1 **Theoretical studies in the molecular Platonic solids: Pure and mixed carbon, nitrogen,**
2 **phosphorus, and silicon tetrahedranes**
3
4 Sierra Rayne [a,*] and Kaya Forest [b,c]
5
6 [a] Ecologica Research, PO Box 74, 318 Rose Street, Mortlach, Saskatchewan, Canada, S0H 3E0
7 [b] Department of Chemistry, Okanagan College, 583 Duncan Avenue West, Penticton, British Columbia,
8 Canada, V2A 8E1
9 [c] Department of Environmental Engineering, Saskatchewan Institute of Applied Science and
10 Technology, Palliser Campus, PO Box 1420, 600 6th Avenue NW, Moose Jaw, Saskatchewan, Canada,
11 S6H 4R4
12
13 [*] Corresponding author. Tel.: +1 306 690 0573. E-mail address: rayne.sierra@gmail.com (S. Rayne).
14
15

16  **Abstract**

18  Calculations were conducted at the G4MP2 and G4 composite method levels of theory on the 35
19  potential carbon, nitrogen, silicon, and phosphorus tetrahedrane derivatives with the general form
20  $C_aN_bSi_cP_dH_{(4-b-d)}$ (where a+b+c+d=4). At both levels of theory, optimized electronic ground state neutral
21  singlet gas phase (298.15 K, 1 atm) geometries were obtained for 24 of the 35 possible C/N/Si/P
22  tetrahedrane derivatives. Corresponding enthalpies of formation were calculated using the atomization
23  method. Triplet state neutral tetrahedron starting geometries for all compounds either resulted in cage
24  opening or failed to converge. Only 9 cationic and 3 anionic forms converged to stable geometries that
25  retained the tetrahedron cage and were absent imaginary frequencies, thereby allowing the calculation
26  of adiabatic ionization energies and electron affinities.

28  **Keywords:** Tetrahedranes; Carbon, nitrogen, phosphorus, and silicon derivatives; Enthalpy of
29  formation; Adiabatic ionization energy; Electron affinity

31 The Platonic solids are set of five congruent regular polygons (tetrahedron, cube, octahedron,
32 dodecahedron, and icosahedron), each with the same number of faces meeting at all vertices (Figure 1).
33 Tetrahedrane is the simplest Platonic solid molecule (Figure 2). Using carbon, nitrogen, silicon, and
34 phosphorus, 35 potential tetrahedrane derivatives of the general form $C_aN_bSi_cP_dH_{(4-b-d)}$ (where
35 a+b+c+d=4) exist. Herein we use a compressed set notation style to denote each possible compound,
36 omitting implied hydrogen atoms on tetravalent carbon and silicon atoms (e.g., {C,C,N,P} is $C_2H_2NP$
37 and {N,Si,Si,Si} is $Si_3H_3N$) (Figure 3).
38
39 At the G4MP2 [1] and G4 [2] levels of theory in Gaussian 09 [3], optimized electronic ground state
40 neutral singlet ($S_0$) gas phase geometries and thermochemical data were obtained for 24 of the 35
41 possible C/N/Si/P tetrahedrane derivatives (Table 1 and Figure 4). Structures where a≥1 and c≥1 (i.e.,
42 the organosilicon members {C,C,C,Si}, {C,C,N,Si}, {C,C,P,Si}, {C,C,Si,Si}, {C,N,N,Si}, {C,N,P,Si},
43 {C,N,Si,Si}, {C,P,P,Si}, {C,P,Si,Si}, and {C,Si,Si,Si}), as well as {P,Si,Si,Si}, converged to ring-
44 opened non-tetrahedrane geometries. Holme et al. [4] reported a {C,C,Si,Si} structure with geometry
45 optimized using the Schlegel method and the 3-21G basis set, with subsequent single point calculations
46 with the 6-31G* basis set and at the MP3/6-31G* level. We were not able to obtain converged
47 {C,C,Si,Si} tetrahedron geometries at any of the HF/3-21G, HF/6-311++G(d,p) [5, 6], M062X/6-311+
48 +G(d,p) [5-7], B3LYP/6-311++G(d,p) [5, 6, 8-10], CBS-Q//B3 [11-18], G4MP2, or G4 levels of theory.
49 Triplet state neutral tetrahedron starting geometries for all compounds either resulted in cage opening
50 or failed to converge.
51
52 Gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_fH°_{(g)}$) were calculated using the atomization
53 approach at both the G4MP2 and G4 levels of theory [19-21] (Table 1). These levels of theory should
54 achieve effective thermochemical accuracy [1, 2, 22-28]. With the exception of phosphorus
55 tetrahedrane (G4MP2/G4 $\Delta_fH°_{(g)}$=48.6/61.2 kJ/mol), all tetrahedranes examined are expected to have
56 substantially endothermic $\Delta_fH°_{(g)}$ (from about 180 to 750 kJ/mol), and no tetrahedranes considered have
57 exothermic $\Delta_fH°_{(g)}$. The mixed element tetrahedranes adopt distorted tetrahedron geometries, with
58 increasing degrees of distortion as atomic size differences increase among the constituents (all
59 geometries at the G4MP2 and G4 levels are provided in the Supplementary Materials).
60
61 Calculations at the G4MP2 and G4 levels were also conducted on all cationic and anionic forms of
62 these 24 C/N/P/Si tetrahedranes. Only 9 of the cations converged yielding non-cage opened tetrahedral
63 geometries absent imaginary frequencies at the G4/G4MP2 levels ({C,N,N,N}, {C,P,P,P}, {C,N,P,P},
64 {N,N,P,P}, {P,P,P,P}, {P,P,Si,Si}, {N,N,P,Si}, {N,P,P,Si}, and {N,P,Si,Si}). Adiabatic ionization
65 energies (AIEs) were calculated for these derivatives and are provided in Table 1. AIEs at the
66 G4/G4MP2 levels are expected to be at or near thermochemical accuracy [1, 2, 24, 29]. Only three
67 anionic structures converged at these levels of theory ({N,N,P,P}, {P,P,Si,Si}, and {N,P,Si,Si}),
68 providing the estimated electron affinities (EAs) also given in Table 1.
69
70 For the carbon and nitrogen tetrahedranes and their mixed derivatives ({C,C,C,C}, {C,C,C,N},
71 {C,C,N,N}, {C,N,N,N}, and {N,N,N,N}), a modest set of prior theoretical $\Delta_fH°_{(g)}$ estimates exist in the
72 literature (Table 2). The only other high-level $\Delta_fH°_{(g)}$ estimates for the C/N/P/Si tetrahedranes are on the
73 pure carbon and nitrogen members, for which our $\Delta_fH°_{(g)}$ data is in excellent agreement with previous
74 calculations using the CBS-Q ({C,C,C,C}), G2 ({C,C,C,C} and {N,N,N,N}), G3 ({N,N,N,N}), and
75 W2 ({N,N,N,N}) methods. An experimental $\Delta_fH°_{(g)}$ datapoint is only available for {P,P,P,P} (59.0
76 kJ/mol), which is in excellent agreement with our G4 estimate (61.2 kJ/mol) and reasonable agreement
77 with our G4MP2 estimate (48.6 kJ/mol). In addition, the experimental AIE for the phosphorus

78    tetrahedrane (9.08 to 9.34 eV) is in excellent agreement with our G4MP2 (9.16 eV) and G4 (9.20 eV)
79    estimates. No other theoretical AIEs for these compounds appear to be available in the literature. We
80    also conducted CBS-Q//B3 [17, 18] calculations on the pure C/N/P/Si tetrahedranes, and the
81    corresponding atomization approach $\Delta_f H°_{(g)}$ estimates are also given in Table 2, as is the $\Delta_f H°_{(g)}$
82    estimate (765.0 kJ/mol) from our W1BD [30] calculation on {N,N,N,N}. These latter calculations are
83    also in strong agreement with our G4MP2 and G4 estimates.
84

**Acknowledgements**

**Appendix A. Supplementary Material**

93    Supplementary data is associated with this article.

95  **Figure Captions**
96
97  **Figure 1.** Geometrical shapes of the five Platonic solids (imagery from
98  http://en.wikipedia.org/wiki/Platonic_solid).
99
100 **Figure 2.** Three- and two-dimensional general representations of tetrahedrane.
101
102 **Figure 3.** Example structures and set notation naming styles for the {C,C,N,P} and {N,Si,Si,Si}
103 tetrahedranes.
104
105 **Figure 4.** Three-dimensional representations of the C/N/P/Si tetrahedranes at the G4 level of theory.
106

107 **Table 1.** G4MP2/G4 calculated C/N/P/Si tetrahedrane gas phase (298.15 K, 1 atm) enthalpies of
108 formation ($\Delta_f H^\circ_g$), adiabatic ionization energies (AIEs), and electron affinities (EAs).
109

| compound | $\Delta_f H^\circ_{(g)}$ (kJ/mol) | | AIE (eV) | | EA (eV) | |
|---|---|---|---|---|---|---|
| | G4MP2 | G4 | G4MP2 | G4 | G4MP2 | G4 |
| {C,C,C,C} | 532.4 | 536.5 | n/c[a] | n/c | n/c | n/c |
| {C,C,C,N} | 543.8 | 546.7 | n/c | n/c | n/c | n/c |
| {C,C,N,N} | 583.1 | 585.7 | n/c | n/c | n/c | n/c |
| {C,N,N,N} | 650.7 | 653.4 | 11.24 | 11.24 | n/c | n/c |
| {C,C,C,P} | 415.1 | 420.2 | n/c | n/c | n/c | n/c |
| {C,C,P,P} | 300.9 | 307.8 | n/c | n/c | n/c | n/c |
| {C,P,P,P} | 180.6 | 190.0 | 8.86 | 8.90 | n/c | n/c |
| {C,C,N,P} | 436.3 | 439.7 | n/c | n/c | n/c | n/c |
| {C,N,N,P} | 482.4 | 484.7 | n/c | n/c | n/c | n/c |
| {C,N,P,P} | 326.4 | 330.5 | 9.21 | 9.26 | n/c | n/c |
| {N,N,N,N} | 746.7 | 751.0 | n/c | n/c | n/c | n/c |
| {N,N,N,P} | 559.7 | 561.3 | n/c | n/c | n/c | n/c |
| {N,N,P,P} | 374.8 | 376.6 | 9.60 | 9.66 | 0.41 | 0.39 |
| {N,P,P,P} | 205.4 | 210.2 | n/c | n/c | n/c | n/c |
| {P,P,P,P} | 48.6 | 61.2 | 9.16 | 9.20 | n/c | n/c |
| {N,N,N,Si} | 728.6 | 727.9 | n/c | n/c | n/c | n/c |
| {N,N,Si,Si} | 601.2 | 601.7 | n/c | n/c | n/c | n/c |
| {N,Si,Si,Si} | 535.5 | 536.2 | n/c | n/c | n/c | n/c |
| {P,P,P,Si} | 198.2 | 207.9 | n/c | n/c | n/c | n/c |
| {P,P,Si,Si} | 331.0 | 338.7 | 7.94 | 7.99 | 1.51 | 1.48 |
| {N,N,P,Si} | 510.2 | 511.1 | 8.75 | 8.80 | n/c | n/c |
| {N,P,P,Si} | 340.6 | 344.2 | 8.59 | 8.65 | n/c | n/c |
| {N,P,Si,Si} | 451.8 | 454.1 | 8.11 | 8.15 | 1.63 | 1.62 |
| {Si,Si,Si,Si} | 638.0 | 638.8 | n/c | n/c | n/c | n/c |

110 [a] Cationic/anionic structure did not converge with a tetrahedrane geometry absent imaginary
111 frequencies.
112

113　**Table 2.** Comparison of G4MP2/G4 calculated C/N/P/Si tetrahedrane gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_f H°_g$) and
114　adiabatic ionization energies (AIEs) with prior calculations and experimental reports from the literature.
115

| compound | level of theory | $\Delta_f H°_g$ (kJ/mol) | AIE (eV) | Ref. | comments |
|---|---|---|---|---|---|
| {C,C,C,C} | BP/6-31G* | 485.3 | n/a[a] | [31] | |
| | SCF/6-31G* | 518.4 | n/a | [32] | homodesmic reaction set |
| | BLYP/6-31G* | 523.4 | n/a | [31] | |
| | MINDO/3 | 528.4 | n/a | [33] | |
| | G4MP2 | 532.4 | n/c[b] | current work | |
| | G4MP2 | 533.9 | n/a | [28] | using alternate atomization approach |
| | G2 | 535.1 | n/a | [34] | |
| | B3LYP/aug-cc-pVDZ | 535.6 | n/a | [35] | |
| | G4 | 536.5 | n/c | current work | |
| | CBS-Q | 537.2 | n/a | [36] | |
| | G4 | 537.6 | n/a | [28] | using alternate atomization approach |
| | SCF/4-31G | 541.0 | n/a | [37] | isodesmic reaction set 2 |
| | CBS-Q//B3 | 546.5 | n/c | current work | |
| | RMP2/6-31G* | 553.5 | n/a | [32] | homodesmic reaction set |
| | SCF/6-31G* | 555.2 | n/a | [38] | isodesmic reaction set 2 |
| | RMP2/6-31G* | 555.2 | n/a | [32] | isodesmic reaction set |
| | SCF/DZ+D | 560.7 | n/a | [39] | |
| | SCF/4-31G | 572.8 | n/a | [37] | isodesmic reaction set 1 |
| | SCF/6-31G* | 587.4 | n/a | [32] | isodesmic reaction set |
| | SCF/6-31G* | 591.2 | n/a | [40] | |
| | B3LYP/6-31G* | 600.0 | n/a | [31] | |
| | SVWN/6-31G* | 609.6 | n/a | [31] | |
| | SCF(MO) | 611.3 | n/a | [41] | |
| | SCF/6-31G* | 651.0 | n/a | [38] | isodesmic reaction set 1 |
| | SCF/6-31G | 661.9 | n/a | [38] | isodesmic reaction set 2 |
| | AM1 | 666.5 | n/a | [38] | |
| | SCF/4-21G | 693.7 | n/a | [38] | isodesmic reaction set 2 |
| | SCF/4-31G | 697.1 | n/a | [40] | |
| | SCF/6-31G | 705.4 | n/a | [38] | isodesmic reaction set 1 |
| | SCF/4-21G | 720.1 | n/a | [38] | isodesmic reaction set 1 |

|            | Method          | Value  |        | Ref          |                          |
| ---------- | --------------- | ------ | ------ | ------------ | ------------------------ |
|            | tight-binding MD | 771.9 | n/a    | [42]         |                          |
| {C,C,C,N}  | G4MP2           | 543.8  | n/c    | current work |                          |
|            | G4              | 546.7  | n/c    | current work |                          |
|            | SCF/6-31G*      | 595.0  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G*      | 667.3  | n/a    | [38]         | isodesmic reaction set 1 |
|            | AM1             | 705.0  | n/a    | [38]         |                          |
|            | SCF/6-31G       | 739.3  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/4-21G       | 771.1  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G       | 777.4  | n/a    | [38]         | isodesmic reaction set 1 |
|            | SCF/4-21G       | 794.5  | n/a    | [38]         | isodesmic reaction set 1 |
| {C,C,N,N}  | G4MP2           | 583.1  | n/c    | current work |                          |
|            | G4              | 585.7  | n/c    | current work |                          |
|            | SCF/6-31G*      | 662.3  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G*      | 674.9  | n/a    | [38]         | isodesmic reaction set 3 |
|            | SCF/6-31G*      | 724.3  | n/a    | [38]         | isodesmic reaction set 1 |
|            | AM1             | 772.8  | n/a    | [38]         |                          |
|            | SCF/4-21G       | 820.5  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G       | 829.3  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G       | 860.6  | n/a    | [38]         | isodesmic reaction set 3 |
|            | SCF/4-21G       | 881.6  | n/a    | [38]         | isodesmic reaction set 3 |
|            | SCF/6-31G       | 897.0  | n/a    | [38]         | isodesmic reaction set 1 |
|            | SCF/4-21G       | 907.9  | n/a    | [38]         | isodesmic reaction set 1 |
| {C,N,N,N}  | G4MP2           | 650.7  | 11.24  | current work |                          |
|            | G4              | 653.4  | 11.24  | current work |                          |
|            | SCF/6-31G*      | 781.6  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G*      | 821.3  | n/a    | [38]         | isodesmic reaction set 1 |
|            | AM1             | 867.3  | n/a    | [38]         |                          |
|            | SCF/4-21G       | 964.4  | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/6-31G       | 1002.5 | n/a    | [38]         | isodesmic reaction set 2 |
|            | SCF/4-21G       | 1061.9 | n/a    | [38]         | isodesmic reaction set 1 |
|            | SCF/6-31G       | 1072.8 | n/a    | [38]         | isodesmic reaction set 1 |
| {N,N,N,N}  | G2              | 732.6  | n/a    | [43]         |                          |
|            | G4MP2           | 746.7  | n/c    | current work |                          |
|            | CBS-Q//B3       | 747.8  | n/c    | current work |                          |

| | | | | | |
|---|---|---|---|---|---|
| | G4 | 751.0 | n/c | current work | |
| | W2 | 755.6 | n/a | [44] | |
| | W1BD | 765.0 | n/a | current work | |
| | G3 | 769.9 | n/a | [45] | |
| | SCF/6-31G* | 929.7 | n/a | [38] | isodesmic reaction set 2 |
| | SCF/6-31G* | 960.2 | n/a | [38] | isodesmic reaction set 1 |
| | AM1 | 981.6 | n/a | [38] | |
| | SCF/4-21G | 1086.6 | n/a | [38] | isodesmic reaction set 2 |
| | SCF/6-31G | 1214.2 | n/a | [38] | isodesmic reaction set 2 |
| | SCF/4-21G | 1261.9 | n/a | [38] | isodesmic reaction set 1 |
| | SCF/6-31G | 1322.1 | n/a | [38] | isodesmic reaction set 1 |
| {P,P,P,P} | CBS-Q//B3 | 48.3 | n/c | current work | |
| | G4MP2 | 48.6 | 9.16 | current work | |
| | experimental | 59.0 | 9.08 to 9.34 | [46-51] | |
| | G4 | 61.2 | 9.20 | current work | |
| {Si,Si,Si,Si} | MINDO/3 | 600.0 | n/a | [52] | |
| | CBS-Q//B3 | 635.6 | n/c | current work | |
| | G4MP2 | 638.0 | n/c | current work | |
| | G4 | 638.8 | n/c | current work | |

116    [a] Not available. [b] Stable cationic tetrahedrane geometries could not be obtained.
117

118   **Figures**
119



| Tetrahedron | Cube | Octahedron | Dodecahedron | Icosahedron |

120
121   Figure 1.
122
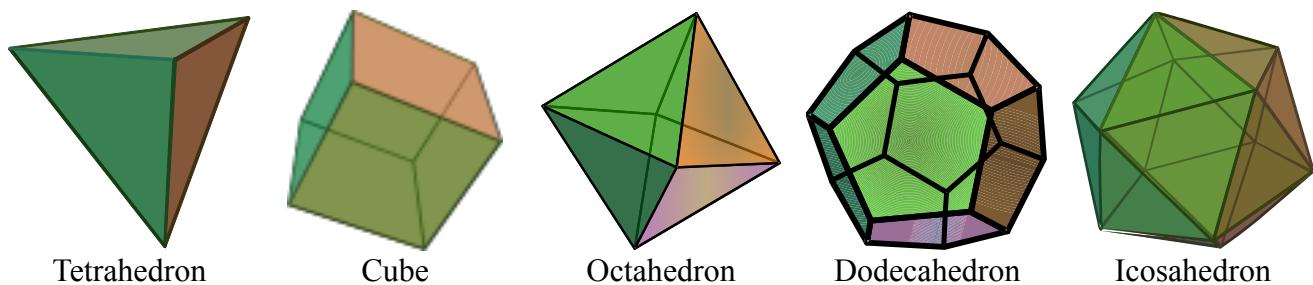
123
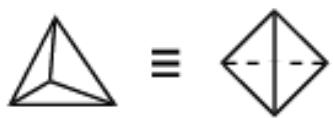


124
125
126     Figure 2.
127

128

{C,C,N,P}                    {N,Si,Si,Si}
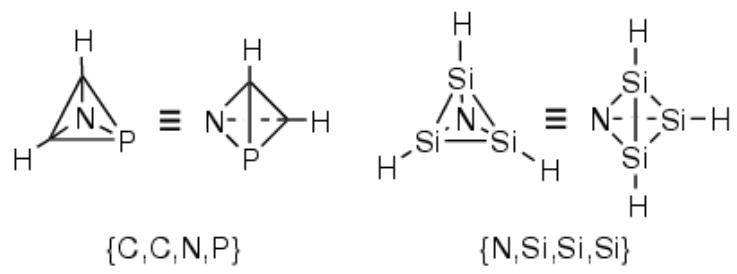
129
130
131    Figure 3.
132
133

134



{C,C,C,C}     {C,C,C,N}     {C,C,N,N}     {C,N,N,N}     {C,C,C,P}     {C,C,P,P}

{C,P,P,P}     {C,C,N,P}     {C,N,N,P}     {C,N,P,P}     {N,N,N,N}     {N,N,N,P}

{N,N,P,P}     {N,P,P,P}     {P,P,P,P}     {N,N,N,Si}     {N,N,Si,Si}     {N,Si,Si,Si}

{P,P,P,Si}     {P,P,Si,Si}     {N,N,P,Si}     {N,P,P,Si}     {N,P,Si,Si}     {Si,Si,Si,Si}

135

136    Figure 4.

137

13
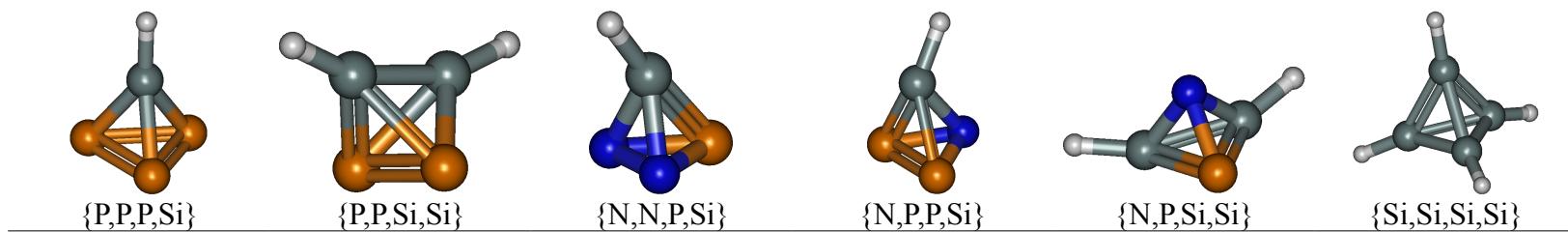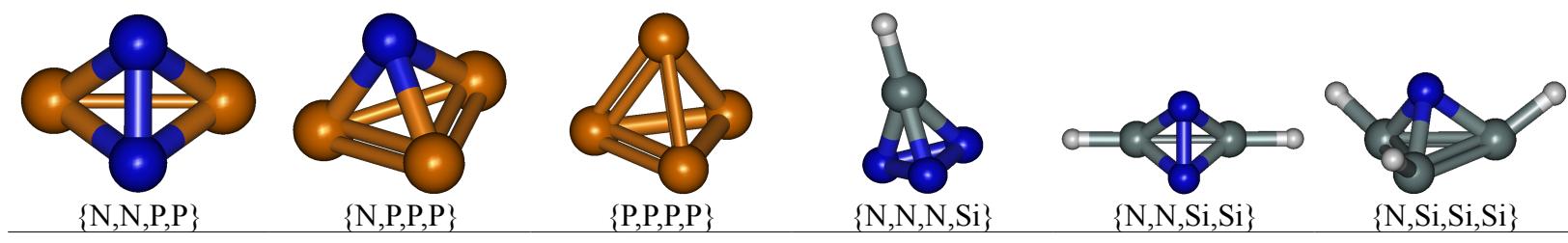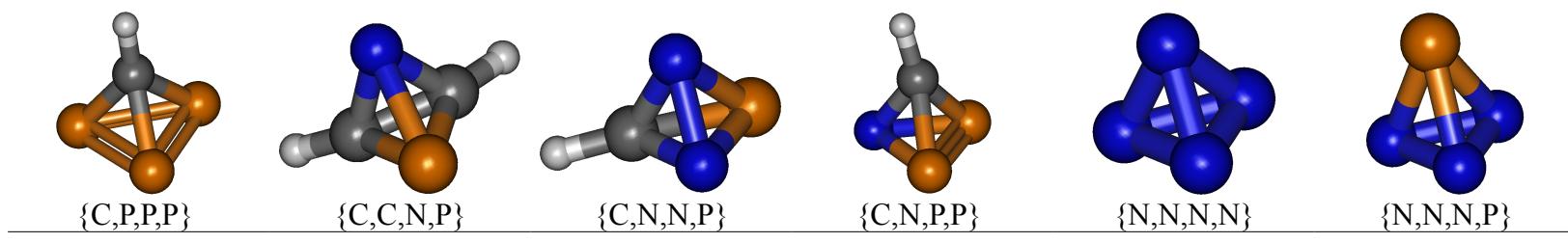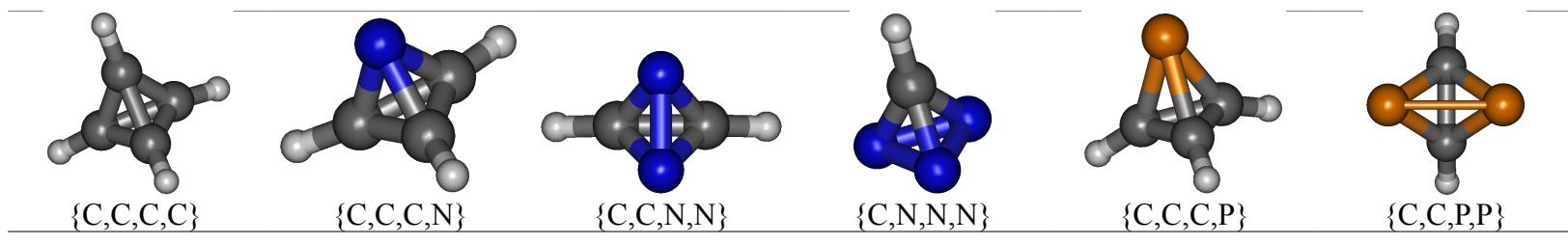
138 **References**
139
140 [1] L.A. Curtiss, P.C. Redfern, K. Raghavachari, Gaussian-4 theory using reduced order perturbation
141 theory, J. Chem. Phys. 127 (2007) 124105-124108.
142 [2] L.A. Curtiss, P.C. Redfern, K. Raghavachari, Gaussian-4 theory, J. Chem. Phys. 126 (2007) 84108-
143 84112.
144 [3] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, G. Scalmani,
145 V. Barone, B. Mennucci, G.A. Petersson, et al., Gaussian 09, Revision B.01, Gaussian, Inc.,
146 Wallingford, CT, 2009.
147 [4] T.A. Holme, M.S. Gordon, S. Yabushita, M.W. Schmidt, Theoretical studies of cyclic $C_2Si_2H_4$
148 molecules, Organometallics 3 (1984) 583-586.
149 [5] A.D. McLean, G.S. Chandler, Contracted Gaussian basis sets for molecular calculations. I. Second
150 row atoms, Z=11-18, J. Chem. Phys. 72 (1980) 5639-5648.
151 [6] K. Raghavachari, J.S. Binkley, R. Seeger, J.A. Pople, Self-consistent molecular orbital methods. 20.
152 Basis set for correlated wave-functions, J. Chem. Phys. 72 (1980) 650-654.
153 [7] Y. Zhao, D. Truhlar, The M06 suite of density functionals for main group thermochemistry,
154 thermochemical kinetics, noncovalent interactions, excited states, and transition elements: Two new
155 functionals and systematic testing of four M06-class functionals and 12 other functionals, Theor. Chem.
156 Acc. 120 (2008) 215-241.
157 [8] A.D. Becke, Density-functional thermochemistry. III. The role of exact exchange, J. Chem. Phys. 98
158 (1993) 5648-5652.
159 [9] C. Lee, W. Yang, R.G. Parr, Development of the Colle-Salvetti correlation energy formula into a
160 functional of the electron density, Phys. Rev. B 37 (1988) 785-789.
161 [10] B. Miehlich, A. Savin, H. Stoll, H. Preuss, Results obtained with the correlation energy density
162 functionals of Becke and Lee, Yang and Parr, Chem. Phys. Lett. 157 (1989) 200-206.
163 [11] M.R. Nyden, G.A. Petersson, Complete basis set correlation energies. I. The asymptotic
164 convergence of pair natural orbital expansions, J. Chem. Phys. 75 (1981) 1843-1862.
165 [12] G.A. Petersson, A. Bennett, T.G. Tensfeldt, M.A. Al-Laham, W.A. Shirley, J. Mantzaris, A
166 complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-
167 row atoms, J. Chem. Phys. 89 (1988) 2193-2218.
168 [13] G.A. Petersson, M.A. Al-Laham, A complete basis set model chemistry. II. Open-shell systems and
169 the total energies of the first-row atoms, J. Chem. Phys. 94 (1991) 6081-6090.
170 [14] G.A. Petersson, T.G. Tensfeldt, J.A. Montgomery, A complete basis set model chemistry. III. The
171 complete basis set-quadratic configuration interaction family of methods, J. Chem. Phys. 94 (1991)
172 6091-6101.
173 [15] J.A. Montgomery, J.W. Ochterski, G.A. Petersson, A complete basis set model chemistry. IV. An
174 improved atomic pair natural orbital method, J. Chem. Phys. 101 (1994) 5900-5909.
175 [16] J.W. Ochterski, G.A. Petersson, J.A. Montgomery, A complete basis set model chemistry. V.
176 Extensions to six or more heavy atoms, J. Chem. Phys. 104 (1996) 2598-2619.
177 [17] J.A. Montgomery, M.J. Frisch, J.W. Ochterski, G.A. Petersson, A complete basis set model
178 chemistry. VI. Use of density functional geometries and frequencies, J. Chem. Phys. 110 (1999) 2822-
179 2827.
180 [18] J.A. Montgomery, M.J. Frisch, J.W. Ochterski, G.A. Petersson, A complete basis set model
181 chemistry. VII. Use of the minimum population localization method, J. Chem. Phys. 112 (2000) 6532-
182 6542.
183 [19] A. Nicolaides, A. Rauk, M.N. Glukhovtsev, L. Radom, Heats of formation from G2, G2(MP2), and
184 G2(MP2,SVP) total energies, J. Phys. Chem. 100 (1996) 17460-17464.

185  [20] R. Notario, O. Castano, J.L.M. Abboud, R. Gomperts, L.M. Frutos, R. Palmeiro, Organic
186  thermochemistry at high ab initio levels. 1. A G2(MP2) and G2 study of cyclic saturated and
187  unsaturated hydrocarbons (including aromatics), J. Org. Chem. 64 (1999) 9011-9014.
188  [21] J.W. Ochterski, Thermochemistry in Gaussian, Gaussian, Inc., Wallingford, CT, 2000.
189  [22] S. Rayne, K. Forest, Performance of Gaussian-3 and Gaussian-4 level theoretical methods in
190  estimating gas phase enthalpies of formation for representative $C_1$ and $C_2$ chlorofluorocarbons and
191  hydrochlorofluorocarbons, J. Mol. Struct. (Theochem) 953 (2010) 47-48.
192  [23] S. Rayne, K. Forest, Estimated gas-phase standard state enthalpies of formation for organic
193  compounds using the Gaussian-4 (G4) and W1BD theoretical methods, J. Chem. Eng. Data 55 (2010)
194  5359-5364.
195  [24] S. Rayne, K. Forest, Thermochemistry of mono- and disubstituted acetylenes and polyynes at the
196  Gaussian-4 level of theory, Comp. Theor. Chem. 970 (2011) 15-22.
197  [25] S. Rayne, K. Forest, Reply to Comments by O. V. Dorofeeva on J. Chem. Eng. Data, 2010, 55,
198  5359-5364, J. Chem. Eng. Data 56 (2011) 684-685.
199  [26] S. Rayne, K. Forest, Computational note on a G4MP2 study into the gas phase enthalpies of
200  formation and isomerization for the $(CH)_{2n}$ (n=1-6) isomers, J. Mol. Struct. (Theochem) 948 (2010)
201  111-112.
202  [27] S. Rayne, K. Forest, Gas-phase enthalpies of formation, acidities, and strain energies of the
203  [m,n]polyprismanes (m≥2; n=3-8; m×n≤16): A CBS-Q//B3, G4MP2, and G4 theoretical study, Theor.
204  Chem. Acc. 127 (2010) 697-709.
205  [28] S. Rayne, K. Forest, A G4MP2 and G4 theoretical study into the thermochemical properties of
206  explosophore substituted tetrahedranes and cubanes, Propell. Explos. Pyrot. (2011) in press.
207  [29] S. Rayne, K. Forest, Estimated adiabatic ionization energies for organic compounds using the
208  Gaussian-4 (G4) and W1BD theoretical methods, J. Chem. Eng. Data 56 (2011) 350-355.
209  [30] E.C. Barnes, G.A. Petersson, J.A. Montgomery, M.J. Frisch, J.M.L. Martin, Unrestricted coupled
210  cluster and Brueckner doubles variations of W1 theory, J. Chem. Theory Comput. 5 (2009) 2687-2693.
211  [31] D.W. Ball, On the $\Delta H_f$ values of tetrahedrane and cubane: Density functional theory calculations,
212  J. Mol. Struct. (Theochem) 364 (1996) 183-188.
213  [32] R.L. Disch, J.M. Schulman, M.L. Sabio, Ab initio heats of formation of medium-sized
214  hydrocarbons. 2. Use of second-order correlation energies, J. Am. Chem. Soc. 107 (1985) 1904-1906.
215  [33] H. Kollmar, F. Carrion, M.J.S. Dewar, R.C. Bingham, Ground states of molecules. 58. The $C_4H_4$
216  potential surface, J. Am. Chem. Soc. 103 (1981) 5292-5303.
217  [34] M.N. Glukhovtsev, S. Laiter, A. Pross, Thermochemistry of cyclobutadiene and tetrahedrane: A
218  high-level computational study, J. Phys. Chem. 99 (1995) 6828-6831.
219  [35] G. Zhou, J.L. Zhang, N.B. Wong, A. Tian, Computational studies on a kind of novel energetic
220  materials tetrahedrane and nitro derivatives, J. Mol. Struct. (Theochem) 668 (2004) 189-195.
221  [36] B.S. Jursic, Computing the heat of formation for cubane and tetrahedrane with density functional
222  theory and complete basis set ab initio methods, J. Mol. Struct. (Theochem) 499 (2000) 137-140.
223  [37] J.M. Schulman, T.J. Venanzi, Theoretical study of the tetrahedrane molecule, J. Am. Chem. Soc.
224  96 (1974) 4739-4746.
225  [38] I. Alkorta, J. Elguero, I. Rozas, A.T. Balaban, Theoretical studies on aza-analogs of Platonic
226  hydrocarbons: Part II. Tetrahedrane and its azaderivatives, J. Mol. Struct. (Theochem) 208 (1990) 63-
227  77.
228  [39] H. Kollmar, An MO theoretical study on the stability of tetrahedrane, J. Am. Chem. Soc. 102
229  (1980) 2617-2621.
230  [40] W.J. Hehre, J.A. Pople, Molecular orbital theory of the electronic structure of organic compounds.
231  XXVI. Geometries, energies and polarities of $C_4$ hydrocarbons, J. Am. Chem. Soc. 97 (1975) 6941-

232   6955.

233   [41] N.C. Baird, M.J.S. Dewar, Ground states of o-bonded molecules. II. Strain energies of
234   cyclopropanes and cyclopropenes, J. Am. Chem. Soc. 89 (1967) 3966-3970.

235   [42] M.M. Maslov, K.P. Katin, On the thermal stability of tetrahedrane: Tight-binding molecular
236   dynamics study, Chem. Phys. 387 (2011) 66-68.

237   [43] M.N. Glukhovtsev, S. Laiter, Thermochemistry of tetrazete and tetraazatetrahedrane: A high-level
238   computational study, J. Phys. Chem. 100 (1996) 1569-1577.

239   [44] T.J. Lee, J.M.L. Martin, An accurate quartic force field, fundamental frequencies, and binding
240   energy for the high energy density material $TdN_4$, Chem. Phys. Lett. 357 (2002) 319-325.

241   [45] M.T. Nguyen, T.L. Nguyen, A.M. Mebel, R. Flammang, Azido-nitrene is probably the $N_4$ molecule
242   observed in mass spectrometric experiments, J. Phys. Chem. A  107 (2003) 5452-5460.

243   [46] J.D. Cox, D.D. Wagman, V.A. Medvedev, CODATA Key Values for Thermodynamics,
244   Hemisphere, New York, NY, 1984.

245   [47] M.W. Chase, NIST-JANAF themochemical tables (4th ed.), J. Phys. Chem. Ref. Data 9 (1998) 1-
246   1951.

247   [48] R.R. Hart, M.B. Robin, N.A. Kuebler, 3p orbitals, bent bonds, and the electronic spectrum of the
248   $P_2$ molecule, J. Chem. Phys. 42 (1965) 3631-3638.

249   [49] C.R. Brundle, N.A. Kuebler, M.B. Robin, H. Basch, Ionization potentials of the tetraphosphorus
250   molecule, Inorg. Chem. 11 (1972) 20-25.

251   [50] S. Evans, P.J. Joachim, A.F. Orchard, D.W. Turner, A study of the orbital electronic structure of the
252   $P_4$ molecule by photoelectron spectroscopy, Int. J. Mass Spectrom. Ion Phys. 9 (1972) 41-49.

253   [51] J. Smets, P. Coppens, J. Drowart, Photoionization with mass spectrometric analysis of the
254   tetraphosphorus molecule, Chem. Phys. 20 (1977) 243-251.

255   [52] M.J.S. Dewar, D.H. Lo, C.A. Ramsden, Ground states of molecules. XXIX. MINDO/3
256   calculations of compounds containing third row elements, J. Am. Chem. Soc. 97 (1975) 1311-1318.

257

Supplementary Material

**Theoretical studies in the molecular Platonic solids: Pure and mixed carbon, nitrogen, phosphorus, and silicon tetrahedranes**

Sierra Rayne [a,*] and Kaya Forest [b,c]

[a] Ecologica Research, PO Box 74, 318 Rose Street, Mortlach, Saskatchewan, Canada, S0H 3E0
[b] Department of Chemistry, Okanagan College, 583 Duncan Avenue West, Penticton, British Columbia, Canada, V2A 8E1
[c] Department of Environmental Engineering, Saskatchewan Institute of Applied Science and Technology, Palliser Campus, PO Box 1420, 600 6th Avenue NW, Moose Jaw, Saskatchewan, Canada, S6H 4R4

[*] Corresponding author. Tel.: +1 306 690 0573. E-mail address: rayne.sierra@gmail.com (S. Rayne).

**G4MP2 archive entries for neutral singlet tetrahedranes**

**{C,C,C,C}**
\\0,1\C,0,-5.0005344619,0.1205928132,-0.4952
170489\C,0,-3.9804743098,1.1689905043,-0.2928088981\C,0,-3.7767984306,
0.1294760058,-1.3217095374\C,0,-4.8068877084,1.1694152257,-1.516581712
8\H,0,-5.7209981089,-0.5019178161,-0.0089835144\H,0,-3.4949266825,1.78
60453485,0.4327958945\H,0,-5.2984152574,1.7869282065,-2.2377640422\H,0
,-3.0503350405,-0.4825602878,-1.8123111406\\Version=EM64L-G09RevA.02\S
tate=1-A\MP2/GTBas1=-154.1076814\CCSD(T)/GTBas1=-154.1562088\MP2/GTBas
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-153.6503097\MP2/GTMP2LargeXP=-154.
2933051\HF/GFHFB3=-153.6501563\HF/GFHFB4=-153.661683\G4MP2=-154.391776
2\FreqCoord=-9.449640651,0.2278873905,-0.9358245988,-7.5220063246,2.20
90719051,-0.5533286267,-7.137114693,0.2446741917,-2.497669053,-9.08370
13204,2.2098745122,-2.8659240953,-10.8111196325,-0.9484872137,-0.01697
63819,-6.6044542845,3.3751365697,0.817865712,-10.0125537749,3.37680492
93,-4.2287611898,-5.76429784,-0.9119067866,-3.4247717234\PG=C01 [X(C4H
4)]\NImag=0\\

**{C,C,C,N}**
\\0,1\N,0,-3.1660029157,0.0760818851,-0.3989702709\C
,0,-2.3591002689,1.3233335015,-0.3018283529\C,0,-1.6932248824,0.047085
9563,-0.1861078748\C,0,-2.2091992813,0.4788416168,-1.4640526466\H,0,-2
.5621492371,2.2907502201,0.1081332401\H,0,-1.0489254145,-0.6016286804,
0.3700113352\H,0,-2.2138980001,0.3796555007,-2.5295854301\\Version=EM6
4L-G09RevA.02\State=1-A\MP2/GTBas1=-170.15366\CCSD(T)/GTBas1=-170.1961
669\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-169.6610992\MP2/GTMP2
LargeXP=-170.3461761\HF/GFHFB3=-169.661231\HF/GFHFB4=-169.6732698\G4MP
2=-170.4502337\FreqCoord=-5.9828784466,0.1437739265,-0.7539445472,-4.4
580534282,2.5007379003,-0.5703729261,-3.1997313091,0.0889795621,-0.351
6929146,-4.1747816147,0.9048795167,-2.7666585462,-4.8417603697,4.32889
05549,0.2043422097,-1.9821817673,-1.1369134397,0.6992200896,-4.1836609
063,0.7174449211,-4.7802236927\PG=C01 [X(C3H3N1)]\NImag=0\\

**{C,C,N,N}**
\\0,1\N,0,-3.1852379407,-0.1086445812,-0.4858913076\
N,0,-2.5861095844,1.2731114036,-0.3027076459\C,0,-1.7681765811,0.07085
46722,-0.1906492754\C,0,-2.2463289604,0.4453874799,-1.4546133263\H,0,-
1.0487586447,-0.3326616133,0.4925165371\H,0,-2.1867382886,0.5614926389
,-2.5176549819\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-186.186
7\CCSD(T)/GTBas1=-186.2236068\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Larg
eXP=-185.6563514\MP2/GTMP2LargeXP=-186.3870642\HF/GFHFB3=-185.6569898\
HF/GFHFB4=-185.6695394\G4MP2=-186.498147\FreqCoord=-6.0192273761,-0.20
53085044,-0.9182015017,-4.8870388642,2.4058318894,-0.5720345492,-3.341
369493,0.1338959257,-0.3602749179,-4.2449465395,0.84166036,-2.74882081
59,-1.981866618,-0.628639344,0.9307213711,-4.1323364897,1.0610673131,-
4.7576784129\PG=C01 [X(C2H2N2)]\NImag=0\\

**{C,N,N,N}**
\\0,1\N,0,-2.9780069549,-0.2201839059,-0.4386589341\
N,0,-2.6599332563,1.2342736821,-0.3040911673\N,0,-1.5587647262,0.22338
0492,-0.2888253719\C,0,-2.3070684462,0.4950938331,-1.4583296728\H,0,-2
.2190066165,0.5732358988,-2.5236548539\\Version=EM64L-G09RevA.02\State
=1-A\MP2/GTBas1=-202.2094057\CCSD(T)/GTBas1=-202.2402606\MP2/GTBas2=0.
\MP2/GTBas3=0.\HF/GTMP2LargeXP=-201.63567\MP2/GTMP2LargeXP=-202.417070
8\HF/GFHFB3=-201.6372508\HF/GFHFB4=-201.6503402\G4MP2=-202.535297\Freq
Coord=-5.6276175666,-0.4160872811,-0.8289452513,-5.0265453862,2.332439

2322,-0.5746490256,-2.945638438,0.4221279532,-0.5458008531,-4.35972753
31,0.9355917546,-2.7558436931,-4.1933147922,1.0832588583,-4.7690165278
\PG=C01 [X(C1H1N3)]\NImag=0\\

**{C,C,C,P}**
\\0,1\C,0,-2.9906188303,-0.1690351501,-0.3126064916\
P,0,-2.8208642819,1.648573017,-0.0060642461\C,0,-1.6011569371,0.265427
3008,-0.1662581957\C,0,-2.3273393472,0.5416683501,-1.4058686999\H,0,-2
.2010871111,0.4963727143,-2.4698307814\H,0,-0.6507273229,-0.0953721091
,0.1751712777\H,0,-3.6158361695,-1.022494123,-0.1371428631\\Version=EM
64L-G09RevA.02\State=1-A\MP2/GTBas1=-456.418893\CCSD(T)/GTBas1=-456.46
78104\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-455.9919668\MP2/GTM
P2LargeXP=-456.6272723\HF/GFHFB3=-455.9965839\HF/GFHFB4=-456.0079833\G
4MP2=-456.7441835\FreqCoord=-5.6514505571,-0.3194301405,-0.5907406565,
-5.3306609508,3.1153515122,-0.0114597643,-3.025748107,0.5015849068,-0.
3141824572,-4.3980339846,1.0236048365,-2.6567068215,-4.1594518346,0.93
80084898,-4.6673037714,-1.2296964274,-0.1802271669,0.3310257412,-6.832
9401017,-1.9322338649,-0.2591624523\PG=C01 [X(C3H3P1)]\NImag=0\\

**{C,C,P,P}**
\\0,1\P,0,-3.2353089328,-0.2748628248,-0.0379006887\
C,0,-2.8022791785,1.4757258991,-0.3848452238\P,0,-1.1974756635,0.61266
50726,-0.1537612788\C,0,-2.470131347,0.5724411356,-1.4766527908\H,0,-2
.5320568969,0.5693337158,-2.5498105671\H,0,-3.2232179813,2.4578870016,
-0.2683694508\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-758.7252
377\CCSD(T)/GTBas1=-758.7753774\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
rgeXP=-758.334237\MP2/GTMP2LargeXP=-758.9590328\HF/GFHFB3=-758.3440612
\HF/GFHFB4=-758.355247\G4MP2=-759.0955203\FreqCoord=-6.1138478383,-0.5
19415463,-0.071621922,-5.2955401952,2.7887177966,-0.7272520765,-2.2629
010547,1.1577691984,-0.2905667067,-4.6678717581,1.0817569735,-2.790469
368,-4.784894088,1.0758848011,-4.8184436625,-6.0909992513,4.6447332986
,-0.5071447645\PG=C01 [X(C2H2P2)]\NImag=0\\

**{C,P,P,P}**
\\0,1\P,0,-3.1180632671,-0.4429272777,-0.0935042641\
P,0,-2.8124333282,1.7444160123,-0.2107219518\P,0,-1.0712149079,0.38133
49214,-0.2439134895\C,0,-2.4058858128,0.500846062,-1.4909170843\H,0,-2
.464882691,0.4516302875,-2.5647332102\\Version=EM64L-G09RevA.02\State=
1-A\MP2/GTBas1=-1061.0292576\CCSD(T)/GTBas1=-1061.081391\MP2/GTBas2=0.
\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1060.6808672\MP2/GTMP2LargeXP=-1061.29
26444\HF/GFHFB3=-1060.6961438\HF/GFHFB4=-1060.7069321\G4MP2=-1061.4492
66\FreqCoord=-5.8922856399,-0.8370112516,-0.1766974513,-5.3147287574,3
.2964685251,-0.398206779,-2.0243028055,0.7206185663,-0.4609296952,-4.5
464652932,0.946461892,-2.8174249762,-4.6579532356,0.8534575567,-4.8466
433713\PG=C01 [X(C1H1P3)]\NImag=0\\

**{C,C,N,P}**
\\0,1\C,0,-3.7634746815,-0.2589692749,-0.550759964
5\C,0,-3.0469788961,0.9512365603,-0.8222944871\N,0,-2.2893020172,-0.28
15307993,-0.5393906868\P,0,-3.0501362308,-0.206366989,-2.2120004686\H,
0,-4.4675801986,-0.705778276,0.1253917912\H,0,-2.8928279759,1.95407877
89,-0.4713961843\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-472.4
583275\CCSD(T)/GTBas1=-472.5011489\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
2LargeXP=-471.9960721\MP2/GTMP2LargeXP=-472.6757621\HF/GFHFB3=-472.001
1482\HF/GFHFB4=-472.0132171\G4MP2=-472.7989453\FreqCoord=-7.111936456,
-0.4893810065,-1.0407854979,-5.7579556464,1.7975765866,-1.5539113812,-
4.326153848,-0.5320161087,-1.0193006766,-5.7639221441,-0.3899770921,-4

.1800750914,-8.4425030521,-1.3337276521,0.2369561448,-5.4666526239,3.6
926737343,-0.8908096884\PG=C01 [X(C2H2N1P1)]\NImag=0\\

**{C,N,N,P}**
\\0,1\C,0,-3.8103239496,-0.2303405234,-0.547479913
3\N,0,-3.1855798036,1.0346497707,-0.8515105182\P,0,-2.0581174381,-0.36
22643985,-0.6049056776\N,0,-3.3005654569,-0.051870761,-1.8862825147\H,
0,-4.7883833518,-0.4803340878,-0.1776013762\\Version=EM64L-G09RevA.02\
State=1-A\MP2/GTBas1=-488.4875939\CCSD(T)/GTBas1=-488.5242589\MP2/GTBa
s2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-487.9853597\MP2/GTMP2LargeXP=-488
.7140162\HF/GFHFB3=-487.991417\HF/GFHFB4=-488.0041318\G4MP2=-488.84431
95\FreqCoord=-7.2004687424,-0.4352805064,-1.0345870993,-6.0198734032,1
.95520471,-1.6091216787,-3.8892783074,-0.6845805009,-1.143106067,-6.23
71647972,-0.0980215326,-3.564557362,-9.0487331541,-0.9076998782,-0.335
6179618\PG=C01 [X(C1H1N2P1)]\NImag=0\\

**{C,N,P,P}**
\\0,1\C,0,-3.8571389103,-0.2579769375,-0.575210336
1\N,0,-3.2044616003,1.037496599,-0.7728993681\P,0,-2.0701680371,-0.360
9295373,-0.4441288426\P,0,-3.2541133399,-0.0375499872,-2.2509976104\H,
0,-4.7570881124,-0.4712001371,-0.0245438428\\Version=EM64L-G09RevA.02\
State=1-A\MP2/GTBas1=-774.7613032\CCSD(T)/GTBas1=-774.8049569\MP2/GTBa
s2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-774.3343299\MP2/GTMP2LargeXP=-775
.0054822\HF/GFHFB3=-774.345085\HF/GFHFB4=-774.3570611\G4MP2=-775.14869
18\FreqCoord=-7.2889361969,-0.4875057604,-1.086990004,-6.0555548278,1.
9605844359,-1.460568134,-3.9120506392,-0.6820579787,-0.8392818803,-6.1
493830179,-0.0709591921,-4.2537690094,-8.9895937225,-0.8904392129,-0.0
463811412\PG=C01 [X(C1H1N1P2)]\NImag=0\\

**{N,N,N,N}**
\\0,1\N,0,-5.1718054384,0.3932767075,-0.569228
0885\N,0,-3.8531628707,0.9028348403,-0.2484104784\N,0,-4.0215933611,-0
.0359974768,-1.3400409621\N,0,-4.5147383298,1.321105929,-1.468550471\\
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-218.2206439\CCSD(T)/GTB
as1=-218.2443231\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-217.5990
55\MP2/GTMP2LargeXP=-218.4361431\HF/GFHFB3=-217.6021086\HF/GFHFB4=-217
.6159468\G4MP2=-218.5616731\FreqCoord=-9.7732958912,0.7431852716,-1.07
56851943,-7.281422571,1.7061105914,-0.4694277727,-7.5997100704,-0.0680
253726,-2.5323104252,-8.5316190049,2.4965283983,-2.7751582025\PG=C01 [
X(N4)]\NImag=0\\

**{N,N,N,P}**
\\0,1\N,0,-3.8110489228,-0.4175315525,-0.5981983722\N,
0,-3.2894315128,0.9485082601,-0.794627295\P,0,-2.0441387804,-0.2992700
509,-0.6244785401\N,0,-3.2407807841,-0.0259366567,-1.9013157928\\Versi
on=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-504.5045937\CCSD(T)/GTBas1=-
504.5346154\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-503.9566481\M
P2/GTMP2LargeXP=-504.7396562\HF/GFHFB3=-503.9642692\HF/GFHFB4=-503.977
7037\G4MP2=-504.8778241\FreqCoord=-7.2018387431,-0.7890202861,-1.13043
10965,-6.216124692,1.7924208464,-1.5016279652,-3.8628624726,-0.5655384
36,-1.1800934166,-6.1241881386,-0.0490131779,-3.5929661404\PG=C01 [X(N
3P1)]\NImag=0\\

**{N,N,P,P}**
\\0,1\N,0,-3.8017359793,-0.4166478744,-0.5060111225\N,
0,-3.2743455693,0.9645068166,-0.704613588\P,0,-2.0101577497,-0.2968458
521,-0.5173875208\P,0,-3.2991607036,-0.0452430952,-2.190607768\\Versio

n=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-790.7880175\CCSD(T)/GTBas1=-7
90.8247004\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-790.3201517\MP
2/GTMP2LargeXP=-791.0426056\HF/GFHFB3=-790.3325676\HF/GFHFB4=-790.3453
819\G4MP2=-791.1932152\FreqCoord=-7.1842398304,-0.7873503765,-0.956222
4418,-6.1876163904,1.8226537366,-1.3315267108,-3.7986476309,-0.5609573
641,-0.9777207189,-6.2345101982,-0.0854970594,-4.139648746\PG=C01 [X(N
2P2)]\NImag=0\\

**{N,P,P,P}**
\\0,1\P,0,-4.046626524,-0.5639672283,-0.355276768\N,0,
-3.2152570845,1.0106580057,-0.7433442007\P,0,-1.9136032741,-0.25161657
82,-0.5531432277\P,0,-3.2099131174,0.0106958008,-2.2668558037\\Version
=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1077.0655107\CCSD(T)/GTBas1=-1
077.1107711\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1076.6801459\
MP2/GTMP2LargeXP=-1077.3389782\HF/GFHFB3=-1076.6969113\HF/GFHFB4=-1076
.7086343\G4MP2=-1077.5027431\FreqCoord=-7.6470158925,-1.0657436094,-0.
6713757928,-6.0759553364,1.9098668447,-1.4047169617,-3.616186115,-0.47
54864233,-1.0452892126,-6.0658567023,0.0202121344,-4.2837366517\PG=C01
 [X(N1P3)]\NImag=0\\

**{P,P,P,P}**
\\0,1\P,0,-5.4617911768,0.0964442504,-0.286729
1491\P,0,-3.5592092276,1.1810249217,0.0184745095\P,0,-3.7329944198,-0.
3115183481,-1.6036361937\P,0,-4.8073151758,1.615269176,-1.7543291666\\
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1363.3346931\CCSD(T)/GT
Bas1=-1363.3892759\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1363.0
335513\MP2/GTMP2LargeXP=-1363.6307366\HF/GFHFB3=-1363.0545142\HF/GFHFB
4=-1363.0646994\G4MP2=-1363.8075489\FreqCoord=-10.3212895191,0.1822532
203,-0.5418395662,-6.7259306898,2.2318136581,0.0349117634,-7.054337109
1,-0.5886843632,-3.0304332229,-9.0845091168,3.0524163735,-3.3152016718
\PG=C01 [X(P4)]\NImag=0\\

**{N,N,N,Si}**
\\0,1\N,0,-3.8238329346,-0.4426861498,-0.5766419771
\N,0,-3.2805124824,0.9801595084,-0.7812400906\Si,0,-2.0871162203,-0.28
48544046,-0.6383422904\N,0,-3.229176748,-0.0350319909,-1.9337638714\H,
0,-0.7750016148,-0.7221469631,-0.1952717704\\Version=EM64L-G09RevA.02\
State=1-A\MP2/GTBas1=-453.1873797\CCSD(T)/GTBas1=-453.2225718\MP2/GTBa
s2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-452.6757116\MP2/GTMP2LargeXP=-453
.4238482\HF/GFHFB3=-452.6811093\HF/GFHFB4=-452.6945899\G4MP2=-453.5583
203\FreqCoord=-7.2259970242,-0.8365555859,-1.0896954134,-6.1992701672,
1.8522330375,-1.4763298153,-3.9440780638,-0.5382968125,-1.206292108,-6
.1022596884,-0.0662008686,-3.6542841227,-1.4645408045,-1.364659988,-0.
3690101676\PG=C01 [X(H1N3Si1)]\NImag=0\\

**{N,N,Si,Si}**
\\0,1\N,0,-3.6373923576,-0.5562157704,-0.6000548392
\N,0,-3.0685677155,0.9334591495,-0.8142649874\Si,0,-1.8532165054,-0.37
45931118,-0.6413559838\Si,0,-3.1646612139,-0.1087831456,-2.275323994\H
,0,-0.8558994312,-0.6034644442,0.4153334914\H,0,-4.0034929286,0.039036
924,-3.4748136298\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-688.
2029495\CCSD(T)/GTBas1=-688.2467856\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM
P2LargeXP=-687.8024197\MP2/GTMP2LargeXP=-688.4559308\HF/GFHFB3=-687.81
10667\HF/GFHFB4=-687.8243534\G4MP2=-688.5962786\FreqCoord=-6.873675393
7,-1.0510954768,-1.1339393107,-5.7987526025,1.7639821487,-1.5387378257
,-3.5020716602,-0.7078783926,-1.2119871632,-5.9803429976,-0.2055703531
,-4.2997392122,-1.6174155223,-1.1403825304,0.7848665526,-7.5655052099,

0.0737690954,-6.5664461231\PG=C01 [X(H2N2Si2)]\NImag=0\\

**{N,Si,Si,Si}**
\\0,1\Si,0,-4.0496286088,-1.0459564848,-0.428426898
7\N,0,-3.1427838166,0.4734759047,-0.8727235323\Si,0,-1.7896967934,-0.7
2943986,-0.642628868\Si,0,-3.1639038269,-0.4385177337,-2.4542645189\H,
0,-0.6897654573,-0.009028291,0.0551304018\H,0,-3.4045125609,0.56737658
74,-3.5247907109\H,0,-5.157288936,-0.6371701225,0.4777341269\\Version=
EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-923.210731\CCSD(T)/GTBas1=-923.
2655452\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-922.8946512\MP2/G
TMP2LargeXP=-923.4624787\HF/GFHFB3=-922.9065176\HF/GFHFB4=-922.9187493
\G4MP2=-923.6113985\FreqCoord=-7.6526890104,-1.9765713033,-0.809609506
6,-5.9390007083,0.8947397903,-1.6492084657,-3.3820368004,-1.3784415658
,-1.2143925655,-5.9789117437,-0.8286784212,-4.6378877983,-1.3034678103
,-0.0170609974,0.1041813611,-6.4335963562,1.0721863644,-6.6608891194,-
9.7458636772,-1.2040770316,0.9027866642\PG=C01 [X(H3N1Si3)]\NImag=0\\

**{P,P,P,Si}**
\\0,1\P,0,-0.5964201736,-0.5399950024,1.14247899\P,
0,-0.5964442694,-0.5400281989,-1.1424522548\P,0,-0.1509293118,1.388331
5789,-0.0000183602\Si,0,1.2543529273,-0.2903866604,-0.0000091043\H,0,2
.6830408276,-0.6215217172,-0.0000192708\\Version=EM64L-G09RevA.02\Stat
e=1-A\MP2/GTBas1=-1312.0387659\CCSD(T)/GTBas1=-1312.0971302\MP2/GTBas2
=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1311.7602946\MP2/GTMP2LargeXP=-1312
.3232299\HF/GFHFB3=-1311.7797154\HF/GFHFB4=-1311.7899313\G4MP2=-1312.4
952685\FreqCoord=-1.1270707883,-1.0204426677,2.1589724037,-1.127116322
7,-1.0205054,-2.1589218815,-0.2852150648,2.6235664658,-0.0000346957,2.
3703835065,-0.5487512608,-0.0000172045,5.0702123675,-1.1745058312,-0.0
000364165\PG=C01 [X(H1P3Si1)]\NImag=0\\

**{P,P,Si,Si}**
\\0,1\Si,0,1.084860211,-0.7602469679,-0.2061814183\
P,0,-0.0013590325,0.4875719366,1.3380547633\P,0,0.0000755672,1.1015986
86,-0.9005196791\Si,0,-1.0835819809,-0.761382803,-0.2085047079\H,0,-2.
4610695337,-1.2598322092,-0.34629464\H,0,2.4631247689,-1.2566786425,-0
.3434443181\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1260.74818
79\CCSD(T)/GTBas1=-1260.8093466\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
rgeXP=-1260.4913523\MP2/GTMP2LargeXP=-1261.0227115\HF/GFHFB3=-1260.509
4579\HF/GFHFB4=-1260.5197163\G4MP2=-1261.1894906\FreqCoord=2.050088691
2,-1.4366585627,-0.3896264143,-0.0025681993,0.9213774303,2.5285570535,
0.0001428013,2.081719825,-1.7017355708,-2.0476731864,-1.43880498,-0.39
40167953,-4.6507474127,-2.3807378489,-0.6544020309,4.6546312444,-2.374
7784714,-0.6490157031\PG=C01 [X(H2P2Si2)]\NImag=0\\

**{N,N,P,Si}**
\\0,1\N,0,-3.7111163769,-0.4587613907,-0.46438217
02\N,0,-3.1748939003,0.945536687,-0.6663159514\Si,0,-1.9635349012,-0.3
59519971,-0.8294780596\P,0,-3.5133824628,0.0330663591,-2.2148624582\H,
0,-0.8327123588,-0.6648816844,0.0497786394\\Version=EM64L-G09RevA.02\S
tate=1-A\MP2/GTBas1=-739.4866263\CCSD(T)/GTBas1=-739.528689\MP2/GTBas2
=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-739.0514468\MP2/GTMP2LargeXP=-739.7
389132\HF/GFHFB3=-739.0619301\HF/GFHFB4=-739.0749685\G4MP2=-739.886487
7\FreqCoord=-7.0129935996,-0.8669333887,-0.8775551227,-5.9996799726,1.
7868053871,-1.2591546661,-3.7105432157,-0.6793942845,-1.5674863659,-6.
6393306547,0.0624863629,-4.1854834679,-1.5735983056,-1.2564442944,0.09
40679957\PG=C01 [X(H1N2P1Si1)]\NImag=0\\

**{N,P,P,Si}**
\\0,1\P,0,0.6070451407,1.1468533719,-0.1753232399
\N,0,0.0725506781,0.0010616569,1.1285038498\Si,0,-1.2038607002,-0.0245
784661,-0.2138454029\P,0,0.6529523503,-1.1217600942,-0.1756003448\H,0,
-2.6070974689,-0.0517564685,0.2253751378\\Version=EM64L-G09RevA.02\Sta
te=1-A\MP2/GTBas1=-1025.7716994\CCSD(T)/GTBas1=-1025.8210164\MP2/GTBas
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1025.4097301\MP2/GTMP2LargeXP=-102
6.0365588\HF/GFHFB3=-1025.4247003\HF/GFHFB4=-1025.4366421\G4MP2=-1026.
1960239\FreqCoord=1.1471490662,2.1672387875,-0.3313129082,0.1371009123
,0.0020062408,2.1325632161,-2.2749670255,-0.0464465697,-0.4041092462,1
.2339011199,-2.1198193649,-0.3318365605,-4.9267002179,-0.097805551,0.4
258972876\PG=C01 [X(H1N1P2Si1)]\NImag=0\\

**{N,P,Si,Si}**
\\0,1\P,0,-0.036941887,1.3231793911,-0.1714377811
\N,0,0.0010276117,0.0043285898,1.1352368828\Si,0,-1.0575391686,-0.6608
524239,-0.1944411847\Si,0,1.0938588905,-0.5996029978,-0.1941798971\H,0
,-2.3844190337,-1.2168389214,0.1259174888\H,0,2.4496135871,-1.08353363
77,0.1219744914\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-974.48
52148\CCSD(T)/GTBas1=-974.5374182\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2
LargeXP=-974.1520927\MP2/GTMP2LargeXP=-974.7445132\HF/GFHFB3=-974.1654
746\HF/GFHFB4=-974.1775518\G4MP2=-974.8982908\FreqCoord=-0.0698100493,
2.5004466738,-0.3239704551,0.0019419047,0.0081798493,2.1452868044,-1.9
984594034,-1.2488300955,-0.3674405881,2.067093731,-1.1330854543,-0.366
9468261,-4.5058989597,-2.2994923093,0.2379495691,4.629098811,-2.047581
831,0.2304983839\PG=C01 [X(H2N1P1Si2)]\NImag=0\\

**{Si,Si,Si,Si}**
\\0,1\Si,0,-0.4778,1.17664,-0.63336\Si,0,-0.17837,-1.
10971,-0.86627\Si,0,1.37948,0.15027,0.29823\Si,0,-0.72326,-0.21724,1.2
0144\H,0,2.81227,0.30621,0.60913\H,0,-0.36409,-2.26103,-1.76811\H,0,-1
.47363,-0.44276,2.4502\H,0,-0.97532,2.3982,-1.29174\\Version=EM64L-G09
RevA.02\State=1-A\MP2/GTBas1=-1158.1483954\CCSD(T)/GTBas1=-1158.217880
2\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1157.9330784\MP2/GTMP2L
argeXP=-1158.4021808\HF/GFHFB3=-1157.9484746\HF/GFHFB4=-1157.9588193\G
4MP2=-1158.5629058\FreqCoord=-0.9029111463,2.223527357,-1.1968769435,-
0.3370704503,-2.0970479869,-1.6370130571,2.6068394058,0.283969146,0.56
35730246,-1.3667633229,-0.4105241051,2.2703925651,5.3144201117,0.57865
30392,1.1510888793,-0.6880303877,-4.2727274782,-3.3412436728,-2.784757
1212,-0.8366951426,4.6302069708,-1.8430876919,4.5319412119,-2.44103483
49\PG=C01 [X(H4Si4)]\NImag=0\\

**G4 archive entries for neutral singlet tetrahedranes**

**{C,C,C,C}**
\\0,1\C,0,-5.0006717441,0.1202784191,-0.4958094221\C,0,-3.98021
01366,1.1692355172,-0.2931641893\C,0,-3.7765904466,0.1293052963,-1.321
1683098\C,0,-4.8072334247,1.169662657,-1.5161702623\H,0,-5.7205744311,
-0.5012203634,-0.0073954722\H,0,-3.495847312,1.785356412,0.4340620402\
H,0,-5.2974344555,1.7862517793,-2.2390692918\H,0,-3.0508080495,-0.4818
997175,-1.8138650929\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1
54.1076814\MP4/GTBas1=-154.1557168\CCSD(T)/G3Bas1=-154.1562099\MP2/GTB
as2=-154.117593\MP4/GTBas2=-154.1653314\MP2/GTBas3=-154.2326793\MP4/GT
Bas3=-154.2854519\HF/GTLargeXP=-153.6507085\MP2/GTLargeXP=-154.4700503
\HF/GFHFB1=-153.6616791\HF/GFHFB2=-153.6639952\G4=-154.5473859\FreqCoo
rd=-9.4499000767,0.2272932717,-0.9369440218,-7.5215071095,2.2095349123
,-0.5540000297,-7.1367216601,0.2443515976,-2.4966462809,-9.0843546295,
2.2103420896,-2.8651465665,-10.8103189976,-0.9471692191,-0.0139754171,
-6.6061940221,3.3738346683,0.8202583807,-10.0107003278,3.3755266673,-4
.231227754,-5.7651916975,-0.9106584895,-3.4277082675\PG=C01 [X(C4H4)]\
NImag=0\\

**{C,C,C,N}**
\\0,1\N,0,-3.1660029159,0.0760818854,-0.3989702707\C,0,-2.359
1002687,1.3233335015,-0.3018283529\C,0,-1.6932248823,0.0470859563,-0.1
86107875\C,0,-2.2091992816,0.4788416166,-1.4640526466\H,0,-2.562149236
6,2.2907502201,0.1081332404\H,0,-1.0489254144,-0.6016286804,0.37001133
5\H,0,-2.2138980005,0.3796555006,-2.5295854301\\Version=EM64L-G09RevA.
02\State=1-A\MP2/GTBas1=-170.15366\MP4/GTBas1=-170.1975124\CCSD(T)/G3B
as1=-170.1961669\MP2/GTBas2=-170.1645486\MP4/GTBas2=-170.2084154\MP2/G
TBas3=-170.2767796\MP4/GTBas3=-170.3260301\HF/GTLargeXP=-169.661495\MP
2/GTLargeXP=-170.5237986\HF/GFHFB1=-169.6732698\HF/GFHFB2=-169.6757821
\G4=-170.607814\FreqCoord=-5.9828784469,0.143773927,-0.7539445469,-4.4
580534278,2.5007379003,-0.5703729261,-3.199731309,0.088979562,-0.35169
29149,-4.1747816151,0.9048795164,-2.7666585462,-4.8417603688,4.3288905
549,0.2043422101,-1.9821817671,-1.1369134397,0.6992200892,-4.183660907
1,0.717444921,-4.7802236927\PG=C01 [X(C3H3N1)]\NImag=0\\

**{C,C,N,N}**
\\0,1\N,0,-3.1852379408,-0.1086445809,-0.4858913074\N,0,-2.58
61095842,1.2731114037,-0.302707646\C,0,-1.7681765812,0.0708546722,-0.1
906492753\C,0,-2.2463289605,0.4453874798,-1.4546133263\H,0,-1.04875864
47,-0.3326616136,0.4925165369\H,0,-2.1867382885,0.5614926388,-2.517654
9819\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-186.1867\MP4/GTBa
s1=-186.2268456\CCSD(T)/G3Bas1=-186.2236068\MP2/GTBas2=-186.1977142\MP
4/GTBas2=-186.23807\MP2/GTBas3=-186.3085663\MP4/GTBas3=-186.3545779\HF
/GTLargeXP=-185.6567564\MP2/GTLargeXP=-186.5656051\HF/GFHFB1=-185.6695
394\HF/GFHFB2=-185.6722422\G4=-186.6574125\FreqCoord=-6.0192273763,-0.
2053085037,-0.9182015013,-4.8870388638,2.4058318896,-0.5720345492,-3.3
41369493,0.1338959257,-0.3602749178,-4.2449465397,0.8416603598,-2.7488
20816,-1.981866618,-0.6286393447,0.9307213706,-4.1323364897,1.06106731
31,-4.7576784129\PG=C01 [X(C2H2N2)]\NImag=0\\

**{C,N,N,N}**
\\0,1\N,0,-2.9780069549,-0.2201839059,-0.4386589341\N,0,-2.65
99332563,1.2342736821,-0.3040911673\N,0,-1.5587647262,0.223380492,-0.2
888253719\C,0,-2.3070684462,0.4950938331,-1.4583296728\H,0,-2.21900661
65,0.5732358988,-2.5236548539\\Version=EM64L-G09RevA.02\State=1-A\MP2/
GTBas1=-202.2094057\MP4/GTBas1=-202.2457983\CCSD(T)/G3Bas1=-202.240260

6\MP2/GTBas2=-202.2199683\MP4/GTBas2=-202.2567471\MP2/GTBas3=-202.3305
149\MP4/GTBas3=-202.3731344\HF/GTLargeXP=-201.6361047\MP2/GTLargeXP=-2
02.5965098\HF/GFHFB1=-201.6503402\HF/GFHFB2=-201.6532327\G4=-202.69607
21\FreqCoord=-5.6276175666,-0.4160872811,-0.8289452513,-5.0265453862,2
.3324392322,-0.5746490256,-2.945638438,0.4221279532,-0.5458008531,-4.3
597275331,0.9355917546,-2.7558436931,-4.1933147922,1.0832588583,-4.769
0165278\PG=C01 [X(C1H1N3)]\NImag=0\\

**{C,C,C,P}**
\\0,1\C,0,-2.99061883,-0.1690351508,-0.312606492\P,0,-2.82086
42811,1.6485730154,-0.0060642418\C,0,-1.6011569366,0.2654272996,-0.166
2581965\C,0,-2.3273393481,0.5416683521,-1.405868699\H,0,-2.2010871131,
0.4963727192,-2.4698307808\H,0,-0.650727322,-0.0953721113,0.175171275\
H,0,-3.6158361691,-1.0224941241,-0.1371428649\\Version=EM64L-G09RevA.0
2\State=1-A\MP2/GTBas1=-456.418893\MP4/GTBas1=-456.4686895\CCSD(T)/G3B
as1=-456.4678104\MP2/GTBas2=-456.428132\MP4/GTBas2=-456.4779821\MP2/GT
Bas3=-456.5509774\MP4/GTBas3=-456.6075726\HF/GTLargeXP=-455.9924125\MP
2/GTLargeXP=-457.0596333\HF/GFHFB1=-456.0065247\HF/GFHFB2=-456.0099476
\G4=-457.1577215\FreqCoord=-5.6514505565,-0.3194301419,-0.5907406572,-
5.3306609493,3.1153515092,-0.0114597563,-3.025748106,0.5015849044,-0.3
141824586,-4.3980339862,1.0236048404,-2.65670682,-4.1594518385,0.93800
84991,-4.6673037703,-1.2296964258,-0.1802271711,0.3310257361,-6.832940
1009,-1.9322338671,-0.2591624557\PG=C01 [X(C3H3P1)]\NImag=0\\

**{C,C,P,P}**
\\0,1\P,0,-3.2353089306,-0.274862825,-0.0379006872\C,0,-2.802
2791787,1.4757258991,-0.3848452239\P,0,-1.1974756624,0.6126650747,-0.1
537612801\C,0,-2.4701313474,0.5724411353,-1.4766527907\H,0,-2.53205689
85,0.5693337147,-2.5498105669\H,0,-3.2232179825,2.4578870012,-0.268369
4511\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-758.7252377\MP4/G
TBas1=-758.7770878\CCSD(T)/G3Bas1=-758.7753774\MP2/GTBas2=-758.7339337
\MP4/GTBas2=-758.7861284\MP2/GTBas3=-758.8674637\MP4/GTBas3=-758.92797
7\HF/GTLargeXP=-758.3346703\MP2/GTLargeXP=-759.6468881\HF/GFHFB1=-758.
3524299\HF/GFHFB2=-758.3568735\G4=-759.7666838\FreqCoord=-6.1138478341
,-0.5194154634,-0.071621919,-5.2955401955,2.7887177966,-0.7272520768,-
2.2629010527,1.1577692023,-0.2905667092,-4.6678717588,1.0817569729,-2.
7904693679,-4.7848940911,1.0758847991,-4.8184436623,-6.0909992535,4.64
47332978,-0.5071447651\PG=C01 [X(C2H2P2)]\NImag=0\\

**{C,P,P,P}**
\\0,1\P,0,-3.1180632671,-0.4429272777,-0.0935042641\P,0,-2.81
24333282,1.7444160123,-0.2107219518\P,0,-1.0712149079,0.3813349214,-0.
2439134895\C,0,-2.4058858128,0.500846062,-1.4909170843\H,0,-2.46488269
1,0.4516302875,-2.5647332102\\Version=EM64L-G09RevA.02\State=1-A\MP2/G
TBas1=-1061.0292576\MP4/GTBas1=-1061.0832886\CCSD(T)/G3Bas1=-1061.0813
91\MP2/GTBas2=-1061.0369257\MP4/GTBas2=-1061.0915803\MP2/GTBas3=-1061.
187058\MP4/GTBas3=-1061.2512007\HF/GTLargeXP=-1060.6812282\MP2/GTLarge
XP=-1062.2360484\HF/GFHFB1=-1060.7030053\HF/GFHFB2=-1060.7082656\G4=-1
062.3777807\FreqCoord=-5.8922856399,-0.8370112516,-0.1766974513,-5.314
7287574,3.2964685251,-0.398206779,-2.0243028055,0.7206185663,-0.460929
6952,-4.5464652932,0.946461892,-2.8174249762,-4.6579532356,0.853457556
7,-4.8466433713\PG=C01 [X(C1H1P3)]\NImag=0\\

**{C,C,N,P}**
\\0,1\C,0,-3.7634746815,-0.2589692749,-0.5507599645\C,0,-3.
0469788961,0.9512365603,-0.8222944871\N,0,-2.2893020172,-0.2815307994,
-0.5393906868\P,0,-3.0501362308,-0.206366989,-2.2120004686\H,0,-4.4675

801986,-0.705778276,0.1253917913\H,0,-2.8928279758,1.9540787789,-0.471
3961843\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-472.4583275\MP
4/GTBas1=-472.5041735\CCSD(T)/G3Bas1=-472.5011489\MP2/GTBas2=-472.4688
865\MP4/GTBas2=-472.5151528\MP2/GTBas3=-472.5896278\MP4/GTBas3=-472.64
29832\HF/GTLargeXP=-471.9965224\MP2/GTLargeXP=-473.1091246\HF/GFHFB1=-
472.0115542\HF/GFHFB2=-472.0153638\G4=-473.2146713\FreqCoord=-7.111936
456,-0.4893810065,-1.0407854979,-5.7579556463,1.7975765866,-1.55391138
12,-4.326153848,-0.5320161087,-1.0193006766,-5.7639221442,-0.389977092
1,-4.1800750915,-8.442503052,-1.3337276521,0.2369561448,-5.4666526239,
3.6926737342,-0.8908096884\PG=C01 [X(C2H2N1P1)]\NImag=0\\

**{C,N,N,P}**
\\0,1\C,0,-3.8103239496,-0.2303405234,-0.5474799133\N,0,-3.
1855798036,1.0346497707,-0.8515105182\P,0,-2.0581174381,-0.3622643985,
-0.6049056776\N,0,-3.3005654569,-0.051870761,-1.8862825147\H,0,-4.7883
833518,-0.4803340878,-0.1776013762\\Version=EM64L-G09RevA.02\State=1-A
\MP2/GTBas1=-488.4875939\MP4/GTBas1=-488.5298671\CCSD(T)/G3Bas1=-488.5
242589\MP2/GTBas2=-488.498689\MP4/GTBas2=-488.5416117\MP2/GTBas3=-488.
6185467\MP4/GTBas3=-488.6689245\HF/GTLargeXP=-487.9858327\MP2/GTLargeX
P=-489.148404\HF/GFHFB1=-488.0022817\HF/GFHFB2=-488.0064631\G4=-489.26
19905\FreqCoord=-7.2004687424,-0.4352805064,-1.0345870993,-6.019873403
2,1.95520471,-1.6091216787,-3.8892783074,-0.6845805009,-1.143106067,-6
.2371647972,-0.0980215326,-3.564557362,-9.0487331541,-0.9076998782,-0.
3356179618\PG=C01 [X(C1H1N2P1)]\NImag=0\\

**{C,N,P,P}**
\\0,1\C,0,-3.8571389103,-0.2579769375,-0.5752103361\N,0,-3.
2044616003,1.037496599,-0.7728993681\P,0,-2.0701680371,-0.3609295373,-
0.4441288426\P,0,-3.2541133399,-0.0375499872,-2.2509976104\H,0,-4.7570
881124,-0.4712001371,-0.0245438428\\Version=EM64L-G09RevA.02\State=1-A
\MP2/GTBas1=-774.7613032\MP4/GTBas1=-774.8095406\CCSD(T)/G3Bas1=-774.8
049569\MP2/GTBas2=-774.7718963\MP4/GTBas2=-774.8209195\MP2/GTBas3=-774
.9039169\MP4/GTBas3=-774.9617298\HF/GTLargeXP=-774.3347709\MP2/GTLarge
XP=-775.6945014\HF/GFHFB1=-774.3539115\HF/GFHFB2=-774.3588637\G4=-775.
8224722\FreqCoord=-7.2889361969,-0.4875057604,-1.086990004,-6.05555482
78,1.9605844359,-1.460568134,-3.9120506392,-0.6820579787,-0.8392818803
,-6.1493830179,-0.0709591921,-4.2537690094,-8.9895937225,-0.8904392129
,-0.0463811412\PG=C01 [X(C1H1N1P2)]\NImag=0\\

**{N,N,N,N}**
\\0,1\N,0,-0.08264,0.84751,-0.25085\N,0,-0.36269,-0.52737,-0.6151
1\N,0,0.86032,-0.19924,0.09059\N,0,-0.41498,-0.1209,0.77537\\Version=E
M64L-G09RevA.02\State=1-A\MP2/GTBas1=-218.2206445\MP4/GTBas1=-218.2524
665\CCSD(T)/G3Bas1=-218.2443235\MP2/GTBas2=-218.2310164\MP4/GTBas2=-21
8.2634248\MP2/GTBas3=-218.3420323\MP4/GTBas3=-218.3800364\HF/GTLargeXP
=-217.599552\MP2/GTLargeXP=-218.6163211\HF/GFHFB1=-217.6159451\HF/GFHF
B2=-217.6190723\G4=-218.7233916\FreqCoord=-0.1561669676,1.6015617949,-
0.4740378004,-0.6853847711,-0.9965848707,-1.1623894416,1.6257691866,-0
.3765090347,0.1711902904,-0.7841985506,-0.2284678895,1.4652369517\PG=C
01 [X(N4)]\NImag=0\\

**{N,N,N,P}**
\\0,1\N,0,-3.8110489228,-0.4175315525,-0.5981983722\N,0,-3.2894
315128,0.9485082601,-0.794627295\P,0,-2.0441387804,-0.2992700509,-0.62
44785401\N,0,-3.2407807841,-0.0259366567,-1.9013157928\\Version=EM64L-
G09RevA.02\State=1-A\MP2/GTBas1=-504.5045937\MP4/GTBas1=-504.5432384\C
CSD(T)/G3Bas1=-504.5346154\MP2/GTBas2=-504.5155611\MP4/GTBas2=-504.555

1525\MP2/GTBas3=-504.6355391\MP4/GTBas3=-504.6828292\HF/GTLargeXP=-503
.9571801\MP2/GTLargeXP=-505.1749982\HF/GFHFB1=-503.9756668\HF/GFHFB2=-
503.9802403\G4=-505.2973535\FreqCoord=-7.2018387431,-0.7890202861,-1.1
304310965,-6.216124692,1.7924208464,-1.5016279652,-3.8628624726,-0.565
538436,-1.1800934166,-6.1241881386,-0.0490131779,-3.5929661404\PG=C01
[X(N3P1)]\NImag=0\\

**{N,N,P,P}**
\\0,1\N,0,-3.8017359794,-0.4166478746,-0.5060111227\N,0,-3.2743
455693,0.9645068167,-0.7046135881\P,0,-2.0101577496,-0.2968458521,-0.5
173875206\P,0,-3.2991607038,-0.0452430951,-2.1906077678\\Version=EM64L
-G09RevA.02\State=1-A\MP2/GTBas1=-790.7880175\MP4/GTBas1=-790.8328878\
CCSD(T)/G3Bas1=-790.8247004\MP2/GTBas2=-790.7994837\MP4/GTBas2=-790.84
5491\MP2/GTBas3=-790.9317318\MP4/GTBas3=-790.9870211\HF/GTLargeXP=-790
.3206331\MP2/GTLargeXP=-791.732767\HF/GFHFB1=-790.3418664\HF/GFHFB2=-7
90.3473628\G4=-791.8693991\FreqCoord=-7.1842398306,-0.7873503769,-0.95
6222442,-6.1876163904,1.8226537369,-1.3315267111,-3.7986476306,-0.5609
573642,-0.9777207186,-6.2345101985,-0.0854970592,-4.1396487457\PG=C01
[X(N2P2)]\NImag=0\\

**{N,P,P,P}**
\\0,1\P,0,-4.046626524,-0.5639672283,-0.355276768\N,0,-3.215257
0845,1.0106580057,-0.7433442007\P,0,-1.9136032741,-0.2516165782,-0.553
1432277\P,0,-3.2099131174,0.0106958008,-2.2668558037\\Version=EM64L-G0
9RevA.02\State=1-A\MP2/GTBas1=-1077.0655107\MP4/GTBas1=-1077.116318\CC
SD(T)/G3Bas1=-1077.1107711\MP2/GTBas2=-1077.0758895\MP4/GTBas2=-1077.1
279344\MP2/GTBas3=-1077.2237139\MP4/GTBas3=-1077.2858869\HF/GTLargeXP=
-1076.680526\MP2/GTLargeXP=-1078.28372\HF/GFHFB1=-1076.70424\HF/GFHFB2
=-1076.710141\G4=-1078.4345461\FreqCoord=-7.6470158925,-1.0657436094,-
0.6713757928,-6.0759553364,1.9098668447,-1.4047169617,-3.616186115,-0.
4754864233,-1.0452892126,-6.0658567023,0.0202121344,-4.2837366517\PG=C
01 [X(N1P3)]\NImag=0\\

**{P,P,P,P}**
\\0,1\P,0,-5.4617533747,0.0964224462,-0.2867197005\P,0,-3.5592318
588,1.1810329903,0.0184884813\P,0,-3.7330484854,-0.3114883335,-1.60363
99554\P,0,-4.807276281,1.615252897,-1.7543488254\\Version=EM64L-G09Rev
A.02\State=1-A\MP2/GTBas1=-1363.334694\MP4/GTBas1=-1363.3908405\CCSD(T
)/G3Bas1=-1363.3892761\MP2/GTBas2=-1363.3409237\MP4/GTBas2=-1363.39768
47\MP2/GTBas3=-1363.5126254\MP4/GTBas3=-1363.5801346\HF/GTLargeXP=-136
3.0338094\MP2/GTLargeXP=-1364.8298528\HF/GFHFB1=-1363.0600914\HF/GFHFB
2=-1363.0658351\G4=-1364.9931901\FreqCoord=-10.3212180836,0.1822120163
,-0.5418217108,-6.7259734566,2.2318289056,0.0349381662,-7.0544392783,-
0.5886276438,-3.0304403314,-9.0844356162,3.0523856106,-3.3152388216\PG
=C01 [X(P4)]\NImag=0\\

**{N,N,N,Si}**
\\0,1\N,0,-3.8238329346,-0.4426861498,-0.5766419771\N,0,-3.2
805124824,0.9801595084,-0.7812400906\Si,0,-2.0871162203,-0.2848544046,
-0.6383422904\N,0,-3.229176748,-0.0350319909,-1.9337638714\H,0,-0.7750
016148,-0.7221469631,-0.1952717704\\Version=EM64L-G09RevA.02\State=1-A
\MP2/GTBas1=-453.1873797\MP4/GTBas1=-453.228138\CCSD(T)/G3Bas1=-453.22
25718\MP2/GTBas2=-453.2007397\MP4/GTBas2=-453.2423459\MP2/GTBas3=-453.
319453\MP4/GTBas3=-453.3692671\HF/GTLargeXP=-452.676256\MP2/GTLargeXP=
-453.8505594\HF/GFHFB1=-452.6918712\HF/GFHFB2=-452.6971375\G4=-453.969
6868\FreqCoord=-7.2259970242,-0.8365555859,-1.0896954134,-6.1992701672
,1.8522330375,-1.4763298153,-3.9440780638,-0.5382968125,-1.206292108,-

6.1022596884,-0.0662008686,-3.6542841227,-1.4645408045,-1.364659988,-0
.3690101676\PG=C01 [X(H1N3Si1)]\NImag=0\\

**{N,N,Si,Si}**
\\0,1\N,0,-3.637392358,-0.5562157701,-0.600054839\N,0,-3.068
5677159,0.9334591496,-0.8142649872\Si,0,-1.8532165048,-0.3745931121,-0
.6413559841\Si,0,-3.1646612148,-0.1087831452,-2.2753239935\H,0,-0.8558
994309,-0.6034644443,0.4153334914\H,0,-4.0034929279,0.0390369236,-3.47
48136302\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-688.2029495\M
P4/GTBas1=-688.2505592\CCSD(T)/G3Bas1=-688.2467856\MP2/GTBas2=-688.218
3968\MP4/GTBas2=-688.2666685\MP2/GTBas3=-688.3456132\MP4/GTBas3=-688.4
03849\HF/GTLargeXP=-687.8029415\MP2/GTLargeXP=-689.1288122\HF/GFHFB1=-
687.8200065\HF/GFHFB2=-687.8262986\G4=-689.254917\FreqCoord=-6.8736753
944,-1.0510954763,-1.1339393105,-5.7987526033,1.7639821489,-1.53873782
54,-3.502071659,-0.7078783931,-1.2119871635,-5.9803429993,-0.205570352
3,-4.2997392114,-1.6174155216,-1.1403825307,0.7848665525,-7.5655052086
,0.0737690947,-6.566446124\PG=C01 [X(H2N2Si2)]\NImag=0\\

**{N,Si,Si,Si}**
\\0,1\Si,0,-4.0496286088,-1.0459564848,-0.4284268987\N,0,-3.
1427838166,0.4734759047,-0.8727235323\Si,0,-1.7896967934,-0.72943986,-
0.642628868\Si,0,-3.1639038269,-0.4385177337,-2.4542645189\H,0,-0.6897
654573,-0.009028291,0.0551304018\H,0,-3.4045125609,0.5673765874,-3.524
7907109\H,0,-5.157288936,-0.6371701225,0.4777341269\\Version=EM64L-G09
RevA.02\State=1-A\MP2/GTBas1=-923.210731\MP4/GTBas1=-923.2667597\CCSD(
T)/G3Bas1=-923.2655452\MP2/GTBas2=-923.2226726\MP4/GTBas2=-923.2798349
\MP2/GTBas3=-923.3542877\MP4/GTBas3=-923.422143\HF/GTLargeXP=-922.8950
46\MP2/GTLargeXP=-924.3813687\HF/GFHFB1=-922.914329\HF/GFHFB2=-922.920
3317\G4=-924.5176685\FreqCoord=-7.6526890104,-1.9765713033,-0.80960950
66,-5.9390007083,0.8947397903,-1.6492084657,-3.3820368004,-1.378441565
8,-1.2143925655,-5.9789117437,-0.8286784212,-4.6378877983,-1.303467810
3,-0.0170609974,0.1041813611,-6.4335963562,1.0721863644,-6.6608891194,
-9.7458636772,-1.2040770316,0.9027866642\PG=C01 [X(H3N1Si3)]\NImag=0\\

**{P,P,P,Si}**
\\0,1\P,0,-0.5964201736,-0.5399950024,1.14247899\P,0,-0.5964
442694,-0.5400281989,-1.1424522548\P,0,-0.1509293118,1.3883315789,-0.0
000183602\Si,0,1.2543529273,-0.2903866604,-0.0000091043\H,0,2.68304082
76,-0.6215217172,-0.0000192708\\Version=EM64L-G09RevA.02\State=1-A\MP2
/GTBas1=-1312.0387659\MP4/GTBas1=-1312.0967548\CCSD(T)/G3Bas1=-1312.09
71302\MP2/GTBas2=-1312.0447842\MP4/GTBas2=-1312.103392\MP2/GTBas3=-131
2.2075878\MP4/GTBas3=-1312.2778661\HF/GTLargeXP=-1311.7605575\MP2/GTLa
rgeXP=-1313.5134964\HF/GFHFB1=-1311.7854342\HF/GFHFB2=-1311.7910786\G4
=-1313.6729638\FreqCoord=-1.1270707883,-1.0204426677,2.1589724037,-1.1
271163227,-1.0205054,-2.1589218815,-0.2852150648,2.6235664658,-0.00003
46957,2.3703835065,-0.5487512608,-0.0000172045,5.0702123675,-1.1745058
312,-0.0000364165\PG=C01 [X(H1P3Si1)]\NImag=0\\

**{P,P,Si,Si}**
\\0,1\Si,0,1.0848602108,-0.7602469679,-0.2061814184\P,0,-0.0
013590325,0.4875719369,1.338054764\P,0,0.0000755671,1.1015986858,-0.90
05196793\Si,0,-1.0835819806,-0.761382803,-0.2085047079\H,0,-2.46106953
34,-1.2598322093,-0.3462946402\H,0,2.4631247686,-1.2566786425,-0.34344
43182\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1260.7481879\MP4
/GTBas1=-1260.8075257\CCSD(T)/G3Bas1=-1260.8093466\MP2/GTBas2=-1260.75
40593\MP4/GTBas2=-1260.8139864\MP2/GTBas3=-1260.9104078\MP4/GTBas3=-12
60.9825071\HF/GTLargeXP=-1260.4916183\MP2/GTLargeXP=-1262.2042875\HF/G

FHFB1=-1260.5152751\HF/GFHFB2=-1260.5208591\G4=-1262.3589051\FreqCoord
=2.0500886908,-1.4366585627,-0.3896264144,-0.0025681992,0.9213774308,2
.5285570547,0.0001428012,2.0817198246,-1.7017355711,-2.0476731859,-1.4
3880498,-0.3940167954,-4.6507474121,-2.3807378489,-0.6544020312,4.6546
312438,-2.3747784714,-0.6490157033\PG=C01 [X(H2P2Si2)]\NImag=0\\

**{N,N,P,Si}**
\\0,1\N,0,-3.7111163769,-0.4587613907,-0.4643821702\N,0,-3
.1748939003,0.945536687,-0.6663159514\Si,0,-1.9635349012,-0.359519971,
-0.8294780596\P,0,-3.5133824628,0.0330663591,-2.2148624582\H,0,-0.8327
123588,-0.6648816844,0.0497786394\\Version=EM64L-G09RevA.02\State=1-A\
MP2/GTBas1=-739.4866263\MP4/GTBas1=-739.5338779\CCSD(T)/G3Bas1=-739.52
8689\MP2/GTBas2=-739.4996805\MP4/GTBas2=-739.5478973\MP2/GTBas3=-739.6
289139\MP4/GTBas3=-739.6866214\HF/GTLargeXP=-739.0519331\MP2/GTLargeXP
=-740.4205204\HF/GFHFB1=-739.0712123\HF/GFHFB2=-739.0769679\G4=-740.55
40044\FreqCoord=-7.0129935996,-0.8669333887,-0.8775551227,-5.999679972
6,1.7868053871,-1.2591546661,-3.7105432157,-0.6793942845,-1.5674863659
,-6.6393306547,0.0624863629,-4.1854834679,-1.5735983056,-1.2564442944,
0.0940679957\PG=C01 [X(H1N2P1Si1)]\NImag=0\\

**{N,P,P,Si}**
\\0,1\P,0,0.6070451407,1.1468533719,-0.1753232399\N,0,0.07
25506781,0.0010616569,1.1285038498\Si,0,-1.2038607002,-0.0245784661,-0
.2138454029\P,0,0.6529523503,-1.1217600942,-0.1756003448\H,0,-2.607097
4689,-0.0517564685,0.2253751378\\Version=EM64L-G09RevA.02\State=1-A\MP
2/GTBas1=-1025.7716994\MP4/GTBas1=-1025.8248082\CCSD(T)/G3Bas1=-1025.8
210164\MP2/GTBas2=-1025.7827022\MP4/GTBas2=-1025.8369077\MP2/GTBas3=-1
025.9230547\MP4/GTBas3=-1025.9879098\HF/GTLargeXP=-1025.410119\MP2/GTL
argeXP=-1026.9725474\HF/GFHFB1=-1025.4322374\HF/GFHFB2=-1025.4381676\G
4=-1027.1192773\FreqCoord=1.1471490662,2.1672387875,-0.3313129082,0.13
71009123,0.0020062408,2.1325632161,-2.2749670255,-0.0464465697,-0.4041
092462,1.2339011199,-2.1198193649,-0.3318365605,-4.9267002179,-0.09780
5551,0.4258972876\PG=C01 [X(H1N1P2Si1)]\NImag=0\\

**{N,P,Si,Si}**
\\0,1\P,0,-0.036941887,1.3231793911,-0.1714377811\N,0,0.00
10276117,0.0043285898,1.1352368828\Si,0,-1.0575391686,-0.6608524239,-0
.1944411847\Si,0,1.0938588905,-0.5996029978,-0.1941798971\H,0,-2.38441
90337,-1.2168389214,0.1259174888\H,0,2.4496135871,-1.0835336377,0.1219
744914\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-974.4852148\MP4
/GTBas1=-974.5392016\CCSD(T)/G3Bas1=-974.5374182\MP2/GTBas2=-974.49681
96\MP4/GTBas2=-974.5518183\MP2/GTBas3=-974.633271\MP4/GTBas3=-974.6992
377\HF/GTLargeXP=-974.1524911\MP2/GTLargeXP=-975.6718188\HF/GFHFB1=-97
4.1729694\HF/GFHFB2=-974.1790755\G4=-975.8130085\FreqCoord=-0.06981004
93,2.5004466738,-0.3239704551,0.0019419047,0.0081798493,2.1452868044,-
1.9984594034,-1.2488300955,-0.3674405881,2.067093731,-1.1330854543,-0.
3669468261,-4.5058989597,-2.2994923093,0.2379495691,4.629098811,-2.047
581831,0.2304983839\PG=C01 [X(H2N1P1Si2)]\NImag=0\\

**{Si,Si,Si,Si}**
\\0,1\Si,0,-0.4778,1.17664,-0.63336\Si,0,-0.17837,-1.10971,-0.
86627\Si,0,1.37948,0.15027,0.29823\Si,0,-0.72326,-0.21724,1.20144\H,0,
2.81227,0.30621,0.60913\H,0,-0.36409,-2.26103,-1.76811\H,0,-1.47363,-0
.44276,2.4502\H,0,-0.97532,2.3982,-1.29174\\Version=EM64L-G09RevA.02\S
tate=1-A\MP2/GTBas1=-1158.1483954\MP4/GTBas1=-1158.2128442\CCSD(T)/G3B
as1=-1158.2178802\MP2/GTBas2=-1158.1528432\MP4/GTBas2=-1158.2179572\MP
2/GTBas3=-1158.2976187\MP4/GTBas3=-1158.3765277\HF/GTLargeXP=-1157.933

3365\MP2/GTLargeXP=-1159.5665887\HF/GFHFB1=-1157.9547147\HF/GFHFB2=-11
57.9599878\G4=-1159.7168637\FreqCoord=-0.9029111463,2.223527357,-1.196
8769435,-0.3370704503,-2.0970479869,-1.6370130571,2.6068394058,0.28396
9146,0.5635730246,-1.3667633229,-0.4105241051,2.2703925651,5.314420111
7,0.5786530392,1.1510888793,-0.6880303877,-4.2727274782,-3.3412436728,
-2.7847571212,-0.8366951426,4.6302069708,-1.8430876919,4.5319412119,-2
.4410348349\PG=C01 [X(H4Si4)]\NImag=0\\

**W1BD archive entries for neutral singlet tetrahedranes**

**{N,N,N,N}**
\\0,1\N,0,-0.0825944219,0.8470092917,-0.2506986769\N,0,-0.3
624734305,-0.527063779,-0.6147624602\N,0,0.8598108199,-0.1991252101,0.
0905369176\N,0,-0.4147329676,-0.1208203026,0.7749242195\\Version=EM64L
-G09RevA.02\State=1-A\BDRef/AVTZ+2d1f=-217.5928463\BDRef/AVQZ+2d1f=-21
7.6052567\BDRefExt=-217.609118\BD/AVTZ+2d1f=-218.4215585\BD/AVQZ+2d1f=
-218.4700851\BDExt=-0.8885075\BD(T)/AVDZ+2d=-218.3000591\BD(T)/AVTZ+2d
1f=0.\TExt=-0.0581249\BD(T)/MTsmall=-218.4816297\DK-BD(T,FU)/MTsmall=-
218.8070567\Core+Rel=-0.325427\W1BD=-218.8682323\FreqCoord=-0.15608083
75,1.6006155934,-0.4737518412,-0.684975514,-0.9960061968,-1.1617326866
,1.6248069757,-0.3762921133,0.1710899791,-0.783731727,-0.2283172833,1.
4643945486\PG=C01 [X(N4)]\NImag=0\\

**G4MP2 archive entries for cationic tetrahedranes**

**{C,N,P,P}+**
\\1,2\C,0,-3.8350242034,-0.3971575142,-0.6144823085\N
,0,-3.0571965327,1.0392568827,-0.8733523127\P,0,-2.1037316904,-0.30347
69593,-0.2752647012\P,0,-3.4012097438,0.0402630482,-2.2704061579\H,0,-
4.7458078297,-0.4690454575,-0.0342745197\\Version=EM64L-G09RevA.02\Sta
te=2-A\MP2/GTBas1=-774.4318316\CCSD(T)/GTBas1=-774.4821077\MP2/GTBas2=
0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-774.0402974\MP2/GTMP2LargeXP=-774.66
26866\HF/GFHFB3=-774.0505951\HF/GFHFB4=-774.0631746\G4MP2=-774.8100851
\FreqCoord=-7.2471454575,-0.7505189335,-1.1612032765,-5.7772641812,1.9
639108901,-1.6503966886,-3.9754767519,-0.5734883407,-0.5201748994,-6.4
273549362,0.0760861344,-4.2904458488,-8.9682770774,-0.8863674585,-0.06
47694555\PG=C01 [X(C1H1N1P2)]\NImag=0\\

**{C,N,N,N}+**
\\1,2\N,0,-3.1135355812,-0.1384017564,-0.5271023287\N,0
,-2.6616809713,1.16638,-0.0876356587\N,0,-1.4790396572,0.3722676039,-0
.354628468\C,0,-2.2538924537,0.336060845,-1.4907020729\H,0,-2.21463133
65,0.5694933075,-2.5534914717\\Version=EM64L-G09RevA.02\State=2-A\MP2/
GTBas1=-201.7893804\CCSD(T)/GTBas1=-201.8413073\MP2/GTBas2=0.\MP2/GTBa
s3=0.\HF/GTMP2LargeXP=-201.2690853\MP2/GTMP2LargeXP=-201.9827889\HF/GF
HFB3=-201.2713785\HF/GFHFB4=-201.2847011\G4MP2=-202.1222322\FreqCoord=
-5.8837295535,-0.261541416,-0.9960790452,-5.0298480888,2.2041387669,-0
.1656073945,-2.7949798919,0.7034838196,-0.6701506834,-4.2592394705,0.6
35062961,-2.8170186634,-4.1850467114,1.0761863858,-4.8253995642\PG=C01
 [X(C1H1N3)]\NImag=0\\

**{N,N,P,P}+**
\\1,2\N,0,-3.7456467162,-0.5703202345,-0.5750317275\N,0,-
3.1381670461,1.0205758357,-0.8037939507\P,0,-2.049710809,-0.2582289373
,-0.35386471\P,0,-3.4518754287,0.0137433362,-2.1859296118\\Version=EM6
4L-G09RevA.02\State=2-A\MP2/GTBas1=-790.4391179\CCSD(T)/GTBas1=-790.48
4923\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-790.0108946\MP2/GTMP
2LargeXP=-790.6829813\HF/GFHFB3=-790.0231215\HF/GFHFB4=-790.0366342\G4
MP2=-790.8404436\FreqCoord=-7.0782464842,-1.0777490513,-1.0866524827,-
5.9302762763,1.9286088273,-1.518950434,-3.8733920806,-0.4879819712,-0.
66870739,-6.5230992051,0.0259711415,-4.1308083121\PG=C01 [X(N2P2)]\NIm
ag=0\\

**{N,N,P,Si}+**
\\1,2\N,0,-3.7418736899,-0.6302247946,-0.5692632878\N,0
,-3.0959450481,1.0623126301,-0.8125390141\Si,0,-2.0622509443,-0.270344
1325,-0.4728030443\P,0,-3.5683979215,0.0580795474,-2.1868491282\H,0,-0
.7271723962,-0.7243832504,-0.0838055256\\Version=EM64L-G09RevB.01\Stat
e=2-A\MP2/GTBas1=-739.1712986\CCSD(T)/GTBas1=-739.2211132\MP2/GTBas2=0
.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-738.7783103\MP2/GTMP2LargeXP=-739.412
4547\HF/GFHFB3=-738.7888667\HF/GFHFB4=-738.8022234\G4MP2=-739.5648155\
FreqCoord=-7.0711164978,-1.190952264,-1.0757517114,-5.8504882633,2.007
4799384,-1.535476209,-3.8970895021,-0.5108763721,-0.8934682686,-6.7432
948048,0.1097544386,-4.1325459462,-1.3741566802,-1.3688859585,-0.15836
94919\PG=C01 [X(H1N2P1Si1)]\NImag=0\\

**{N,P,P,Si}+**
\\1,2\P,0,0.6449202091,1.1254259765,-0.3807630091\N,
0,0.0610202168,-0.18540214,1.1747423238\Si,0,-1.2477444738,0.267408955
6,0.1042228527\P,0,0.7129361596,-1.0860994731,-0.1569427613\H,0,-2.649

5421116,-0.171513319,0.0478505939\\Version=EM64L-G09RevA.02\State=2-A\
MP2/GTBas1=-1025.4562901\CCSD(T)/GTBas1=-1025.5181554\MP2/GTBas2=0.\MP
2/GTBas3=0.\HF/GTMP2LargeXP=-1025.1375427\MP2/GTMP2LargeXP=-1025.71173
44\HF/GFHFB3=-1025.1521539\HF/GFHFB4=-1025.1643588\G4MP2=-1025.8805148
\FreqCoord=1.2187225727,2.1267468784,-0.7195378088,0.1153114982,-0.350
3592691,2.2199412687,-2.3578953393,0.5053296915,0.1969526484,1.3472540
92,-2.0524305572,-0.2965788374,-5.0069089685,-0.324113201,0.0904245178
\PG=C01 [X(H1N1P2Si1)]\NImag=0\\

**{N,P,Si,Si}$^+$**
\\1,2\P,0,-0.0362370379,1.3148005519,-0.3730709119\N
,0,0.0066827695,-0.1961224629,1.2266485336\Si,0,-1.1280330001,-0.57899
54877,-0.0466096618\Si,0,1.1591846918,-0.5161394531,-0.0480349525\H,0,
-2.4592953422,-1.1978460605,0.033535967\H,0,2.5232979189,-1.0590170877
,0.0306010255\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-974.1913
104\CCSD(T)/GTBas1=-974.2549065\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
rgeXP=-973.9007838\MP2/GTMP2LargeXP=-974.4388994\HF/GFHFB3=-973.913722
7\HF/GFHFB4=-973.9260269\G4MP2=-974.6001456\FreqCoord=-0.0684780774,2.
4846129625,-0.7050018516,0.0126286041,-0.3706177434,2.3180297899,-2.13
1673439,-1.0941429039,-0.0880794959,2.1905416049,-0.9753622127,-0.0907
72905,-4.6473946766,-2.2636010037,0.0633737933,4.7683420184,-2.0012522
659,0.0578275576\PG=C01 [X(H2N1P1Si2)]\NImag=0\\

**{C,P,P,P}$^+$**
\\1,2\P,0,-3.1072846593,-0.4323013547,0.0355711174\P,0,
-2.9647577784,1.7252041735,-0.2668794863\P,0,-1.0546634092,0.229922101
4,-0.3032901308\C,0,-2.3082522847,0.6258277012,-1.5017407768\H,0,-2.43
75218684,0.4866473785,-2.5674507235\\Version=EM64L-G09RevA.02\State=2-
A\MP2/GTBas1=-1060.7148572\CCSD(T)/GTBas1=-1060.7726281\MP2/GTBas2=0.\
MP2/GTBas3=0.\HF/GTMP2LargeXP=-1060.3943915\MP2/GTMP2LargeXP=-1060.964
3943\HF/GFHFB3=-1060.4091868\HF/GFHFB4=-1060.4204045\G4MP2=-1061.12364
38\FreqCoord=-5.871917023,-0.8169311672,0.0672196701,-5.6025802516,3.2
601634113,-0.5043291396,-1.9930250057,0.4344898036,-0.573135286,-4.361
9646636,1.1826429617,-2.8378787907,-4.6062487743,0.9196302686,-4.85177
87271\PG=C01 [X(C1H1P3)]\NImag=0\\

**{P,P,Si,Si}$^+$**
\\1,2\Si,0,-1.0069374965,0.8970299775,-0.444939302\P,0
,-0.818213203,-0.9503336492,0.7290035051\P,0,0.8385025049,-0.932248603
5,-0.7291993185\Si,0,0.9869865324,0.9185309223,0.4452069095\H,0,1.7905
109619,1.4072594453,1.5814882433\H,0,-1.8213392997,1.3687119077,-1.580
6700374\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1260.4667344\C
CSD(T)/GTBas1=-1260.533033\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP
=-1260.2369668\MP2/GTMP2LargeXP=-1260.7290362\HF/GFHFB3=-1260.254434\H
F/GFHFB4=-1260.2651901\G4MP2=-1260.8978048\FreqCoord=-1.9028361012,1.6
951409904,-0.8408134265,-1.546198872,-1.7958703319,1.3776169745,1.5845
400961,-1.7616945484,-1.3779870083,1.8651342431,1.7357718877,0.8413191
314,3.3835753558,2.6593349496,2.9885796622,-3.4418324715,2.5864906604,
-2.9870334771\PG=C01 [X(H2P2Si2)]\NImag=0\\

**{P,P,P,P}$^+$**
\\1,2\P,0,-5.3903850679,-0.0023159995,-0.2035280935\P,0,-3.
6527563424,1.2785587162,0.0776960664\P,0,-3.8425925645,-0.3515730647,-
1.6939514512\P,0,-4.6755760251,1.656550348,-1.8064365217\\Version=EM64
L-G09RevA.02\State=2-A\MP2/GTBas1=-1363.0046698\CCSD(T)/GTBas1=-1363.0
652396\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1362.7323345\MP2/G
TMP2LargeXP=-1363.2910591\HF/GFHFB3=-1362.7525764\HF/GFHFB4=-1362.7633

736\G4MP2=-1363.4708406\FreqCoord=-10.1863515292,-0.0043766048,-0.3846
123571,-6.9027091174,2.4161258185,0.146824287,-7.2614475872,-0.6643768
08,-3.2011043251,-8.835558201,3.1304264831,-3.4136703024\PG=C01 [X(P4)
]\NImag=0\\

**G4 archive entries for cationic tetrahedranes**

**{C,N,N,N}⁺**

\\1,2\N,0,-3.1135355814,-0.1384017563,-0.5271023291\N,0
,-2.6616809714,1.1663799999,-0.0876356573\N,0,-1.4790396571,0.37226760
42,-0.3546284683\C,0,-2.2538924538,0.3360608454,-1.4907020731\H,0,-2.2
146313362,0.5694933067,-2.5534914722\\Version=EM64L-G09RevA.02\State=2
-A\MP2/GTBas1=-201.7893804\MP4/GTBas1=-201.8403064\CCSD(T)/G3Bas1=-201
.8413073\MP2/GTBas2=-201.7963635\MP4/GTBas2=-201.8481277\MP2/GTBas3=-2
01.9020514\MP4/GTBas3=-201.958851\HF/GTLargeXP=-201.2695012\MP2/GTLarg
eXP=-202.161182\HF/GFHFB1=-201.2847011\HF/GFHFB2=-201.2876901\G4=-202.
2829621\FreqCoord=-5.8837295538,-0.2615414156,-0.996079046,-5.02984808
91,2.2041387668,-0.1656073918,-2.7949798917,0.7034838201,-0.670150684,
-4.2592394707,0.6350629619,-2.817018664,-4.1850467108,1.0761863842,-4.
825399565\PG=C01 [X(C1H1N3)]\NImag=0\\

**{C,N,P,P}⁺**

\\1,2\C,0,-3.8350242034,-0.3971575142,-0.6144823085\N
,0,-3.0571965327,1.0392568827,-0.8733523127\P,0,-2.1037316904,-0.30347
69593,-0.2752647012\P,0,-3.4012097438,0.0402630482,-2.2704061579\H,0,-
4.7458078297,-0.4690454575,-0.0342745197\\Version=EM64L-G09RevA.02\Sta
te=2-A\MP2/GTBas1=-774.4318316\MP4/GTBas1=-774.4848376\CCSD(T)/G3Bas1=
-774.4821077\MP2/GTBas2=-774.43965\MP4/GTBas2=-774.4933602\MP2/GTBas3=
-774.5643647\MP4/GTBas3=-774.6256364\HF/GTLargeXP=-774.0407979\MP2/GTL
argeXP=-775.3507621\HF/GFHFB1=-774.0595183\HF/GFHFB2=-774.0650469\G4=-
775.4823543\FreqCoord=-7.2471454575,-0.7505189335,-1.1612032765,-5.777
2641812,1.9639108901,-1.6503966886,-3.9754767519,-0.5734883407,-0.5201
748994,-6.4273549362,0.0760861344,-4.2904458488,-8.9682770774,-0.88636
74585,-0.0647694555\PG=C01 [X(C1H1N1P2)]\NImag=0\\

**{C,P,P,P}⁺**

\\1,2\P,0,-3.1072846593,-0.4323013547,0.0355711174\P,0,
-2.9647577784,1.7252041735,-0.2668794863\P,0,-1.0546634092,0.229922101
4,-0.3032901308\C,0,-2.3082522847,0.6258277012,-1.5017407768\H,0,-2.43
75218684,0.4866473785,-2.5674507235\\Version=EM64L-G09RevA.02\State=2-
A\MP2/GTBas1=-1060.7148572\MP4/GTBas1=-1060.7730373\CCSD(T)/G3Bas1=-10
60.7726281\MP2/GTBas2=-1060.7205918\MP4/GTBas2=-1060.779327\MP2/GTBas3
=-1060.8624861\MP4/GTBas3=-1060.92957\HF/GTLargeXP=-1060.3947513\MP2/G
TLargeXP=-1061.9069123\HF/GFHFB1=-1060.4164045\HF/GFHFB2=-1060.4218278
\G4=-1062.0508423\FreqCoord=-5.871917023,-0.8169311672,0.0672196702,-5
.6025802516,3.2601634113,-0.5043291396,-1.9930250057,0.4344898036,-0.5
73135286,-4.3619646636,1.1826429617,-2.8378787907,-4.6062487742,0.9196
302687,-4.8517787271\PG=C01 [X(C1H1P3)]\NImag=0\\

**{N,N,P,P}⁺**

\\1,2\N,0,-3.7456467167,-0.570320234,-0.5750317269\N,0,-3
.1381670467,1.0205758358,-0.80379395\P,0,-2.0497108086,-0.2582289376,-
0.3538647106\P,0,-3.4518754281,0.0137433358,-2.1859296124\\Version=EM6
4L-G09RevA.02\State=2-A\MP2/GTBas1=-790.4391179\MP4/GTBas1=-790.490707
6\CCSD(T)/G3Bas1=-790.484923\MP2/GTBas2=-790.4480008\MP4/GTBas2=-790.5
005263\MP2/GTBas3=-790.5751633\MP4/GTBas3=-790.6352675\HF/GTLargeXP=-7
90.0114482\MP2/GTLargeXP=-791.3722761\HF/GFHFB1=-790.032515\HF/GFHFB2=
-790.0387202\G4=-791.5145106\FreqCoord=-7.078246485,-1.0777490504,-1.0
866524816,-5.9302762774,1.9286088275,-1.5189504328,-3.8733920798,-0.48
79819716,-0.6687073911,-6.523099204,0.0259711409,-4.1308083132\PG=C01
[X(N2P2)]\NImag=0\\

**{N,N,P,Si}⁺**

\\1,2\N,0,-3.7419095694,-0.6301790362,-0.569174249\N
,0,-3.0956292363,1.0623480997,-0.8125529206\Si,0,-2.0622947305,-0.2705
547798,-0.473043662\P,0,-3.568563891,0.0581732066,-2.1867972253\H,0,-0
.7272425727,-0.7243474902,-0.0836919431\\Version=EM64L-G09RevA.02\Stat
e=2-A\MP2/GTBas1=-739.1712893\MP4/GTBas1=-739.2223124\CCSD(T)/G3Bas1=-
739.221113\MP2/GTBas2=-739.1810189\MP4/GTBas2=-739.2328065\MP2/GTBas3=
-739.307047\MP4/GTBas3=-739.3673542\HF/GTLargeXP=-738.7788556\MP2/GTLa
rgeXP=-740.0925918\HF/GFHFB1=-738.7978599\HF/GFHFB2=-738.8043547\G4=-7
40.2304928\FreqCoord=-7.0711843002,-1.1908657931,-1.0755834525,-5.8498
914656,2.0075469662,-1.5355024885,-3.8971722459,-0.5112744378,-0.89392
29701,-6.7436084418,0.1099314287,-4.1324478639,-1.3742892946,-1.368818
3816,-0.158154852\PG=C01 [X(H1N2P1Si1)]\NImag=0\\

**{N,P,P,Si}⁺**

\\1,2\P,0,0.644920209,1.1254259765,-0.3807630094\N,0
,0.0610202168,-0.18540214,1.1747423239\Si,0,-1.2477444738,0.2674089555
,0.104222853\P,0,0.7129361596,-1.086099473,-0.1569427612\H,0,-2.649542
1116,-0.1715133189,0.0478505937\\Version=EM64L-G09RevA.02\State=2-A\MP
2/GTBas1=-1025.4562901\MP4/GTBas1=-1025.5147453\CCSD(T)/G3Bas1=-1025.5
181554\MP2/GTBas2=-1025.4637227\MP4/GTBas2=-1025.523208\MP2/GTBas3=-10
25.6029774\MP4/GTBas3=-1025.6711168\HF/GTLargeXP=-1025.1379324\MP2/GTL
argeXP=-1026.6465382\HF/GFHFB1=-1025.1599355\HF/GFHFB2=-1025.1660574\G
4=-1026.8014293\FreqCoord=1.2187225725,2.1267468783,-0.7195378094,0.11
53114983,-0.3503592691,2.219941269,-2.3578953392,0.5053296914,0.196952
649,1.3472540918,-2.0524305571,-0.2965788372,-5.0069089684,-0.32411320
09,0.0904245173\PG=C01 [X(H1N1P2Si1)]\NImag=0\\

**{N,P,Si,Si}⁺**

\\1,2\P,0,-0.0362370378,1.3148005517,-0.3730709127\N
,0,0.0066827695,-0.1961224622,1.2266485336\Si,0,-1.1280330001,-0.57899
54876,-0.0466096616\Si,0,1.1591846918,-0.5161394532,-0.0480349525\H,0,
-2.4592953422,-1.1978460605,0.0335359676\H,0,2.5232979188,-1.059017088
2,0.0306010255\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-974.191
3104\MP4/GTBas1=-974.2488594\CCSD(T)/G3Bas1=-974.2549065\MP2/GTBas2=-9
74.1987116\MP4/GTBas2=-974.2571116\MP2/GTBas3=-974.3324414\MP4/GTBas3=
-974.4009125\HF/GTLargeXP=-973.9011794\MP2/GTLargeXP=-975.364985\HF/GF
HFB1=-973.9213305\HF/GFHFB2=-973.9277291\G4=-975.513442\FreqCoord=-0.0
684780773,2.484612962,-0.7050018532,0.0126286042,-0.3706177421,2.31802
97899,-2.1316734391,-1.0941429038,-0.0880794955,2.190541605,-0.9753622
129,-0.090772905,-4.6473946767,-2.2636010037,0.0633737945,4.7683420182
,-2.0012522667,0.0578275575\PG=C01 [X(H2N1P1Si2)]\NImag=0\\

**{P,P,P,P}⁺**

\\1,2\P,0,-5.3903850679,-0.0023159995,-0.2035280935\P,0,-3.
6527563424,1.2785587162,0.0776960664\P,0,-3.8425925645,-0.3515730647,-
1.6939514512\P,0,-4.6755760251,1.656550348,-1.8064365217\\Version=EM64
L-G09RevA.02\State=2-A\MP2/GTBas1=-1363.0046698\MP4/GTBas1=-1363.06533
91\CCSD(T)/G3Bas1=-1363.0652396\MP2/GTBas2=-1363.0102079\MP4/GTBas2=-1
363.0715251\MP2/GTBas3=-1363.1747674\MP4/GTBas3=-1363.2456424\HF/GTLar
geXP=-1362.7325985\MP2/GTLargeXP=-1364.4891574\HF/GFHFB1=-1362.7587549
\HF/GFHFB2=-1362.7646247\G4=-1364.655149\FreqCoord=-10.1863515292,-0.0
043766048,-0.3846123571,-6.9027091174,2.4161258185,0.146824287,-7.2614
475872,-0.664376808,-3.2011043251,-8.835558201,3.1304264831,-3.4136703
024\PG=C01 [X(P4)]\NImag=0\\

**{P,P,Si,Si}⁺**

\\1,2\Si,0,1.0510579658,-0.9270893103,0.0562870507\P,0
,0.1677402825,0.6472246756,1.3084734843\P,0,-0.1689855035,1.2232916497
,-0.7949812452\Si,0,-1.0497819522,-0.7705737344,-0.52045278\H,0,-2.398
3521268,-1.3273370943,-0.3033645681\H,0,2.4003713341,-1.2944861863,-0.
4128519417\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1260.466734
1\MP4/GTBas1=-1260.5290831\CCSD(T)/G3Bas1=-1260.533048\MP2/GTBas2=-126
0.4722274\MP4/GTBas2=-1260.5351946\MP2/GTBas3=-1260.6190725\MP4/GTBas3
=-1260.6930457\HF/GTLargeXP=-1260.237176\MP2/GTLargeXP=-1261.9089359\H
F/GFHFB1=-1260.2608601\HF/GFHFB2=-1260.2664108\G4=-1262.0652793\FreqCo
ord=1.9862117052,-1.7519448972,0.1063671107,0.3169831953,1.2230773834,
2.4726565375,-0.319336322,2.3116861986,-1.5022968342,-1.9838003889,-1.
4561733233,-0.9835132193,-4.5322286898,-2.5083035943,-0.5732759521,4.5
360444388,-2.4462243749,-0.7801771033\PG=C01 [X(H2P2Si2)]\NImag=0\\

**G4MP2 archive entries for anionic tetrahedranes**

**{N,N,P,P}⁻**
\\\-1,2\N,0,-3.8276934506,-0.4307291783,-0.4890681868\N,0,
-3.2829996652,0.9957400113,-0.6941867911\P,0,-2.0002439552,-0.30342240
13,-0.5367972972\P,0,-3.2744629289,-0.0558184317,-2.1985677249\\Versio
n=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-790.7556331\CCSD(T)/GTBas1=-7
90.7912675\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-790.2932374\MP
2/GTMP2LargeXP=-791.0492432\HF/GFHFB3=-790.3065222\HF/GFHFB4=-790.3194
319\G4MP2=-791.208366\FreqCoord=-7.2332923424,-0.8139601845,-0.9242049
334,-6.2039702617,1.8816759209,-1.3118229202,-3.7799132743,-0.57338524
1,-1.0143998806,-6.187838168,-0.1054815491,-4.1546908846\PG=C01 [X(N2P
2)]\NImag=0\\

**{N,P,Si,Si}⁻**
\\\-1,2\P,0,-0.0312243604,1.1136261495,-0.0620341434\
N,0,0.0136098173,-0.4453672726,0.9667620679\Si,0,-1.193049548,-0.80711
97307,-0.3538215594\Si,0,1.2372549852,-0.7360012061,-0.3563475905\H,0,
-2.5691552273,-0.7496375175,0.3152128259\H,0,2.6081643332,-0.608820422
7,0.3132983995\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-974.517
8014\CCSD(T)/GTBas1=-974.5736833\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2L
argeXP=-974.1893135\MP2/GTMP2LargeXP=-974.7928619\HF/GFHFB3=-974.20287
35\HF/GFHFB4=-974.2147061\G4MP2=-974.9583568\FreqCoord=-0.0590054899,2
.1044484371,-0.1172275418,0.0257188274,-0.8416221737,1.8269155439,-2.2
545369086,-1.5252352474,-0.6686258472,2.3380730786,-1.390840713,-0.673
3993541,-4.8549997725,-1.416609607,0.5956659145,4.9287162993,-1.150503
8631,0.5920481729\PG=C01 [X(H2N1P1Si2)]\NImag=0\\

**{P,P,Si,Si}⁻**
\\\-1,2\Si,0,1.2427126443,-1.0299314683,-0.3056436421\P
,0,-0.0005272987,0.1236821554,1.2413215007\P,0,-0.0000981788,0.7975360
369,-0.9219058299\Si,0,-1.2410072511,-1.0317770496,-0.3052943124\H,0,-
2.7189078246,-0.6558643825,-0.1899329486\H,0,2.7198779089,-0.652615291
9,-0.1854347677\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1260.7
762195\CCSD(T)/GTBas1=-1260.8413846\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM
P2LargeXP=-1260.518112\MP2/GTMP2LargeXP=-1261.0658404\HF/GFHFB3=-1260.
5364204\HF/GFHFB4=-1260.5463906\G4MP2=-1261.2448268\FreqCoord=2.348386
5596,-1.9462884107,-0.5775827779,-0.0009964502,0.2337254012,2.34575767
93,-0.0001855311,1.5071246908,-1.7421495388,-2.3451638335,-1.949776053
9,-0.5769226404,-5.137991169,-1.2394040632,-0.3589212565,5.1398243628,
-1.2332641719,-0.3504209264\PG=C01 [X(H2P2Si2)]\NImag=0\\

**G4 archive entries for anionic tetrahedranes**

**{N,N,P,P}⁻**
\\\-1,2\N,0,-3.8276934506,-0.4307291785,-0.4890681869\N,0,
-3.2829996651,0.9957400114,-0.6941867911\P,0,-2.0002439553,-0.30342240
12,-0.5367972971\P,0,-3.274462929,-0.0558184317,-2.1985677248\\Version
=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-790.7556331\MP4/GTBas1=-790.79
85827\CCSD(T)/G3Bas1=-790.7912675\MP2/GTBas2=-790.7985933\MP4/GTBas2=-
790.8420344\MP2/GTBas3=-790.9069524\MP4/GTBas3=-790.9624842\HF/GTLarge
XP=-790.2937014\MP2/GTLargeXP=-791.7386547\HF/GFHFB1=-790.3158402\HF/G
FHFB2=-790.3215974\G4=-791.8837388\FreqCoord=-7.2332923423,-0.81396018
49,-0.9242049335,-6.2039702614,1.8816759212,-1.3118229203,-3.779913274
5,-0.5733852409,-1.0143998805,-6.1878381681,-0.1054815491,-4.154690884
6\PG=C01 [X(N2P2)]\NImag=0\\

**{N,P,Si,Si}⁻**
\\\-1,2\P,0,-0.0312243604,1.1136261495,-0.0620341434\
N,0,0.0136098173,-0.4453672726,0.9667620679\Si,0,-1.193049548,-0.80711
97307,-0.3538215594\Si,0,1.2372549852,-0.7360012061,-0.3563475905\H,0,
-2.5691552273,-0.7496375174,0.3152128259\H,0,2.6081643332,-0.608820422
7,0.3132983994\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-974.517
8014\MP4/GTBas1=-974.5727047\CCSD(T)/G3Bas1=-974.5736833\MP2/GTBas2=-9
74.539261\MP4/GTBas2=-974.5955597\MP2/GTBas3=-974.6717509\MP4/GTBas3=-
974.7403157\HF/GTLargeXP=-974.1896713\MP2/GTLargeXP=-975.7194095\HF/GF
HFB1=-974.2107176\HF/GFHFB2=-974.2163026\G4=-975.8726065\FreqCoord=-0.
0590054899,2.104448437,-0.1172275419,0.0257188274,-0.8416221737,1.8269
155439,-2.2545369086,-1.5252352475,-0.6686258472,2.3380730786,-1.39084
0713,-0.6733993541,-4.8549997725,-1.4166096069,0.5956659145,4.92871629
93,-1.150503863,0.5920481728\PG=C01 [X(H2N1P1Si2)]\NImag=0\\

**{P,P,Si,Si}⁻**
\\\-1,2\Si,0,1.2427126443,-1.0299314682,-0.3056436423\P
,0,-0.0005272987,0.123682155,1.2413215009\P,0,-0.0000981789,0.79753603
71,-0.9219058295\Si,0,-1.2410072511,-1.0317770495,-0.3052943126\H,0,-2
.7189078246,-0.6558643825,-0.1899329487\H,0,2.7198779089,-0.6526152919
,-0.1854347678\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1260.77
62195\MP4/GTBas1=-1260.8373184\CCSD(T)/G3Bas1=-1260.8413846\MP2/GTBas2
=-1260.7900366\MP4/GTBas2=-1260.8518574\MP2/GTBas3=-1260.9448708\MP4/G
TBas3=-1261.0200516\HF/GTLargeXP=-1260.5183364\MP2/GTLargeXP=-1262.246
7168\HF/GFHFB1=-1260.5424995\HF/GFHFB2=-1260.5476163\G4=-1262.4132549\
FreqCoord=2.3483865596,-1.9462884105,-0.5775827783,-0.0009964502,0.233
7254004,2.3457576796,-0.0001855312,1.5071246913,-1.7421495381,-2.34516
38335,-1.9497760538,-0.5769226408,-5.137991169,-1.2394040633,-0.358921
2566,5.1398243628,-1.2332641717,-0.3504209267\PG=C01 [X(H2P2Si2)]\NIma
g=0\\