3.28450200 |
| H | 4.49262400 | -0.97771000 | 5.53562200 |
| H | 4.97241800 | -3.36615100 | 5.08857400 |
| C | 2.60572100 | -1.49199700 | -1.30260700 |
| C | 2.56405800 | -2.71724000 | -1.98510600 |
| C | 3.85332100 | -0.85182600 | -1.15970000 |
| C | 3.71698500 | -3.26472800 | -2.55532600 |
| H | 1.61679000 | -3.23289400 | -2.11725700 |
| C | 5.00799500 | -1.38661600 | -1.72433700 |
| H | 3.91727900 | 0.09746000 | -0.63143500 |
| C | 4.94526600 | -2.59761700 | -2.43497800 |
| H | 3.64585900 | -4.17186400 | -3.15082900 |

| | | | |
|---|---|---|---|
| H | -2.64208700 | 6.53651200 | 2.44495900 |
| C | 3.19713400 | -0.42958200 | 1.81148100 |
| C | 3.77906100 | -1.71655000 | 1.93548400 |
| C | 4.05930200 | 0.69113900 | 1.91008800 |
| C | 5.16201400 | -1.87963900 | 2.15572700 |
| H | 3.15887200 | -2.60785800 | 1.87757600 |
| C | 5.44299200 | 0.53813200 | 2.13030300 |
| H | 3.65920300 | 1.69881600 | 1.82771900 |
| C | 6.00219800 | -0.75090900 | 2.25032600 |
| H | 5.58053800 | -2.87728400 | 2.27425100 |
| H | 6.07928400 | 1.41590100 | 2.22731700 |
| H | 7.06694600 | -0.87299100 | 2.44325800 |
| C | -1.88593400 | -2.61126200 | 1.77442800 |
| C | -1.33470900 | -3.90898700 | 1.78721900 |
| C | -3.27144900 | -2.47971900 | 2.01586600 |
| C | -2.11730400 | -5.03611400 | 2.09934100 |
| H | -0.27587800 | -4.06087600 | 1.59092600 |
| C | -4.06317600 | -3.59624700 | 2.33824200 |
| H | -3.74442400 | -1.50071500 | 2.00413400 |
| C | -3.48068500 | -4.87831900 | 2.40879100 |
| H | -1.65667500 | -6.02017100 | 2.16214000 |
| H | -5.11466100 | -3.46235900 | 2.58570000 |
| H | -4.07405900 | -5.73542400 | 2.72182900 |
| C | -1.88588100 | -2.61131900 | -1.77428000 |
| C | -3.27139000 | -2.47978300 | -2.01575600 |
| C | -1.33465800 | -3.90904500 | -1.78700800 |
| C | -4.06311200 | -3.59632200 | -2.33810600 |
| H | -3.74436400 | -1.50077800 | -2.00407500 |
| C | -2.11724700 | -5.03618300 | -2.09910500 |
| H | -0.27583200 | -4.06092800 | -1.59068700 |
| C | -3.48062100 | -4.87839700 | -2.40859300 |
| H | -5.11459100 | -3.46244200 | -2.58559400 |
| H | -1.65661900 | -6.02024200 | -2.16185700 |
| H | -4.07399100 | -5.73551200 | -2.72161100 |
| Mg | 4.96914100 | -0.65317100 | 0.00014100 |
| Mg | -3.42901400 | -4.36495500 | 0.00008700 |
| Mg | -1.87196000 | 4.57582400 | -0.00004100 |
| C | -5.55701200 | -5.78791500 | 0.00002900 |
| H | -6.08094300 | -6.12998500 | 0.89574400 |
| H | -6.08076400 | -6.12996400 | -0.89579900 |
| H | -5.58746600 | -4.68098600 | 0.00003300 |
| H | -4.55537400 | -6.25899200 | 0.00011700 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| H | 5.94375400 | -0.83650500 | -1.66405400 |
| H | 5.79523400 | -2.90841800 | -3.04811700 |
| C | -0.11272900 | 3.08364900 | -1.39204600 |
| C | -0.98787900 | 4.05581300 | -0.88004500 |
| C | 0.60047300 | 3.39136800 | -2.56920700 |
| C | -1.19793800 | 5.26883800 | -1.54938100 |
| H | -1.56382800 | 3.84251400 | 0.01966000 |
| C | 0.42856300 | 4.61010200 | -3.22171000 |
| H | 1.28112500 | 2.65849700 | -2.99551700 |
| C | -0.48656500 | 5.55344600 | -2.72434700 |
| H | -1.97821000 | 5.94888800 | -1.20681300 |
| H | 0.95916700 | 4.80951300 | -4.14845200 |
| H | -0.72970700 | 6.43448400 | -3.31777500 |
| C | -2.91444700 | -1.05370800 | -1.34285900 |
| C | -4.06084500 | -0.30346700 | -1.01878500 |
| C | -3.05840500 | -2.12651500 | -2.24055800 |
| C | -5.29376000 | -0.56963200 | -1.61477600 |
| H | -3.98136600 | 0.53408500 | -0.32816400 |
| C | -4.29068500 | -2.41048900 | -2.83259000 |
| H | -2.19296800 | -2.72240300 | -2.51793800 |
| C | -5.41686900 | -1.62676500 | -2.53023200 |
| H | -6.14143300 | 0.08467900 | -1.41891700 |
| H | -4.36396400 | -3.19803300 | -3.57918800 |
| H | -6.31924600 | -1.71931500 | -3.13885100 |
| C | -2.74988400 | -1.32914300 | 2.84436500 |
| C | -3.27925600 | -2.52668700 | 2.33343700 |
| C | -3.29893000 | -0.79813700 | 4.01901800 |
| C | -4.32378300 | -3.17819000 | 2.98961300 |
| H | -2.83383400 | -2.97643800 | 1.44577800 |
| C | -4.34499500 | -1.44714900 | 4.67383500 |
| H | -2.90399600 | 0.12265100 | 4.43963100 |
| C | -4.85922700 | -2.63664200 | 4.16171100 |
| H | -4.69081800 | -4.13451100 | 2.62338100 |
| H | -4.74800700 | -1.03406000 | 5.59293700 |
| H | -5.65194600 | -3.15598400 | 4.69125800 |
| Mg | 0.71718100 | 7.18495600 | -1.15012800 |
| Mg | -6.91899600 | -3.08396300 | -1.09568100 |
| Mg | 6.24935100 | -4.20192000 | -0.97636600 |
| C | 5.37438900 | -2.31422100 | 1.29748500 |
| C | 8.21480800 | -6.05878300 | 0.87188700 |
| C | 2.61122400 | 4.66726300 | -0.59307500 |
| C | -0.80963700 | 6.28008300 | 1.42416900 |
| C | -4.25388200 | -4.71315700 | -0.57029900 |
| C | -6.07095300 | -1.30070200 | 1.35944500 |
| O | -1.66930800 | 5.76363100 | 1.97409600 |
| O | 0.04021900 | 6.83525800 | 0.81431600 |
| O | 3.08619100 | 3.63421100 | -0.44443700 |
| O | 2.14661000 | 5.73899700 | -0.73196400 |
| O | 5.48679800 | -3.36261600 | 0.75448800 |
| O | 5.31887200 | -1.28216000 | 1.78657100 |
| O | 7.54226900 | -5.36794100 | 0.18167800 |
| O | 8.86164800 | -6.72166700 | 1.53609300 |
| O | -5.39789400 | -4.44746800 | -0.66580900 |
| O | -3.14432600 | -4.98067800 | -0.47191700 |
| O | -6.48552000 | -2.22052000 | 0.74115300 |
| O | -5.71075700 | -0.37648600 | 1.92891300 |
| C | 4.05195800 | -6.47948600 | -0.38777000 |
| C | -8.87843200 | -5.00903100 | 0.62602000 |
| C | -1.44570200 | 9.49881500 | -1.74028500 |
| O | 4.86135500 | -5.72924200 | -0.80982600 |
| O | 3.25986900 | -7.19895800 | 0.01111800 |
| O | -8.24056900 | -4.32076700 | -0.09867400 |
| O | -9.49446400 | -5.67107700 | 1.31951000 |
| O | -2.06735000 | 10.42634900 | -1.96393500 |
| O | -0.80775000 | 8.52408100 | -1.50875600 |
| C | 8.93576900 | -2.46143600 | -1.17663900 |
| O | 7.81033300 | -2.82346100 | -1.06903900 |

| | | | |
|---|---|---|---|
| O | 10.01102200 | -2.09723600 | -1.27779700 |
| C | -7.84584500 | -4.88360000 | -3.59850200 |
| O | -7.36400700 | -4.12431800 | -2.82368800 |
| O | -8.29837400 | -5.60971500 | -4.35058900 |
| C | 2.39391100 | 8.36909600 | -3.62750600 |
| O | 1.70345900 | 7.74080400 | -2.89547100 |
| O | 3.05695500 | 8.96260300 | -4.33991100 |
| C | 7.39668100 | -5.87724900 | -3.50266900 |
| C | 2.36748500 | 9.40890900 | 0.52032600 |
| C | -9.52202900 | -1.26551000 | -1.58945500 |
| O | 1.87341300 | 8.66357400 | -0.25846100 |
| O | 2.84757700 | 10.12695300 | 1.26405400 |
| O | 6.97011900 | -5.13664900 | -2.67888500 |
| O | 7.80409300 | -6.58229100 | -4.29905200 |
| O | -8.43716000 | -1.72688400 | -1.44772600 |
| O | -10.55636000 | -0.80846800 | -1.72663300 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-3$Mg^{2+}$-18$N_2$**

6 1

| | | | |
|---|---|---|---|
| Si | 0.94186400 | -1.30742800 | 0.41597300 |
| Si | 1.51853000 | 0.96470500 | -0.06386000 |
| Si | 0.02925200 | 0.42476600 | 1.72226100 |
| Si | -0.27159000 | 1.02210800 | -1.63031500 |
| Si | -0.82441600 | -1.19990500 | -1.15615700 |
| Si | -1.76282000 | 0.54911500 | 0.16015800 |
| C | 3.20924500 | 1.88076900 | -0.08986200 |
| C | 3.75755000 | 2.33470300 | -1.30632600 |
| C | 3.96800300 | 2.06066200 | 1.08559600 |
| C | 5.05372200 | 2.84674100 | -1.37016800 |
| H | 3.19333800 | 2.22703500 | -2.23024000 |
| C | 5.26283700 | 2.57369600 | 1.04044800 |
| H | 3.56445200 | 1.74274400 | 2.04443400 |
| C | 5.82911100 | 2.95060900 | -0.19610200 |
| H | 5.49311300 | 3.07899800 | -2.33878600 |
| H | 5.86356500 | 2.60414900 | 1.94702700 |
| H | 6.91121000 | 3.09590900 | -0.27267900 |
| C | 1.90939400 | -2.92328400 | 0.81564100 |
| C | 1.41129900 | -3.84145300 | 1.76089000 |
| C | 3.13555800 | -3.21778500 | 0.18951500 |
| C | 2.14986900 | -4.96380300 | 2.13974200 |
| H | 0.46474200 | -3.64649700 | 2.25937400 |
| C | 3.88714000 | -4.33582900 | 0.55386800 |
| H | 3.53993500 | -2.53338600 | -0.55144000 |
| C | 3.41019300 | -5.20564100 | 1.55515700 |
| H | 1.79558700 | -5.59485000 | 2.95277400 |
| H | 4.87778700 | -4.48476400 | 0.12933800 |
| H | 4.09044100 | -5.92820500 | 2.01420000 |
| C | -1.48987500 | -2.69502700 | -2.05070300 |
| C | -2.16906000 | -3.69003400 | -1.32568000 |
| C | -1.24563900 | -2.89395600 | -3.41783300 |
| C | -2.58975700 | -4.85792500 | -1.95618100 |
| H | -2.38435400 | -3.54214300 | -0.26863700 |
| C | -1.66778100 | -4.06366700 | -4.04708800 |
| H | -0.73289800 | -2.13060500 | -3.99778200 |
| C | -2.33725700 | -5.04484100 | -3.31722500 |
| H | -3.13722800 | -5.61260800 | -1.39875100 |
| H | -1.48995000 | -4.20339600 | -5.10882900 |
| H | -2.68316700 | -5.94624100 | -3.81425700 |
| C | -0.61045600 | 2.06485900 | -3.13386200 |
| C | -1.22982100 | 3.32111500 | -3.00919300 |
| C | -0.24419200 | 1.60916900 | -4.41150600 |
| C | -1.47276500 | 4.10012700 | -4.13623900 |

**HPPS-3$Mg^{2+}$-9$CH_4$**

6 1

| | | | |
|---|---|---|---|
| Si | 1.34766000 | -0.14859700 | -1.15255300 |
| Si | -0.83989900 | -1.10684100 | -1.14925100 |
| Si | -0.57377600 | 1.26589300 | -1.15601200 |
| Si | -0.82826700 | -1.17407300 | 1.21064300 |
| Si | 1.35330800 | -0.19738900 | 1.20290400 |
| Si | -0.59083800 | 1.19815300 | 1.19917700 |
| C | -1.74775700 | -2.52833100 | -2.03348500 |
| C | -1.56031500 | -3.83506000 | -1.52870600 |
| C | -2.57207500 | -2.37383900 | -3.15781900 |
| C | -2.18167500 | -4.94441000 | -2.13997000 |
| H | -0.83975100 | -4.00734400 | -0.72728700 |
| C | -3.19763600 | -3.47084500 | -3.76489400 |
| H | -2.72235800 | -1.38809900 | -3.59033000 |
| C | -3.01294000 | -4.75564000 | -3.26061700 |
| H | -1.88771300 | -5.95830300 | -1.85788900 |
| H | -3.80698800 | -3.32074400 | -4.65201000 |
| H | -3.45778900 | -5.61123400 | -3.76274700 |
| C | 3.02370000 | -0.40925000 | -2.01747400 |
| C | 3.46252900 | 0.31994300 | -3.13201400 |
| C | 3.88160900 | -1.41110900 | -1.50819800 |
| C | 4.70897600 | 0.07977400 | -3.72447800 |
| H | 2.82067700 | 1.08042400 | -3.56913600 |
| C | 5.13469400 | -1.66400300 | -2.10546400 |
| H | 3.52903200 | -2.07438600 | -0.71598300 |
| C | 5.55232300 | -0.90370000 | -3.21472800 |
| H | 5.00645500 | 0.64415700 | -4.60373400 |
| H | 5.70544000 | -2.55111200 | -1.82102900 |
| H | 6.49763300 | -1.12370900 | -3.70462300 |
| C | 3.07108100 | -0.25649200 | 2.02430200 |
| C | 4.07506400 | 0.57067800 | 1.47104500 |
| C | 3.41260200 | -1.03994500 | 3.13692400 |
| C | 5.37120000 | 0.60858300 | 2.02527200 |
| H | 3.82070900 | 1.27287600 | 0.67479700 |
| C | 4.70181800 | -1.01557800 | 3.68508800 |
| H | 2.66329100 | -1.67164700 | 3.60690000 |
| C | 5.68612200 | -0.19878600 | 3.13475300 |
| H | 6.07664500 | 1.38068900 | 1.70901200 |
| H | 4.92673000 | -1.61366600 | 4.56365600 |
| H | 6.67002200 | -0.13893600 | 3.59346600 |
| C | -1.93367100 | -2.50965300 | 2.00121900 |
| C | -3.20961900 | -2.70772900 | 1.42630400 |
| C | -1.58540000 | -3.30228700 | 3.10523000 |
| C | -4.09994500 | -3.66822800 | 1.94941300 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H | -1.52297600 | 3.68944000 | -2.02778400 | H | -3.55683600 | -2.03979700 | 0.63588500 |
| C | -0.49067500 | 2.39036800 | -5.53636400 | C | -2.46118000 | -4.26539600 | 3.62372700 |
| H | 0.22990200 | 0.63775300 | -4.53128400 | H | -0.62261300 | -3.16446500 | 3.59021400 |
| C | -1.10468300 | 3.63470200 | -5.39869000 | C | -3.71577100 | -4.45724600 | 3.05080500 |
| H | -1.94985600 | 5.07001000 | -4.03507500 | H | -5.14160000 | -3.68346000 | 1.61929200 |
| H | -0.20991300 | 2.02971000 | -6.52072400 | H | -2.17201400 | -4.84458700 | 4.49607000 |
| H | -1.30060100 | 4.24092500 | -6.27760700 | H | -4.41478900 | -5.16717300 | 3.48584800 |
| C | -3.49649300 | 1.35450900 | 0.31298800 | C | -1.18931100 | 2.77616600 | 2.08053900 |
| C | -4.05914600 | 1.64977100 | 1.57200600 | C | -2.05748000 | 2.79600600 | 3.18241800 |
| C | -4.18104500 | 1.79992900 | -0.83790600 | C | -0.70965600 | 4.01514500 | 1.59771000 |
| C | -5.19958200 | 2.44312500 | 1.68813800 | C | -2.44703000 | 3.99791700 | 3.78794200 |
| H | -3.56063400 | 1.31829700 | 2.48034200 | H | -2.42885400 | 1.86277000 | 3.59760700 |
| C | -5.32347300 | 2.59140900 | -0.73919000 | C | -1.09036800 | 5.22804600 | 2.20959400 |
| H | -3.77056400 | 1.60029000 | -1.82575700 | H | 0.05278300 | 4.03271500 | 0.81657700 |
| C | -5.83214100 | 2.94268400 | 0.53065300 | C | -1.97362700 | 5.21581800 | 3.30597600 |
| H | -5.54758500 | 2.74752200 | 2.67308900 | H | -3.09763500 | 3.97794300 | 4.65770800 |
| H | -5.76082800 | 3.01714400 | -1.64051000 | H | -0.57409100 | 6.15537400 | 1.94974300 |
| H | -6.53984000 | 3.77272600 | 0.61945600 | H | -2.23434600 | 6.14363500 | 3.80926400 |
| C | 0.10959200 | 0.76135700 | 3.54842200 | C | -1.31816300 | 2.82379000 | -1.95957400 |
| C | 0.61069300 | -0.19916000 | 4.44130000 | C | -0.74569400 | 3.50689400 | -3.04188800 |
| C | -0.34596500 | 1.99181400 | 4.05347100 | C | -2.52986500 | 3.32606100 | -1.43139500 |
| C | 0.65945500 | 0.06608100 | 5.80672800 | C | -1.34055400 | 4.65178000 | -3.58750300 |
| H | 0.96061800 | -1.15968900 | 4.06942500 | H | 0.17334900 | 3.13820500 | -3.48984900 |
| C | -0.30276600 | 2.25049800 | 5.41911800 | C | -3.13833200 | 4.47377800 | -1.98068400 |
| H | -0.73448600 | 2.75194600 | 3.37775000 | H | -3.06037500 | 2.76089200 | -0.66294700 |
| C | 0.20094900 | 1.28824800 | 6.29517400 | C | -2.53187600 | 5.14359200 | -3.06080800 |
| H | 1.04746600 | -0.67924900 | 6.49339700 | H | -0.88553100 | 5.14117100 | -4.44405500 |
| H | -0.65970700 | 3.19994200 | 5.80532600 | H | -4.15653400 | 4.74330600 | -1.68986700 |
| H | 0.23325100 | 1.49116600 | 7.36094900 | H | -3.02033300 | 6.00111200 | -3.51691100 |
| Mg | 5.78726100 | 5.27783300 | -0.02239600 | Mg | -3.51089800 | -4.81448100 | -0.11119000 |
| Mg | -7.74901400 | 1.63239700 | 0.46689800 | Mg | -2.35506000 | 5.39668300 | 0.14440100 |
| Mg | 2.71398300 | -6.96310600 | 0.18359900 | Mg | 5.85337500 | -0.58693000 | -0.04014600 |
| N | 2.84289800 | -9.09553000 | 2.91974200 | C | -5.01411900 | -6.88328000 | -0.16414700 |
| N | 0.62350300 | -5.08408300 | -1.76288400 | H | -6.07003400 | -6.87694200 | -0.44535900 |
| N | 2.79315000 | -8.41596200 | 2.05827000 | H | -4.43558800 | -6.56413000 | -1.05225800 |
| N | 1.28428700 | -5.67047800 | -1.10936800 | H | -4.90877500 | -6.26838600 | 0.75035400 |
| N | -9.35826000 | 3.97588200 | -1.51275800 | H | -4.69407200 | -7.89705500 | 0.08891200 |
| N | -8.83754200 | 3.23143900 | -0.89555900 | C | -5.50990200 | -3.48308200 | -1.16300200 |
| N | -7.80636400 | 0.67166600 | 2.65423700 | H | -6.03047200 | -2.76893600 | -0.52244700 |
| N | -7.86403600 | 0.24482100 | 3.66432700 | H | -5.95268900 | -3.48851300 | -2.16115200 |
| N | 4.76885100 | 6.00163800 | -2.08973800 | H | -4.45956300 | -3.16616300 | -1.28547700 |
| N | 4.33469600 | 6.34580500 | -3.03787100 | H | -5.66829900 | -4.49285300 | -0.75735100 |
| N | 7.87060900 | 5.27995600 | 1.11946200 | C | 5.78609600 | -2.99203000 | 0.99573800 |
| N | 8.83871300 | 5.30439800 | 1.63771900 | H | 5.00246300 | -2.24072000 | 1.19594300 |
| N | 5.90886300 | -8.33699400 | 0.35009800 | H | 6.09701900 | -3.38516000 | 1.96595600 |
| N | 4.90724600 | -7.89010900 | 0.28996300 | H | 5.37151500 | -3.79121900 | 0.37855200 |
| N | 3.46505300 | 5.27427300 | 0.28636600 | H | 6.70261600 | -2.62189200 | 0.51354900 |
| N | 2.37788300 | 5.19714600 | 0.41258500 | C | 8.40171700 | -0.80471900 | -0.06637700 |
| N | -6.47141200 | -0.33961300 | 0.39214400 | H | 9.09764100 | 0.00036500 | -0.31487600 |
| N | -5.82149700 | -1.22272700 | 0.35308800 | H | 8.94882500 | -1.71970200 | 0.17347000 |
| N | -10.73894500 | 0.11321100 | 0.42571600 | H | 7.85369700 | -0.50075700 | 0.84610300 |
| N | -9.75089200 | 0.59162400 | 0.44008500 | H | 7.79600000 | -1.00507900 | -0.97096100 |
| N | 2.27999800 | -8.85678800 | -0.94970300 | C | -3.36497600 | 7.74958200 | 0.20209500 |
| N | 2.09180100 | -9.79751600 | -1.48332500 | H | -4.40726900 | 7.97559200 | 0.43990500 |
| N | 5.97516400 | 7.50611000 | 0.13788100 | H | -2.81413800 | 8.67032600 | -0.00507900 |
| N | 6.09207900 | 8.59483100 | 0.21749000 | H | -2.91596000 | 7.28757400 | 1.10216600 |
| N | 0.43970500 | -7.43884500 | 0.88884100 | H | -3.35761500 | 7.14663600 | -0.72610200 |
| N | -0.59218400 | -7.65177200 | 1.19777500 | C | -0.18622200 | 6.50477600 | -0.84370500 |
| N | -7.90371900 | 0.39843400 | -2.81543400 | H | -0.45818400 | 5.45423800 | -1.04567300 |
| N | -7.84115100 | 0.77244700 | -1.78491800 | H | 0.00940500 | 6.97116900 | -1.81136800 |
| N | 7.48623300 | 5.46312100 | -1.65390000 | H | -0.95787700 | 7.12104900 | -0.36021400 |
| N | 8.28162700 | 5.56776800 | -2.40402200 | H | 0.71036600 | 6.52994300 | -0.22179900 |
| N | 5.20510000 | 5.76453400 | 3.39881300 | C | -4.63616900 | 4.53949900 | 1.11003300 |
| N | 5.36782300 | 5.60661500 | 2.32438600 | H | -5.10072800 | 4.66989800 | 2.08954600 |
| N | -9.42384300 | 3.84267400 | 2.56466300 | H | -3.68190600 | 4.01090200 | 1.27992400 |
| N | -8.88421200 | 3.14707800 | 1.90784700 | H | -5.27335900 | 3.93055600 | 0.46621900 |
| N | 3.83018100 | -6.52406500 | -1.90706900 | H | -4.56374600 | 5.54528900 | 0.67165600 |

| | | | |
|---|---|---|---|
| N | 4.34698400 | -6.34439700 | -2.85912600 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| C | -1.65231300 | -6.34745500 | 0.93670500 |
| H | -0.78709700 | -6.56762800 | 0.30884400 |
| H | -2.54256400 | -6.79511300 | 0.47190500 |
| H | -1.54692800 | -6.83368100 | 1.90877800 |
| H | -1.69902800 | -5.26193300 | 1.13108200 |
| C | 6.18977900 | 1.81366300 | -1.06607700 |
| H | 5.27708700 | 1.21642900 | -1.23649400 |
| H | 5.94382400 | 2.67351200 | -0.44038900 |
| H | 7.03754200 | 1.28463400 | -0.60801900 |
| H | 6.53586700 | 2.14573500 | -2.04695300 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 64 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-3Li$^+$-1CO$_2$**

3 1

| | | | |
|---|---|---|---|
| Si | -0.75081400 | -0.54253000 | 1.34716300 |
| Si | 1.59915400 | -0.80619800 | 1.15910500 |
| Si | 0.66190700 | 1.35794500 | 1.21714000 |
| Si | 1.39905800 | -0.82165400 | -1.18613800 |
| Si | -0.95527500 | -0.54628200 | -0.99851100 |
| Si | 0.47002100 | 1.34447500 | -1.12775500 |
| C | 3.07557800 | -1.85402600 | 1.70861700 |
| C | 2.94903900 | -3.25099700 | 1.83751300 |
| C | 4.37169000 | -1.30246200 | 1.68020600 |
| C | 4.07957400 | -4.07058800 | 1.92885900 |
| H | 1.96314900 | -3.70864600 | 1.85984000 |
| C | 5.50430800 | -2.11876000 | 1.77247600 |
| H | 4.50382800 | -0.22840800 | 1.57572700 |
| C | 5.36036900 | -3.50645100 | 1.88956900 |
| H | 3.96259700 | -5.14495100 | 2.03436500 |
| H | 6.49539700 | -1.67539000 | 1.75527700 |
| H | 6.23815000 | -4.14110700 | 1.96254000 |
| C | -2.25554800 | -1.19247300 | 2.29214300 |
| C | -3.27871300 | -0.32456800 | 2.72069500 |
| C | -2.48916700 | -2.58114200 | 2.35757300 |
| C | -4.49616300 | -0.82583200 | 3.19365900 |
| H | -3.12965200 | 0.75129200 | 2.68288000 |
| C | -3.70930700 | -3.08493700 | 2.81928000 |
| H | -1.71691800 | -3.27827900 | 2.04025500 |
| C | -4.71739900 | -2.20585300 | 3.23461600 |
| H | -5.27145300 | -0.14154500 | 3.52415300 |
| H | -3.87100300 | -4.15768800 | 2.86670000 |
| H | -5.66246600 | -2.59565700 | 3.59958000 |
| C | -2.55915900 | -1.21836900 | -1.71957900 |
| C | -3.35637500 | -0.51638200 | -2.63225200 |
| C | -3.01259400 | -2.47404700 | -1.25639900 |
| C | -4.56448300 | -1.05294800 | -3.08353000 |
| H | -3.02881200 | 0.44719500 | -3.01302800 |
| C | -4.22582400 | -3.00576100 | -1.69906000 |
| H | -2.38424900 | -3.06915100 | -0.59278900 |
| C | -5.00206600 | -2.29256900 | -2.61831000 |
| H | -5.15894800 | -0.50773200 | -3.81083800 |
| H | -4.54336100 | -3.99084100 | -1.36683200 |
| H | -5.93193600 | -2.71429300 | -2.98852400 |
| C | 2.76744300 | -1.87941700 | -1.95521400 |
| C | 4.04577300 | -1.32788000 | -2.17185700 |
| C | 2.62449100 | -3.27927100 | -2.03105800 |
| C | 5.14646800 | -2.14612000 | -2.44848600 |
| H | 4.18995400 | -0.25179000 | -2.11716300 |
| C | 3.72350500 | -4.10085400 | -2.30775600 |
| H | 1.65191100 | -3.73690200 | -1.86916700 |
| C | 4.98887600 | -3.53591100 | -2.50981200 |
| H | 6.12275900 | -1.70235200 | -2.61808200 |
| H | 3.59317300 | -5.17704700 | -2.36991400 |

**HPPS-3Li$^+$-9CO$_2$**

3 1

| | | | |
|---|---|---|---|
| Si | -1.08021200 | -0.92927600 | 0.97107800 |
| Si | 1.24260600 | -0.85637000 | 1.38842100 |
| Si | 0.04860700 | 1.15026500 | 1.10779900 |
| Si | 1.66709900 | -0.87409500 | -0.93640600 |
| Si | -0.65423100 | -0.92761500 | -1.36640300 |
| Si | 0.46106600 | 1.13990200 | -1.21116500 |
| C | 2.41136100 | -1.37779200 | 2.75022300 |
| C | 2.64322300 | -2.73819100 | 3.01061700 |
| C | 3.13182600 | -0.41629900 | 3.47602200 |
| C | 3.56815100 | -3.12569600 | 3.97575400 |
| H | 2.08937700 | -3.50102700 | 2.46740800 |
| C | 4.06428600 | -0.80470300 | 4.43616400 |
| H | 2.94978800 | 0.64277300 | 3.30381600 |
| C | 4.28166600 | -2.15823500 | 4.68691600 |
| H | 3.72924800 | -4.17923200 | 4.18492400 |
| H | 4.60725400 | -0.05334600 | 5.00094800 |
| H | 5.00026900 | -2.46345300 | 5.44144500 |
| C | -2.49169600 | -1.70884500 | 1.97221700 |
| C | -3.65866400 | -0.98849300 | 2.29190600 |
| C | -2.39607200 | -3.04032300 | 2.41350000 |
| C | -4.68758700 | -1.57174000 | 3.03436000 |
| H | -3.76851200 | 0.03748200 | 1.94969400 |
| C | -3.42568900 | -3.63298100 | 3.15285500 |
| H | -1.50854100 | -3.62363100 | 2.18175300 |
| C | -4.57059800 | -2.89772100 | 3.46944800 |
| H | -5.57457800 | -0.99599100 | 3.28079000 |
| H | -3.33012200 | -4.66117500 | 3.48797200 |
| H | -5.36279700 | -3.35090400 | 4.05774400 |
| C | -1.63468200 | -1.69173700 | -2.76211000 |
| C | -1.86865700 | -0.98995400 | -3.95323800 |
| C | -2.13455400 | -3.00051100 | -2.63939200 |
| C | -2.59061100 | -1.57480900 | -4.99121200 |
| H | -1.47971300 | 0.01806500 | -4.07623800 |
| C | -2.86224100 | -3.58152600 | -3.67431100 |
| H | -1.93330000 | -3.56968200 | -1.73216200 |
| C | -3.09304100 | -2.86562100 | -4.84997200 |
| H | -2.76278300 | -1.02361400 | -5.90997400 |
| H | -3.22763500 | -4.60063400 | -3.58524100 |
| H | -3.65392100 | -3.32161600 | -5.65941800 |
| C | 3.17935200 | -1.62489700 | -1.78817100 |
| C | 3.97183900 | -0.88585200 | -2.68748900 |
| C | 3.56621500 | -2.94478400 | -1.49096800 |
| C | 5.11000800 | -1.44739600 | -3.27075500 |
| H | 3.69800200 | 0.13725300 | -2.93509300 |
| C | 4.70953400 | -3.50775000 | -2.06686800 |
| H | 2.97683300 | -3.54052000 | -0.79780900 |
| C | 5.48287400 | -2.75929300 | -2.95883400 |
| H | 5.70258500 | -0.86536600 | -3.97017100 |
| H | 4.99065300 | -4.52866800 | -1.82704400 |

| | | | |
|---|---|---|---|
| H | 5.84103700 | -4.17186300 | -2.72880700 |
| C | 0.59124700 | 3.10812100 | -1.80616700 |
| C | 1.85376300 | 3.70089900 | -2.00675000 |
| C | -0.54487400 | 3.94134900 | -1.82162500 |
| C | 1.97837300 | 5.07932200 | -2.21239000 |
| H | 2.75066400 | 3.08674400 | -1.99653400 |
| C | -0.42416500 | 5.32041600 | -2.02638300 |
| H | -1.53274100 | 3.51545800 | -1.66450700 |
| C | 0.83917700 | 5.89379600 | -2.21587700 |
| H | 2.95899600 | 5.51746100 | -2.37152400 |
| H | -1.31147300 | 5.94585500 | -2.04088900 |
| H | 0.93424000 | 6.96300300 | -2.37820400 |
| C | 0.87891600 | 3.12572000 | 1.85806200 |
| C | -0.24719600 | 3.95591400 | 2.02291500 |
| C | 2.15419700 | 3.72422400 | 1.87064600 |
| C | -0.10580600 | 5.33791100 | 2.18939000 |
| H | -1.24578900 | 3.52594000 | 2.01139200 |
| C | 2.29961800 | 5.10599000 | 2.03696600 |
| H | 3.04384400 | 3.11255300 | 1.74275100 |
| C | 1.16881300 | 5.91712000 | 2.18963700 |
| H | -0.98521800 | 5.96124500 | 2.32099400 |
| H | 3.29105300 | 5.54871100 | 2.05124800 |
| H | 1.28081400 | 6.98878600 | 2.32254100 |
| Li | 4.26364900 | -2.87103300 | -0.24399600 |
| Li | 0.90851100 | 4.78666500 | -0.00210300 |
| Li | -4.16874500 | -1.64281500 | 0.81403900 |
| C | -6.48158500 | -0.36557800 | -0.66339800 |
| O | -5.64105800 | -0.58578500 | 0.13023800 |
| O | -7.30635000 | -0.13610900 | -1.42809500 |

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| H | 6.36544200 | -3.19833600 | -3.41362700 |
| C | 0.48545900 | 2.64061400 | -2.33148200 |
| C | 1.59003200 | 3.50736800 | -2.32832400 |
| C | -0.61635300 | 2.95468000 | -3.14159900 |
| C | 1.59863800 | 4.64937900 | -3.12454300 |
| H | 2.45485000 | 3.28380700 | -1.70623800 |
| C | -0.61117000 | 4.09867000 | -3.93766600 |
| H | -1.48137300 | 2.29405300 | -3.16374400 |
| C | 0.49875800 | 4.94245200 | -3.93395800 |
| H | 2.46427400 | 5.30498100 | -3.12893500 |
| H | -1.46198500 | 4.32396900 | -4.57314100 |
| H | 0.50978500 | 5.82802200 | -4.56177700 |
| C | -0.15972600 | 2.73347600 | 2.12291300 |
| C | -1.21588700 | 2.93384500 | 3.03202200 |
| C | 0.73736100 | 3.79593100 | 1.90283400 |
| C | -1.36784000 | 4.15053700 | 3.70084400 |
| H | -1.92524800 | 2.13175400 | 3.22205800 |
| C | 0.58440900 | 5.01711700 | 2.56742100 |
| H | 1.55574000 | 3.67645900 | 1.19704200 |
| C | -0.46879300 | 5.19675100 | 3.46749600 |
| H | -2.18101800 | 4.28193200 | 4.40837800 |
| H | 1.28937800 | 5.82319500 | 2.38743900 |
| H | -0.58317000 | 6.14156800 | 3.98986100 |
| Li | 5.41770000 | -1.53380200 | -0.69284100 |
| Li | -1.42705300 | 4.58439500 | 1.08667700 |
| Li | -4.50571600 | -2.96265000 | 0.96386300 |
| C | 4.20805400 | 1.15730500 | 0.52872600 |
| C | -2.96126600 | 2.16273300 | -0.38083200 |
| C | -4.12617800 | -5.45702900 | -0.79260900 |
| O | 3.54066900 | 2.04304900 | 0.85725600 |
| O | 4.89950900 | 0.27817000 | 0.19421600 |
| O | -2.52219100 | 3.17971300 | -0.01379700 |
| O | -3.42342300 | 1.16528300 | -0.74269100 |
| O | -3.97047100 | -4.67431400 | 0.06833000 |
| O | -4.26388100 | -6.22406800 | -1.63873100 |
| C | -0.37041200 | 6.29678700 | -1.23447100 |
| C | 6.01439200 | -2.92096500 | 1.97778800 |
| C | -4.57945300 | -1.32751200 | -1.72439100 |
| O | -0.60170600 | 5.36188700 | -0.56284600 |
| O | -0.14428100 | 7.22527400 | -1.87518400 |
| O | 5.42446100 | -2.42916600 | 1.08968300 |
| O | 6.59818300 | -3.41292000 | 2.83829700 |
| O | -4.82460300 | -0.82172400 | -2.72821500 |
| O | -4.35130400 | -1.82315900 | -0.68504700 |
| C | -3.69927300 | 6.67374500 | 1.64960800 |
| C | 8.45603800 | -0.83013100 | -1.07972800 |
| C | -7.61548900 | -3.50370700 | 1.03385100 |
| O | -8.72025100 | -3.69048900 | 1.28533400 |
| O | -6.48527400 | -3.31027600 | 0.77379300 |
| O | -4.47961600 | 7.41747300 | 2.04476900 |
| O | -2.90317500 | 5.91005600 | 1.24394800 |
| O | 7.37355800 | -1.14575100 | -0.74824900 |
| O | 9.51406200 | -0.52062200 | -1.40132400 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**HPPS-3Li$^+$-1N$_2$**

3 1

| | | | |
|---|---|---|---|
| Si | 0.94970700 | -0.59453900 | 1.26059800 |
| Si | -0.39528300 | 1.35934800 | 1.21261500 |
| Si | -1.41252900 | -0.77021400 | 1.17291900 |
| Si | -0.30418600 | 1.36012100 | -1.13944700 |
| Si | 1.05527800 | -0.58248200 | -1.09079400 |
| Si | -1.31470200 | -0.76955200 | -1.17830500 |

**HPPS-3Li$^+$-1CH$_4$**

3 1

| | | | |
|---|---|---|---|
| Si | 0.11576400 | 1.42905600 | 1.17518600 |
| Si | -0.99669100 | -0.66644600 | 1.14290200 |
| Si | 1.37954800 | -0.56144700 | 1.17121300 |
| Si | -0.94023300 | -0.65778800 | -1.20984800 |
| Si | 0.15372400 | 1.44350900 | -1.18083700 |
| Si | 1.42800200 | -0.54332400 | -1.18093400 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -0.54858600 | 3.12661400 | 1.87271800 | C | -2.39280700 | -1.64688700 | 1.93828100 |
| C | 0.59548000 | 3.94147900 | 1.98283500 | C | -3.24190200 | -1.17405500 | 2.94630200 |
| C | -1.81376700 | 3.74084500 | 1.95512800 | C | -2.62806500 | -2.93856100 | 1.41342200 |
| C | 0.48037900 | 5.32394600 | 2.16597300 | C | -4.29506200 | -1.96235700 | 3.41740600 |
| H | 1.58643900 | 3.49942700 | 1.91495700 | H | -3.08128200 | -0.19049400 | 3.37923700 |
| C | -1.93272600 | 5.12302300 | 2.13769900 | C | -3.68669500 | -3.72138200 | 1.87796900 |
| H | -2.71670000 | 3.14128800 | 1.87083700 | H | -1.93683700 | -3.36281500 | 0.68409000 |
| C | -0.78512000 | 5.91887100 | 2.23696100 | C | -4.52567500 | -3.22707200 | 2.88222300 |
| H | 1.37344900 | 5.93534700 | 2.25382300 | H | -4.93451800 | -1.58671000 | 4.21015800 |
| H | -2.91613400 | 5.57804400 | 2.20716500 | H | -3.82916800 | -4.72931400 | 1.49507400 |
| H | -0.87632100 | 6.99086500 | 2.38245300 | H | -5.33989500 | -3.83841800 | 3.25858300 |
| C | 2.46963400 | -1.32569600 | 2.12099800 | C | -0.03035900 | 3.19915800 | 1.83093100 |
| C | 2.63351000 | -2.72504000 | 2.17495000 | C | 1.11469600 | 4.01341700 | 1.93608100 |
| C | 3.56308500 | -0.51417500 | 2.48189100 | C | -1.29506000 | 3.81263300 | 1.92604700 |
| C | 3.85273100 | -3.29425100 | 2.55592800 | C | 1.00060400 | 5.39506800 | 2.12637500 |
| H | 1.80622200 | -3.37936600 | 1.91006900 | H | 2.10520200 | 3.57190000 | 1.86033500 |
| C | 4.78035900 | -1.08043900 | 2.87613600 | C | -1.41279700 | 5.19409700 | 2.11557200 |
| H | 3.46809800 | 0.56825500 | 2.45397400 | H | -2.19817600 | 3.21261000 | 1.84516600 |
| C | 4.93205200 | -2.47061500 | 2.90205700 | C | -0.26445300 | 5.98957600 | 2.20983000 |
| H | 3.96025400 | -4.37416400 | 2.59398300 | H | 1.89438900 | 6.00593300 | 2.21051900 |
| H | 5.60986900 | -0.43952500 | 3.15965500 | H | -2.39558200 | 5.64895100 | 2.19416700 |
| H | 5.87704600 | -2.91070900 | 3.20572600 | H | -0.35451800 | 7.06087900 | 2.36096600 |
| C | 2.61337400 | -1.30165700 | -1.86353500 | C | 0.01584600 | 3.21312000 | -1.83736000 |
| C | 3.02447600 | -2.58700400 | -1.44265600 | C | 1.16122200 | 4.02936400 | -1.92099800 |
| C | 3.42699000 | -0.60529800 | -2.76678500 | C | -1.24796000 | 3.82553600 | -1.95026600 |
| C | 4.21762400 | -3.14620900 | -1.90815600 | C | 1.04801100 | 5.41142400 | -2.10830700 |
| H | 2.37883400 | -3.18111500 | -0.79469500 | H | 2.15096100 | 3.58907200 | -1.83086200 |
| C | 4.61138500 | -1.17124500 | -3.24334100 | C | -1.36492100 | 5.20724200 | -2.13712200 |
| H | 3.13164500 | 0.38014500 | -3.11667000 | H | -2.15160000 | 3.22453700 | -1.88513800 |
| C | 5.01257800 | -2.43354100 | -2.81217800 | C | -0.21622100 | 6.00450300 | -2.21022500 |
| H | 4.50193800 | -4.15176300 | -1.60803100 | H | 1.94210300 | 6.02379600 | -2.17585000 |
| H | 5.21846200 | -0.62533700 | -3.95903700 | H | -2.34694400 | 5.66101100 | -2.22978100 |
| H | 5.92880400 | -2.87365200 | -3.19318200 | H | -0.30539100 | 7.07618400 | -2.35913800 |
| C | -0.41745600 | 3.13042900 | -1.80020900 | C | -2.36191100 | -1.55675700 | -2.08315600 |
| C | -1.67736000 | 3.74266800 | -1.95316900 | C | -2.34179900 | -2.96201000 | -2.19108600 |
| C | 0.72968400 | 3.94699800 | -1.84969500 | C | -3.55339300 | -0.88290400 | -2.41598100 |
| C | -1.78875600 | 5.12417200 | -2.14517500 | C | -3.47682300 | -3.67167000 | -2.59759600 |
| H | -2.58222900 | 3.14122300 | -1.91741300 | H | -1.43554800 | -3.51230500 | -1.94899600 |
| C | 0.62209500 | 5.32902200 | -2.04107300 | C | -4.68593400 | -1.58831400 | -2.83809800 |
| H | 1.71615100 | 3.50636000 | -1.72897800 | H | -3.60140900 | 0.20078600 | -2.34606800 |
| C | -0.63845700 | 5.92193000 | -2.18275100 | C | -4.65437200 | -2.98435600 | -2.91785800 |
| H | -2.76763400 | 5.57721200 | -2.26916100 | H | -3.44139500 | -4.75416400 | -2.67629500 |
| H | 1.51748900 | 5.94178700 | -2.08156100 | H | -5.59142200 | -1.05049500 | -3.10234400 |
| H | -0.72314300 | 6.99346800 | -2.33523000 | H | -5.53426900 | -3.53284100 | -3.24003500 |
| C | -2.74784400 | -1.77579700 | -1.89598100 | C | 2.97006500 | -1.42876900 | -1.82564200 |
| C | -4.02362000 | -1.19156100 | -2.02590700 | C | 2.97206300 | -2.83271700 | -1.94448400 |
| C | -2.64139500 | -3.17573400 | -2.01337600 | C | 4.20513800 | -0.75398600 | -1.88504100 |
| C | -5.15609800 | -1.97884400 | -2.26060700 | C | 4.16761100 | -3.54029500 | -2.11124100 |
| H | -4.14035100 | -0.11448700 | -1.93551600 | H | 2.03591900 | -3.38371300 | -1.89973100 |
| C | -3.77227300 | -3.96643900 | -2.24712400 | C | 5.40242200 | -1.45791000 | -2.05463200 |
| H | -1.67176600 | -3.65716700 | -1.91608200 | H | 4.23942000 | 0.32832300 | -1.78925900 |
| C | -5.03356900 | -3.36976700 | -2.36483500 | C | 5.38697300 | -2.85412700 | -2.16040500 |
| H | -6.13004900 | -1.51074700 | -2.36621800 | H | 4.14885100 | -4.62162800 | -2.20757200 |
| H | -3.67009400 | -5.04325300 | -2.34249100 | H | 6.34445600 | -0.92031800 | -2.10591000 |
| H | -5.91069600 | -3.98152100 | -2.55221400 | H | 6.31558900 | -3.40036300 | -2.29431200 |
| C | -2.88375700 | -1.79313300 | 1.77930400 | C | 2.91548600 | -1.43182500 | 1.85274300 |
| C | -2.77807400 | -3.19448400 | 1.87818900 | C | 4.14385600 | -0.74628400 | 1.93281400 |
| C | -4.16871400 | -1.21757400 | 1.82703800 | C | 2.92474200 | -2.83389500 | 1.99079300 |
| C | -3.91759000 | -3.99476300 | 2.01598100 | C | 5.34226200 | -1.43811800 | 2.13982700 |
| H | -1.80145000 | -3.67039700 | 1.83859900 | H | 4.17136100 | 0.33502700 | 1.82406900 |
| C | -5.31036000 | -2.01449400 | 1.96541500 | C | 4.12210000 | -3.52945500 | 2.19392100 |
| H | -4.28586800 | -0.13978300 | 1.74660100 | H | 1.99343400 | -3.39191900 | 1.93566800 |
| C | -5.18757500 | -3.40634100 | 2.05319900 | C | 5.33470900 | -2.83322000 | 2.26269000 |
| H | -3.81615300 | -5.07273100 | 2.09800900 | H | 6.27873500 | -0.89258000 | 2.20690900 |
| H | -6.29219800 | -1.55267900 | 2.00808900 | H | 4.10921000 | -4.60947200 | 2.30479700 |
| H | -6.07257000 | -4.02570700 | 2.16270900 | H | 6.26393200 | -3.37034700 | 2.42591600 |
| Li | -0.64906100 | 4.80171700 | 0.02897500 | Li | -4.06544000 | -2.39906200 | -0.53189800 |

| | | | |
|---|---|---|---|
| Li | -4.18504400 | -2.76917600 | -0.12123900 |
| Li | 4.25237200 | -1.88753700 | 0.53246500 |
| N | 6.70380300 | -0.03656700 | -0.53697900 |
| N | 5.85245900 | -0.65447000 | -0.22474300 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

| | | | |
|---|---|---|---|
| Li | 4.37686500 | -2.32271200 | 0.03968500 |
| Li | -0.15641800 | 4.88102900 | 0.00153900 |
| C | -6.11843100 | -1.52693200 | 0.36198300 |
| H | -6.40212300 | -0.92659900 | -0.50339700 |
| H | -5.16396700 | -1.17920600 | 0.78349800 |
| H | -6.86707700 | -1.40752300 | 1.14647000 |
| H | -6.10805400 | -2.59306200 | 0.09924300 |

Convergence criteria used for SCF calculation:
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

**Bibliography:**


1 H. Zhao, L. Shi, Z. Zhang, X. Luo, L. Zhang, Q. Shen, S. Li, H. Zhang, N. Sun, W. Wei and Y. Sun, *ACS Appl. Mater. Interfaces*, 2018, **10**, 3495–3505.

2 J. Lan, D. Cao, W. Wang and B. Smit, *ACS Nano*, 2010, **4**, 4225–4237.

3 Y. Liu, Z. Meng, X. Guo, G. Xu, D. Rao, Y. Wang, K. Deng and R. Lu, *Phys. Chem. Chem. Phys.*, 2017, **19**, 28323–28329.

4 Z. Xiang, Z. Hu, D. Cao, W. Yang, J. Lu, B. Han and W. Wang, *Angew. Chemie Int. Ed.*, 2011, **50**, 491–494.

5 Y. Liu, Z. Meng, X. Guo, G. Xu, D. Rao, Y. Wang, K. Deng and R. Lu, *Phys. Chem. Chem. Phys.*, 2017, **19**, 28323–28329.

6 D. Saha, Z. Bao, F. Jia and S. Deng, *Environ. Sci. Technol.*, 2010, **44**, 1820–1826.

7 A. Ghosh, K. S. Subrahmanyam, K. S. Krishna, S. Datta, A. Govindaraj, S. K. Pati and C. N. R. Rao, *J. Phys. Chem. C*, 2008, **112**, 15704–15707.

8 A. Rajamani, V. Saravanan, S. Vijayakumar and R. Shankar, *ACS Omega*, 2019, **4**, 13808–13823.

9 P. D. Wakchaure and B. Ganguly, *ACS Omega*, 2020, **5**, 31146–31155.