

# Structures, enthalpies of formation, and ionization energies for the parent and binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives: A G4MP2 theoretical study

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**Keywords:** cubane derivatives, theoretical methods, Gaussian-4 MP2 (G4MP2), structures, enthalpy of formation, ionization energy

Gas phase standard state (298.15 K, 1 atm) structures, enthalpies of formation ( $\Delta_f H_{(g)}^\circ$ ), and ionization energies (IEs) were calculated at the G4MP2 composite method level of theory for the parent and binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives. Increasing nitrogen content increases the  $\Delta_f H_{(g)}^\circ$  for the carbon-nitrogen, nitrogen-phosphorus, and silicon-nitrogen binary cubanes, with the opposite  $\Delta_f H_{(g)}^\circ$  trend for increasing phosphorus content within the carbon-phosphorus, nitrogen-phosphorus, and silicon-phosphorus derivatives. Varying carbon/silicon content in the carbon-silicon cubanes results in no general trends for  $\Delta_f H_{(g)}^\circ$ . Isomerization enthalpies within the homolog groups having more than one isomer vary widely with atomic composition and substitution patterns. Increasing nitrogen content of the carbon-nitrogen and nitrogen-phosphorus derivatives increases the IE, increasing silicon content in the carbon-silicon cubanes and phosphorus content of the carbon-phosphorus cubanes decreases the IE, while no IE clear trends are evident based on relative atomic content for the silicon-nitrogen and silicon-phosphorus compounds. The binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives are predicted to display potentially tunable thermodynamic stability and redox behavior depending on the atom identities and relative positions.

Polyhedral cubane derivatives are high priority synthetic targets because of their possible applications in nanoscale architectures and high energy density materials, as well as being of fundamental interest in or-

ganic chemistry due to the high strain and unusual bonding arrangements in these molecules and potential for a large number of thermal and excited state intramolecular rearrangements [1] [2] [3] [4] [5] [6]. In addition to the parent hydrocarbon cubane with a carbon skeleton [1], the edge atoms in this cubyl structure may be replaced by any atom capable of trivalent bonding or higher, facilitating access to a large number of possible analogs (having up to 8 different atoms). Cubane can be represented in two-dimensional planar graph format where intersections represent vertex atoms on the cube according to the system developed by Balaban et al. [5] [8] (Figure 1).

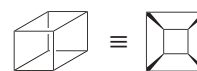


Figure 1: Three dimensional and two dimensional planar graph representations of cubane.

According to this system, there are 20 binary cubanoids having two different atoms (e.g. X and Y) where the number of atoms  $X > 1$ ,  $Y > 1$ , and  $X + Y = 8$  (Figure 2.)

In the current study, we investigated the gas phase standard state (298.15 K, 1 atm) structures (provided in cartesian coordinates as part of the Supporting Information), enthalpies of formation ( $\Delta_f H_{(g)}^\circ$ ), and ionization energies (IEs) for the parent and binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives (Table 1). Prior work has considered a limited subset of these compounds (see, e.g., ref. [7] [8] [9] [10] [11] [12] [13] [14] [15] [16] [17] [18], and references therein). Calculations were conducted using Gaussian 09 [19] at the G4MP2 [20] composite method level of theory. All structures reported herein were confirmed as true minima with no imaginary frequencies. Several neutral and cationic compounds converged with one or more imaginary frequencies; these were omitted from further analysis,

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and the corresponding structural details,  $\Delta_f H_{(g)}^\circ$ , and IEs are not reported.

Several general structure-property trends are evident in the theoretical data. All derivatives - with the single exception of the silicon-nitrogen cubane **10** ( $\Delta_f H_{(g)}^\circ = -4.6$  kcal mol<sup>-1</sup>) - have estimated  $\Delta_f H_{(g)}^\circ > 0$ . Increasing nitrogen content among the carbon-nitrogen and silicon-nitrogen cubanes increases their  $\Delta_f H_{(g)}^\circ$ ; conversely, increasing phosphorus content within the carbon-phosphorus, nitrogen-phosphorus, and silicon-phosphorus cubanes decreases their  $\Delta_f H_{(g)}^\circ$ . Varying carbon/silicon content in the carbon-silicon cubanes results in no general trends for  $\Delta_f H_{(g)}^\circ$ . Isomerization enthalpies ( $\Delta_{isom} H_{(g)}^\circ$ ) within the homolog groups having more than one isomer (**2-4**; **5-7**; **8-13**; **14-16**; and **17-19**) vary widely with atomic composition and substitution patterns. For example,  $\Delta_{isom} H_{(g)}^\circ$  between the silicon-nitrogen isomers **8** and **10** is  $> 250$  kcal mol<sup>-1</sup>, whereas the corresponding  $\Delta_{isom} H_{(g)}^\circ$  between the carbon-nitrogen isomers is  $< 60$  kcal mol<sup>-1</sup>, and  $< 6$  kcal mol<sup>-1</sup> between the carbon-phosphorus isomers.

Based on our previous G4MP2 studies [17] [18] of various strained compounds, the  $\Delta_f H_{(g)}^\circ$  presented herein are expected to be at or near chemical accuracy ( $\pm 1$  kcal mol<sup>-1</sup>). To the best of our knowledge, among the compounds presented herein, only carbon cubane has an experimental  $\Delta_f H_{(g)}^\circ$  reported at  $148.7 \pm 1$  kcal mol<sup>-1</sup> [21], although Karpushenkava et al. [22] have recently proposed an experimental  $\Delta_f H_{(g)}^\circ$  of  $142.7 \pm 1$  kcal mol<sup>-1</sup> for cubane based on revised sublimation data. Our G4MP2  $\Delta_f H_{(g)}^\circ$  estimate of  $144.1$  kcal mol<sup>-1</sup> lies between these two experimental estimates. Previous  $\Delta_f H_{(g)}^\circ$  estimates for the carbon-nitrogen cubanoids have been reported using the semiempirical AM1, PM3, and MNDO methods [8] [10]. As expected for such strained compounds, there is only modest agreement between these prior estimates and the current G4MP2 data. We find reasonable agreement with the MP2/6-31G\*  $\Delta_f H_{(g)}^\circ$  estimates for various carbon-nitrogen cubanoids reported by Engelke [11]. For example, Engelke's [11]  $\Delta_f H_{(g)}^\circ$  MP2/6-31G\* estimate for the carbon-nitrogen compound **20** was  $380.9$  kcal mol<sup>-1</sup>, in excellent agreement with our G4MP2 estimate of  $379.6$  kcal mol<sup>-1</sup>. Similarly, Engelke's [11]  $\Delta_f H_{(g)}^\circ$  value at the MP2/6-31G\* level of theory for N<sub>8</sub> ( $442.6$  kcal mol<sup>-1</sup>) is also in good agreement with our value of  $436.2$  kcal mol<sup>-1</sup>. Differences from several kcal mol<sup>-1</sup> up to  $> 10$  kcal mol<sup>-1</sup> are evident between the MP2/6-31G\* and G4MP2  $\Delta_f H_{(g)}^\circ$  estimates

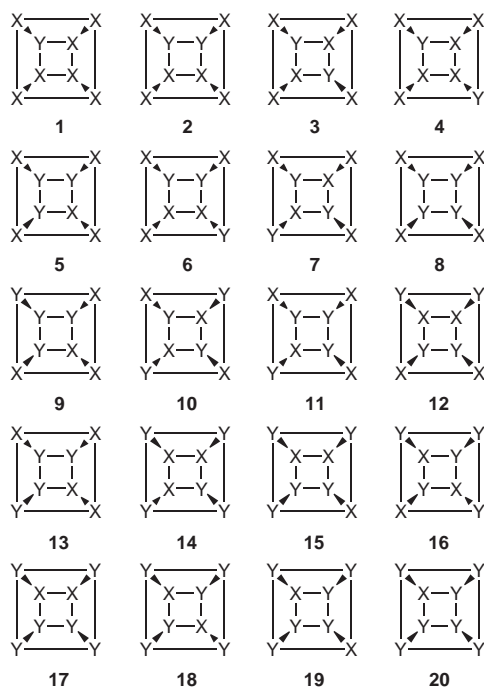


Figure 2: Planar graph representations of the 20 binary cubanoids having two different atoms denoted X and Y where the number of atoms  $X > 1$ ,  $Y > 1$ , and  $X + Y = 8$ .

Table 1: Gas phase standard state (298.15 K, 1 atm) enthalpies of formation ( $\Delta_f H_{(g)}^\circ$ ; values in kcal mol<sup>-1</sup>) and ionization energies (IEs; values in eV) for the parent and binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives.

ID	$\Delta_f H_{(g)}^\circ$						IE					
	X=C Y=N	X=C Y=P	X=C Y=Si	X=N Y=P	X=Si Y=N	X=Si Y=P	X=C Y=N	X=C Y=P	X=C Y=Si	X=N Y=P	X=Si Y=N	X=Si Y=P
all X	144.1	144.1	144.1	436.2	137.7	137.7	8.56	8.56	8.56	10.37	7.36	7.36
1	161.0	134.1	138.7	371.6	106.1	112.8	7.93	7.66	8.03	i <sup>a</sup>	7.18	i
2	192.0	124.7	142.8	329.1	150.7	101.4	7.68	7.63	7.60	8.28	6.65	7.25
3	176.7	123.8	126.7	293.8	74.6	87.9	7.98	7.51	7.75	8.67	i	i
4	179.1	124.9	135.2	305.6	94.6	87.9	7.85	7.09	7.55	i	i	i
5	221.3	114.4	139.0	271.7	169.0	87.6	8.17	7.57	7.45	7.93	6.86	7.35
6	208.9	115.4	132.6	252.0	124.0	75.6	7.85	7.18	7.28	7.82	7.04	7.23
7	191.7	112.5	106.4	202.8	36.5	60.5	i	7.62	i	8.29	8.11	7.77
8	265.3	105.4	147.0	i	252.3	86.8	i	7.55	7.60	i	6.42	7.38
9	249.2	103.5	126.7	198.8	167.8	71.0	8.74	7.85	7.63	8.10	7.63	7.43
10	206.1	99.4	76.7	98.9	-4.6	30.2	9.14	7.71	8.05	i	8.90	8.03
11	237.2	104.3	120.1	182.4	135.2	59.8	8.31	7.31	7.21	7.62	7.24	7.34
12	239.8	107.2	133.1	200.6	170.7	63.6	7.89	7.14	7.06	7.27	6.55	7.02
13	251.9	105.4	137.9	216.8	190.3	73.9	8.32	7.23	7.17	7.61	7.49	i
14	294.3	95.5	136.6	168.7	i	70.5	8.78	7.29	7.49	7.75	i	7.25
15	281.3	95.6	128.6	151.0	212.8	58.3	8.49	7.22	6.94	7.22	7.24	7.14
16	264.3	91.6	97.4	97.5	130.3	39.6	8.89	7.43	7.44	i	8.09	7.52
17	337.9	86.8	138.9	137.0	315.4	67.9	9.02	7.25	i	7.15	7.54	7.14
18	322.2	83.8	116.1	89.5	i	49.9	9.18	7.14	7.16	7.59	i	7.26
19	324.0	85.6	128.9	106.7	266.1	53.8	9.10	7.32	6.61	7.00	8.06	7.32
20	379.6	76.4	130.4	83.5	351.6	60.2	i	i	i	7.20	i	i
all Y	436.2	68.9	137.7	68.9	436.2	68.9	10.37	e <sup>b</sup>	7.36	e	10.37	e

<sup>a</sup>  $\geq 1$  imaginary frequency. <sup>b</sup> cationic structure did not converge.

for the other carbon-nitrogen cubanoids ((CH)<sub>7</sub>N to (CH)<sub>2</sub>N<sub>6</sub>) reported in ref. [11].

Increasing nitrogen content of the carbon-nitrogen and nitrogen-phosphorus derivatives increases the IE, increasing silicon content in the carbon-silicon cubanes and phosphorus content of the carbon-phosphorus cubanes decreases the IE, while no IE clear trends are evident based on relative atomic content for the silicon-nitrogen and silicon-phosphorus compounds. As with the  $\Delta_f H_{(g)}^\circ$  data, the only experimentally available IE is for carbon cubane. The NIST evaluated IE for this compound is 8.6 eV [23], equivalent to our G4MP2 estimate of 8.56 eV. For all binary groups, substantial intra-homolog variability in IE is predicted (up to  $\pm 1.5$  eV), with an overall IE range for all binary compounds between about 6.4 and 9.2 eV. Consequently, the binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives display potentially tunable thermodynamic stability and redox behavior depending on the atom identities and relative positions.

## Acknowledgements

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Supporting Information

**Structures, enthalpies of formation, and ionization energies for the parent and binary mixed carbon, silicon, nitrogen, and phosphorus cubane derivatives:  
A G4MP2 theoretical study**

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## G4MP2 Gaussian 09 ARCHIVE ENTRIES

### carbon cubane

```
\\0,1\C,0,0.99589,0.91352,-0.15753\C,0,1.18979,-0.6454
5,-0.13892\C,0,-0.24214,0.74799,-1.11014\C,0,-0.04861,-0.81092,-1.0911
\C,0,-1.18968,0.64564,0.13858\C,0,-0.99598,-0.91331,0.15777\C,0,0.0483
4,0.81069,1.09133\C,0,0.2424,-0.74816,1.11\H,0,2.14235,-1.16139,-0.250
12\H,0,0.43648,-1.34689,1.99868\H,0,1.79298,1.64484,-0.28316\H,0,0.087
76,1.45974,1.9649\H,0,-2.14219,1.16176,0.24947\H,0,-0.43598,1.34656,-1
.99899\H,0,-0.08827,-1.46016,-1.96452\H,0,-1.79319,-1.64445,0.2837\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-308.4144636\CCSD(T)/GTBas1=-308.5151094\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-307.479805\MP2/GTMP2LargeXP=-308.7706148\HF/GFHFB3=-307.4801856\HF/GFHFB4=-307.5017678\G4MP2=-308.9564709
```

### nitrogen cubane

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\\0,1\N,0,0.8234720647,-0.9699647975,-0.3276050168\N,0,0
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0.9492046361\N,0,0.6761081446,1.1168479946,0.1491485092\N,0,-0.6039623
265,-0.3003840639,1.1276043397\N,0,-0.823468919,0.969968536,0.32760446
33\N,0,-0.676104857,-1.1168440678,-0.1491489489\N,0,-0.8955847777,0.15
35493374,-0.9492065854\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-
436.2705071\CCSD(T)/GTBas1=-436.3598848\MP2/GTBas2=0.\MP2/GTBas3=0.\HF
F/GTMP2LargeXP=-435.0895821\MP2/GTMP2LargeXP=-436.7114442\HF/GFHFB3=-4
35.0927098\HF/GFHFB4=-435.1208519\G4MP2=-436.9940013
```

### phosphorus cubane

```
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9032677352\P,0,-1.103309374,-1.5338788985,0.6405982779\P,0,1.934140539
3,-0.4667175677,0.1430585431\P,0,0.3808711658,-1.606601032,-1.11968375
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```

### silicon cubane

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,-0.4732552061\Si,0,-0.0588572603,-1.7659950936,1.0888246241\Si,0,-0.0
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,-0.466707011\Si,0,0.0589159446,1.7659733601,-1.088925821\Si,0,-1.6551
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18\H,0,2.9755818406,1.7923491386,0.8021019855\H,0,-2.8425947392,1.9924
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```

### carbon cubane<sup>+</sup>

```
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211696,-1.117466341\C,0,0.0750577044,-0.7450390144,-1.1807757488\C,0,-
```

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,0.307454612\C,0,0.059055319,0.8244854284,1.0963221975\C,0,0.221347333  
6,-0.7350989431,1.121734578\H,0,2.1110162292,-1.2117430369,-0.18670616  
43\H,0,0.493079862,-1.385804822,1.9490653145\H,0,1.8025947131,1.643992  
7805,-0.2979992602\H,0,0.0789566367,1.4588808032,1.9776841959\H,0,-2.1  
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689701757\H,0,-0.1527875055,-1.5005050851,-1.9291842416\H,0,-1.7715436  
711,-1.6761694759,0.2059453455\\Version=EM64L-G09RevA.02\State=2-A\MP2  
/GTBas1=-308.1035331\CCSD(T)/GTBas1=-308.2103481\MP2/GTBas2=0.\MP2/GTB  
as3=0.\HF/GTMP2LargeXP=-307.2008526\MP2/GTMP2LargeXP=-308.4446408\HF/G  
FHF3=-307.2010446\HF/GFHF4=-307.2229571\G4MP2=-308.640414

#### nitrogen cubane<sup>+</sup>

\\1,2\N,0,0.8566611538,-1.0039373785,-0.3333592372  
\N,0,0.5833998028,0.2998459227,-1.0716318971\N,0,0.9307755522,-0.16432  
38997,0.9796218081\N,0,0.6510105955,1.0667748735,0.1279450533\N,0,-0.5  
833971122,-0.2998432705,1.0716317151\N,0,-0.8566586202,1.003939691,0.3  
333593351\N,0,-0.6510080486,-1.0667724208,-0.1279450653\N,0,-0.9307733  
234,0.1643264823,-0.979621712\\Version=EM64L-G09RevA.02\State=2-A\MP2/  
GTBas1=-435.9025719\CCSD(T)/GTBas1=-435.9791324\MP2/GTBas2=0.\MP2/GTBa  
s3=0.\HF/GTMP2LargeXP=-434.7081061\MP2/GTMP2LargeXP=-436.3395922\HF/GF  
HF3=-434.7109636\HF/GFHF4=-434.7400768\G4MP2=-436.6124347

#### silicon cubane<sup>+</sup>

\\1,2\Si,0,1.8201108325,1.0951703353,0.48965798  
23\Si,0,0.1019694117,0.4767768876,1.9958894208\Si,0,1.6932552944,-1.07  
90659435,-0.4377839273\Si,0,-0.1409855044,-1.7686562331,1.0374250041\S  
i,0,-0.1019537764,-0.4768526167,-1.9959033916\Si,0,-1.8201121185,-1.09  
52828429,-0.489692516\Si,0,0.1409542021,1.7685611596,-1.0374231905\Si,  
0,-1.6932910913,1.0789341049,0.4377768918\H,0,0.0544600387,0.758466684  
3,3.453712635\H,0,3.0550630227,1.8376123514,0.8230087667\H,0,-2.834461  
2466,1.9586401783,0.799086221\H,0,-0.1234521743,-3.0146649352,1.845841  
2086\H,0,-3.0550629234,-1.8377256704,-0.8230474244\H,0,2.8344280805,-1  
.9588055348,-0.7990202\H,0,0.1233483239,3.0146454504,-1.8457207311\H,  
0,-0.0544803717,-0.7585033752,-3.4537349294\\Version=EM64L-G09RevA.02\  
State=2-A\MP2/GTBas1=-2316.3268709\CCSD(T)/GTBas1=-2316.4543547\MP2/GT  
Bas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2315.9013568\MP2/GTMP2LargeXP=-  
2316.8168622\HF/GFHF3=-2315.931904\HF/GFHF4=-2315.9529328\G4MP2=-231  
7.1182045

### 1. Carbon-nitrogen cubanoids

#### CN1

\\0,1\N,0,0.0090243209,0.0086588479,0.0087444452\C,0  
,1.5409428545,0.0119340013,0.0117367326\C,0,0.0287594651,1.5405208852,  
0.0119222531\C,0,1.5871203403,1.5697973682,-0.0136190656\C,0,0.0196156  
732,1.58730369,1.5704073226\C,0,1.5944346138,1.5776073826,1.5614472483  
\C,0,0.0285750171,0.0287342605,1.5403288208\C,0,1.5869150684,0.0025278  
825,1.5700553116\H,0,2.0705457781,-0.665665641,-0.658848691\H,0,-0.643  
1527986,2.0768016095,-0.6590510251\H,0,2.2138711631,2.1897841976,-0.65  
23903633\H,0,-0.6062109254,2.2205762181,2.1968974432\H,0,2.2290733803,  
2.2057429129,2.1829118565\H,0,-0.6435460378,-0.6361241937,2.0839440621  
\H,0,2.2132320871,-0.6299994217,2.1968136491\\Version=EM64L-G09RevA.02\  
\State=1-A\MP2/GTBas1=-324.4307101\CCSD(T)/GTBas1=-324.5274603\MP2/GTB  
as2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-323.4713269\MP2/GTMP2LargeXP=-32  
4.7986473\HF/GFHF3=-323.4718301\HF/GFHF4=-323.4939268\G4MP2=-324.992  
4159



**CN2**

\\0,1\N,0,0.0141532367,-0.0293124425,0.0134346192\C,  
0,1.5412390585,0.0133593751,0.0144193573\N,0,-0.0220914716,1.527541961  
7,0.0133589611\C,0,1.5052675688,1.556174626,0.0144708844\C,0,-0.001524  
3003,1.520986002,1.5408873104\C,0,1.5588278849,1.5759757547,1.57506123  
31\C,0,0.0344982047,-0.0218271036,1.5409091905\C,0,1.595659281,-0.0039  
90992,1.5750690394\H,0,2.0904664653,-0.6341114318,-0.6684827964\H,0,2.  
0236767968,2.2287818531,-0.6682176929\H,0,-0.6927808896,2.1651574575,2  
.0835032934\H,0,2.1728369425,2.2243648954,2.1962002511\H,0,-0.62576523  
26,-0.6977478133,2.0834921221\H,0,2.239336455,-0.6230521423,2.19609422  
73\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-340.4228811\CCSD(T)  
/GTbas1=-340.5176019\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-339.  
434019\MP2/GTMP2LargeXP=-340.8011982\HF/GFHFB3=-339.4348824\HF/GFHFB4=  
-339.457626\G4MP2=-341.0058191

**CN3**

\\0,1\N,0,0.006973042,0.0063945569,0.008213109\C,0,1  
.5258664699,0.0291214231,0.0243617238\C,0,0.0902038592,1.523175503,0.0  
243995235\N,0,1.6088062919,1.5456250759,-0.0103217491\C,0,0.0425815063  
,1.5913389105,1.5696312073\C,0,1.6048405711,1.541779456,1.5252862207\C  
,0,0.0294287227,0.027933471,1.5435089912\C,0,1.5921185987,-0.021213674  
4,1.5695894476\H,0,2.0879059659,-0.564491697,-0.6983361899\H,0,-0.4805  
581517,2.1084416363,-0.6982698231\H,0,-0.5730623765,2.2394854893,2.189  
0585485\H,0,2.2904527598,2.2005950019,2.0561539398\H,0,-0.6496984199,-  
0.6246646708,2.0901566189\H,0,2.2152411607,-0.6622204819,2.1889684317\  
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-340.449117\CCSD(T)/GTB  
as1=-340.5416754\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-339.4654  
39\MP2/GTMP2LargeXP=-340.8285643\HF/GFHFB3=-339.4659929\HF/GFHFB4=-339  
.4886914\G4MP2=-341.0300923

**CN4**

\\0,1\N,0,0.0081178998,0.0081282226,0.0077062385\C,0  
,1.5453497983,0.011771753,0.0119793095\C,0,0.0258898357,1.5453046952,0  
.0117791714\C,0,1.5730104269,1.5585352776,0.0255999771\C,0,0.053326263  
8,1.5724118648,1.5585041218\N,0,1.5905484359,1.576180059,1.5628314719\  
C,0,0.0258465328,0.0256439138,1.5449357319\C,0,1.5729662215,0.03900197  
19,1.5586945964\H,0,2.0778167926,-0.663889304,-0.6577453276\H,0,-0.644  
8058184,2.0839245116,-0.6580776257\H,0,2.2442634217,2.2234520812,-0.51  
83608596\H,0,-0.4792357049,2.2480191872,2.2282057198\H,0,-0.6453320097  
, -0.6393255559,2.0889240635\H,0,2.2437379041,-0.499558678,2.2285234112  
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-340.4438614\CCSD(T)/G  
Tbas1=-340.5369569\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-339.45  
95711\MP2/GTMP2LargeXP=-340.8240505\HF/GFHFB3=-339.4602688\HF/GFHFB4=-  
339.4828795\G4MP2=-341.0263034

**CN5**

\\0,1\N,0,-0.0123186883,-0.012858425,0.0141271145\N,  
0,1.5338793057,0.0202226166,0.0180957022\N,0,-0.0636313617,1.532844420  
3,0.018166603\C,0,1.4458664918,1.5271628361,0.0369162985\C,0,-0.053132  
5255,1.5333405367,1.5460192406\C,0,1.512311731,1.5972676588,1.58400745  
48\C,0,-0.0116461014,-0.0122225058,1.5405931373\C,0,1.5338783789,0.030  
6701544,1.5459487293\H,0,2.0000744535,2.1125064921,-0.6974682761\H,0,-  
0.7492005971,2.1740756128,2.0845988198\H,0,2.1282228133,2.2477158353,2  
.2002839507\H,0,-0.6625628092,-0.6996971674,2.0778418082\H,0,2.2116589  
09,-0.6294280648,2.0844694173\\Version=EM64L-G09RevA.02\State=1-A\MP2/  
GTbas1=-356.4179189\CCSD(T)/GTbas1=-356.5102199\MP2/GTbas2=0.\MP2/GTba

s3=0.\HF/GTMP2LargeXP=-355.4002307\MP2/GTMP2LargeXP=-356.8069698\HF/GF  
HF3=-355.4013128\HF/GFHFB4=-355.4247116\G4MP2=-357.0220102

**CN6**

\\0,1\N,0,0.0150557789,-0.0333184305,0.0136775907\C,  
0,1.5489888106,0.0133732898,0.0147386792\N,0,-0.023582516,1.529941135,  
0.01175521\C,0,1.4905631957,1.5438172315,0.0555533382\C,0,0.0372000251  
,1.5097130444,1.525237508\N,0,1.5579821201,1.5717717254,1.5767172799\C  
,0,0.0325663511,-0.0222099137,1.548181224\C,0,1.5819154282,0.030030392  
4,1.5646207419\H,0,2.100134991,-0.6282630729,-0.670825871\H,0,2.050406  
3529,2.2717773594,-0.5326682699\H,0,-0.5612959303,2.2104933161,2.10838  
85864\H,0,-0.6315847892,-0.6923579836,2.0915625694\H,0,2.2661501818,-0  
.4957680933,2.2290614132\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas  
1=-356.4387593\CCSD(T)/GTBas1=-356.5295039\MP2/GTBas2=0.\MP2/GTBas3=0.  
\HF/GTMP2LargeXP=-355.4249499\MP2/GTMP2LargeXP=-356.8289291\HF/GFHFB3=  
-355.4259364\HF/GFHFB4=-355.4492277\G4MP2=-357.0417399

**CN7**

\\0,1\N,0,0.0054589351,0.0059453978,0.0056008385\C,0  
,1.5113583346,0.0449831072,0.0449936461\C,0,0.0867172088,1.5272184491,  
0.0226001903\N,0,1.6091219226,1.5464340222,-0.034515047\C,0,0.06195041  
48,1.5911867589,1.5729851367\C,0,1.6093555874,1.5062048705,1.488346886  
9\C,0,0.0863662916,0.0401715501,1.5267647303\N,0,1.6090174166,-0.01593  
20738,1.5474638899\H,0,2.1164078851,-0.6013115991,-0.5933065143\H,0,-0  
.4942751282,2.1140066554,-0.6882517962\H,0,-0.5409459235,2.2339880004,  
2.208314928\H,0,2.3500240094,2.0745231781,2.0500608094\H,0,-0.49515695  
42,-0.6639183168,2.1211423014\\Version=EM64L-G09RevA.02\State=1-A\MP2/  
GTBas1=-356.469183\CCSD(T)/GTBas1=-356.5572273\MP2/GTBas2=0.\MP2/GTBas  
3=0.\HF/GTMP2LargeXP=-355.4615046\MP2/GTMP2LargeXP=-356.8599012\HF/GFH  
FB3=-355.4620314\HF/GFHFB4=-355.4854033\G4MP2=-357.0690568

**CN8**

\\0,1\N,0,-0.0089656558,-0.0094906968,0.0267403315\N  
,0,1.5211123723,-0.0090579969,0.0269157831\N,0,-0.0094234744,1.5205855  
381,0.0268534568\N,0,1.5206590755,1.5210254405,0.0270145248\C,0,-0.019  
3222056,1.5305012824,1.5504340812\C,0,1.5305234235,1.5306671998,1.5505  
857284\C,0,-0.0191614176,-0.0193456948,1.5503084262\C,0,1.5306839209,-  
0.0191763958,1.5504952694\H,0,-0.6894952996,2.2007804312,2.0852936467\  
H,0,2.2007917471,2.2007442514,2.0855803551\H,0,-0.6895385564,-0.689501  
3297,2.0850679508\H,0,2.2007360702,-0.6895320293,2.0854104458\\Version  
=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-372.3872455\CCSD(T)/GTBas1=-37  
2.4790202\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.3375229\MP2  
/GTMP2LargeXP=-372.7861806\HF/GFHFB3=-371.3391266\HF/GFHFB4=-371.36346  
88\G4MP2=-373.0146803

**CN9**

\\0,1\N,0,-0.0015857045,-0.0017873802,-0.0015596273\  
N,0,1.5361482404,0.0223600176,0.0232341783\N,0,-0.0484658622,1.5354955  
958,0.023419938\C,0,1.4613932066,1.5303689641,0.0795349688\C,0,-0.0611  
441432,1.4600464156,1.5322062947\C,0,1.4878507072,1.5579385425,1.63471  
27354\N,0,-0.0485635412,-0.0508024882,1.5349931839\C,0,1.4613618726,0.  
0058887523,1.5323767474\H,0,2.0367489269,2.1330095209,-0.6224943626\H,  
0,-0.8168357909,2.0015151396,2.1003150189\H,0,2.0855933823,2.184018694  
7,2.2915140892\H,0,2.0368987058,-0.7241517746,2.1005468354\\Version=EM  
64L-G09RevA.02\State=1-A\MP2/GTBas1=-372.4153567\CCSD(T)/GTBas1=-372.5  
048725\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.3692083\MP2/GT  
MP2LargeXP=-372.815342\HF/GFHFB3=-371.3703589\HF/GFHFB4=-371.39445\G4M

P2=-373.0403039

**CN10**

\\0,1\N,0,0.0047698944,0.0051388136,0.0045927332\C,0  
,1.5157065018,0.0429323478,0.0418089528\C,0,0.1006242058,1.513341188,0  
.0418273828\N,0,1.6090117101,1.5489257563,-0.053115084\N,0,0.063811140  
3,1.6072449949,1.5501527011\C,0,1.5696614313,1.5117731971,1.4574954187  
\C,0,0.1005709137,0.0965900373,1.5102170788\N,0,1.6087510779,0.0035686  
527,1.5502845918\H,0,2.1209298096,-0.6093652419,-0.5871870773\H,0,-0.5  
280199474,2.1432606703,-0.5870301458\H,0,2.2219792794,2.1399410534,2.0  
635825006\H,0,-0.5282960169,-0.5092514695,2.1620709472\\Version=EM64L-  
G09RevA.02\State=1-A\MP2/GTbas1=-372.4904559\CCSD(T)/GTbas1=-372.57370  
73\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-371.4589175\MP2/GTMP2L  
argeXP=-372.892276\HF/GFHFB3=-371.4593319\HF/GFHFB4=-371.4834527\G4MP2  
=-373.1088947

**CN11**

\\0,1\N,0,0.019497654,-0.0337365198,0.0161168213\C,0  
,1.5143183412,0.0459808223,0.0517416082\N,0,0.0112907226,1.5195887094,  
0.0159931365\N,0,1.5642499114,1.5412018065,-0.0110383683\C,0,0.0406884  
337,1.5172022165,1.5492043114\C,0,1.5756712716,1.4933634969,1.50398227  
74\C,0,0.0936481875,-0.0175963924,1.530039293\N,0,1.6207939516,-0.0325  
189651,1.5563002714\H,0,2.1333686764,-0.5724250696,-0.6004426071\H,0,-  
0.6241760429,2.1788344956,2.099594793\H,0,2.2921989277,2.0867987291,2.  
0710680066\H,0,-0.475850035,-0.7352933293,2.1197404566\\Version=EM64L-  
G09RevA.02\State=1-A\MP2/GTbas1=-372.4359046\CCSD(T)/GTbas1=-372.52389  
27\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-371.3932617\MP2/GTMP2L  
argeXP=-372.8364882\HF/GFHFB3=-371.3943684\HF/GFHFB4=-371.4184084\G4MP  
2=-373.059475

**CN12**

\\0,1\C,0,0.0336289391,0.0260819285,0.034775157\N,0,  
1.5512477351,-0.0356511526,0.0080343487\C,0,0.0680617274,1.5433151559,  
0.0346604474\N,0,1.5869282195,1.53609207,0.0079413186\N,0,-0.018937655  
7,1.5726205052,1.5510008298\C,0,1.4986768166,1.510927841,1.5242768784\  
N,0,-0.054561238,0.0008670708,1.5511072449\C,0,1.4643051051,-0.0063032  
44,1.524383221\H,0,-0.5599225795,-0.66213413,-0.5666900556\H,0,-0.4937  
076068,2.2576516844,-0.5668790907\H,0,2.0922680688,2.1991594318,2.1256  
849658\H,0,2.0261124684,-0.720627161,2.1259047349\\Version=EM64L-G09Re  
vA.02\State=1-A\MP2/GTbas1=-372.4312097\CCSD(T)/GTbas1=-372.5198047\MP  
2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-371.3872364\MP2/GTMP2LargeX  
P=-372.8314939\HF/GFHFB3=-371.3885944\HF/GFHFB4=-371.4125472\G4MP2=-37  
3.0553034

**CN13**

\\0,1\N,0,-0.011236735,-0.0093034103,0.0203137717\N,  
0,1.5222182748,0.0200116303,-0.0100118218\N,0,-0.0711963577,1.53947557  
33,0.0195851363\C,0,1.4426137266,1.5259285567,-0.0042212634\C,0,-0.020  
7621538,1.5412098335,1.5538710804\C,0,1.5332574562,1.5668491341,1.5272  
5007\C,0,0.0691227608,0.0094008161,1.5260866401\N,0,1.5829488365,0.032  
5820302,1.5386853754\H,0,1.9835403748,2.1061351195,-0.7513953479\H,0,-  
0.7052852448,2.1765141603,2.1126841792\H,0,2.2183571833,2.1307851176,2  
.1573847894\H,0,-0.4718781218,-0.7324885611,2.1129673907\\Version=EM64  
L-G09RevA.02\State=1-A\MP2/GTbas1=-372.4102552\CCSD(T)/GTbas1=-372.500  
3732\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-371.3633424\MP2/GTMP  
2LargeXP=-372.8103101\HF/GFHFB3=-371.3646909\HF/GFHFB4=-371.3887336\G4  
MP2=-373.0361033

**CN14**

\\0,1\C,0,0.0060642647,0.0061924742,0.0047554916\C,0  
,1.5442290159,0.0285647147,0.0270430396\C,0,0.070169119,1.5431839772,0  
.0270447843\N,0,1.5852506425,1.5430918033,-0.0274192141\N,0,0.04897798  
8,1.5529504492,1.5341852881\N,0,1.5696688173,1.5279273865,1.5137238667  
\N,0,0.0176965107,0.0175092578,1.5374123647\N,0,1.5534190509,0.0071181  
853,1.5341833244\H,0,-0.6724906199,-0.6542052679,-0.5299106173\H,0,2.2  
598628613,-0.5646857878,-0.5404621086\H,0,-0.5034476505,2.2746528077,-  
0.5404562193\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-388.38236  
72\CCSD(T)/GTBas1=-388.4716617\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar  
geXP=-387.3032592\MP2/GTMP2LargeXP=-388.7925679\HF/GFHFB3=-387.3049837  
\HF/GFHFB4=-387.3299247\G4MP2=-389.0314521

**CN15**

\\0,1\C,0,0.0397654607,0.0352959313,0.0385463179\N,0  
,1.550903784,-0.0102401373,-0.0169970051\C,0,0.063075652,1.5557962808,  
0.0284257223\N,0,1.5834636259,1.5489288111,-0.0308790676\N,0,0.0251448  
451,1.5833366582,1.5492631847\C,0,1.52052825,1.4745001389,1.4675222244  
\N,0,0.0046221944,0.0239001918,1.5509384794\N,0,1.5422136847,-0.015674  
047,1.5213553338\H,0,-0.5574339316,-0.6713726642,-0.5350268489\H,0,-0.  
5183577648,2.2636752268,-0.5603824462\H,0,2.1750741994,2.0752536095,2.  
0999341053\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-388.4051504  
\CCSD(T)/GTBas1=-388.4927608\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar  
geXP=-387.3283023\MP2/GTMP2LargeXP=-388.8156093\HF/GFHFB3=-387.3298516\H  
F/GFHFB4=-387.3546146\G4MP2=-389.0520688

**CN16**

\\0,1\C,0,0.0487682771,0.0429197822,0.0419616221\N,0  
,1.5627272876,-0.0059592445,-0.0058134073\N,0,-0.0353177051,1.53909161  
57,-0.0311517368\C,0,1.4622043868,1.5050688182,0.0531408099\N,0,-0.050  
475482,1.5410755042,1.5146056865\N,0,1.4940400936,1.5792141087,1.55138  
21761\N,0,-0.0355447237,-0.0040297066,1.5393577806\C,0,1.462462737,0.0  
795187998,1.5039954666\H,0,-0.5691637788,-0.5972976033,-0.5872732115\H  
,0,2.0859777611,2.1493999833,-0.5660968684\H,0,2.0865211464,-0.5284020  
576,2.1586916822\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-388.4  
350557\CCSD(T)/GTBas1=-388.5199394\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP  
2LargeXP=-387.3634255\MP2/GTMP2LargeXP=-388.8462949\HF/GFHFB3=-387.364  
5329\HF/GFHFB4=-387.3893688\G4MP2=-389.0791545

**CN17**

\\0,1\C,0,0.0283991612,0.0241197991,0.0274902649\N,0  
,1.5398005431,-0.0134323656,-0.0167503084\C,0,0.0570408924,1.547148155  
2,0.027756615\N,0,1.5687722457,1.5278909917,-0.0164835393\N,0,0.031999  
0734,1.5565150515,1.5400195064\N,0,1.556186669,1.5108551022,1.50856043  
93\N,0,0.0030242784,0.0151925274,1.5397661332\N,0,1.5278472103,0.00355  
29371,1.5083068782\H,0,-0.5687166982,-0.6800672367,-0.5491052261\H,0,-  
0.5131533754,2.2735250381,-0.5485607634\\Version=EM64L-G09RevA.02\Stat  
e=1-A\MP2/GTBas1=-404.3519856\CCSD(T)/GTBas1=-404.4407715\MP2/GTBas2=0  
4472\HF/GFHFB3=-403.2423784\HF/GFHFB4=-403.2682405\G4MP2=-405.0248821

**CN18**

\\0,1\C,0,0.048659493,0.0506116867,0.039493758\N,0,1  
.5500066087,0.0111020568,-0.0478096286\N,0,-0.0446032142,1.5496049218,  
-0.0473754407\C,0,1.4582197664,1.5115882382,0.0100626964\N,0,-0.010026  
2396,1.5475073311,1.5033888068\N,0,1.5160823683,1.5711270699,1.5003013

856\N,0,0.0212470478,0.0217917919,1.531511574\N,0,1.5470946312,0.04514  
96633,1.5029648935\H,0,-0.5841073466,-0.6050671787,-0.5581223636\H,0,2  
.0785268851,2.154684419,-0.6137156814\\Version=EM64L-G09RevA.02\State=  
1-A\MP2/GTbas1=-404.3798235\CCSD(T)/GTbas1=-404.4662136\MP2/GTbas2=0.\  
MP2/GTbas3=0.\HF/GTMP2LargeXP=-403.2704461\MP2/GTMP2LargeXP=-404.80080  
1\HF/GFHFB3=-403.272208\HF/GFHFB4=-403.2979073\G4MP2=-405.0498718

**CN19**

\\0,1\C,0,0.0614761721,0.0593391652,0.0586737536\N,0  
,1.5527444315,-0.0158009926,-0.0151223039\N,0,0.0101491276,1.551937840  
6,-0.0160516136\N,0,1.5545375981,1.5288312477,-0.0381001591\N,0,0.0115  
876309,1.5537590906,1.5289445149\C,0,1.5028574823,1.4786101778,1.45514  
25223\N,0,0.0097787914,0.0091299424,1.5519171349\N,0,1.5541698185,-0.0  
139875179,1.5298778435\H,0,-0.5773513993,-0.5702340244,-0.5604818435\H  
,0,2.1416503469,2.1082150706,2.0743001509\\Version=EM64L-G09RevA.02\St  
ate=1-A\MP2/GTbas1=-404.3768939\CCSD(T)/GTbas1=-404.4637592\MP2/GTbas2  
=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-403.2663762\MP2/GTMP2LargeXP=-404.7  
974491\HF/GFHFB3=-403.268189\HF/GFHFB4=-403.2937373\G4MP2=-405.0468895

**CN20**

\\0,1\C,0,0.0501573676,0.0486202758,0.0478767596\N,0  
,1.5434631964,-0.0174207517,-0.0173666345\N,0,0.0054131406,1.542648188  
7,-0.0177895\N,0,1.5371704597,1.5145816659,-0.0189371218\N,0,0.0260747  
045,1.536663587,1.5142007794\N,0,1.5375139557,1.5150844418,1.492753106  
1\N,0,0.0053082997,0.0049581508,1.5426210265\N,0,1.5371232639,0.003455  
5871,1.5145377448\H,0,-0.5878243881,-0.5804911453,-0.5719961601\\Versi  
on=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-420.3247969\CCSD(T)/GTbas1=-  
420.4126949\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-419.1793896\M  
P2/GTMP2LargeXP=-420.755801\HF/GFHFB3=-419.181795\HF/GFHFB4=-419.20854  
67\G4MP2=-421.0213603

**CN1<sup>+</sup>**

\\1,2\N,0,0.0738784183,0.0725355338,0.07208677  
11\C,0,1.5817736884,0.0089126808,0.0088012037\C,0,0.0258351023,1.58125  
0675,0.0085228557\C,0,1.5910554256,1.5743235064,-0.0290054629\C,0,0.00  
48036378,1.5913557206,1.5743394982\C,0,1.5771012974,1.5599019944,1.543  
9871923\C,0,0.0255768674,0.0255701435,1.5812705027\C,0,1.5909269154,-0  
.012640866,1.5748234046\H,0,2.0930132743,-0.6733226281,-0.6663903699\H  
,0,-0.6510569672,2.0994457746,-0.6667454293\H,0,2.2015800442,2.1785055  
06,-0.692475764\H,0,-0.6458893482,2.2090635847,2.1850991083\H,0,2.2110  
918412,2.1871476188,2.1647318165\H,0,-0.6517468146,-0.643877292,2.1063  
944347\H,0,2.2012566176,-0.6699719523,2.1858602385\\Version=EM64L-G09R  
evA.02\State=2-A\MP2/GTbas1=-324.1438138\CCSD(T)/GTbas1=-324.2511164\M  
P2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-323.2193623\MP2/GTMP2Large  
XP=-324.4943563\HF/GFHFB3=-323.2196978\HF/GFHFB4=-323.2419888\G4MP2=-3  
24.7003332

**CN2<sup>+</sup>**

\\1,2\N,0,0.059401188,0.0471004895,0.059769081  
1\C,0,1.5895828374,0.0117434302,-0.0150569475\N,0,0.0265875013,1.45332  
987,0.0597822585\C,0,1.5534541044,1.5601015548,-0.014970332\C,0,-0.030  
4446024,1.5230509918,1.5895538534\C,0,1.5429071184,1.5656893079,1.5592  
095001\C,0,0.0057462499,-0.0253068373,1.589536524\C,0,1.5793728384,0.0  
055497587,1.5591231973\H,0,2.0891474755,-0.675455968,-0.6901671728\H,0  
,2.0204188124,2.2699266847,-0.6900059941\H,0,-0.7154690522,2.205925556  
7,2.0814944824\H,0,2.1464435767,2.2297151413,2.1703188837\H,0,-0.64662  
94639,-0.7394497579,2.081457614\H,0,2.2132814161,-0.6296202225,2.17015

50519\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-340.158347\\CCSD(T)/GTBas1=-340.2501888\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-339.1855654\\MP2/GTMP2LargeXP=-340.5216117\\HF/GFHFB3=-339.186074\\HF/GFHFB4=-339.2092264\\G4MP2=-340.7227799

**CN3+**

\\1,2\\N,0,0.0517204743,0.0493763486,0.04704359  
98\\C,0,1.5706240256,-0.0175048644,0.0191272294\\C,0,0.0453843486,1.5697436821,0.01916758\\N,0,1.5645345585,1.5030945926,0.0295425332\\C,0,0.0141475308,1.6208599949,1.5636794447\\C,0,1.5854116159,1.5230970801,1.5251114939\\C,0,0.0488560194,0.0466055725,1.5428831265\\C,0,1.6204787018,-0.0508099092,1.5636393876\\H,0,2.0989355981,-0.5765203016,-0.7472522874\\H,0,-0.4921667276,2.1199205798,-0.7471828024\\H,0,-0.5862047996,2.2533965094,2.2080759075\\H,0,2.2698431047,2.1807796549,2.0585208675\\H,0,-0.6290670584,-0.6048265385,2.0920410368\\H,0,2.2286026079,-0.6759124012,2.2080028828\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-340.1709512\\CCSD(T)/GTBas1=-340.263214\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-339.1957459\\MP2/GTMP2LargeXP=-340.534509\\HF/GFHFB3=-339.1961053\\HF/GFHFB4=-339.2190362\\G4MP2=-340.7360338

**CN4+**

\\1,2\\N,0,0.0429148839,0.042342667,0.042048607  
7\\C,0,1.5640051989,0.0084965082,0.0085158627\\C,0,0.0229620361,1.5636805323,0.0087065825\\C,0,1.5764869162,1.5620128655,0.007020775\\C,0,0.0348195291,1.575740895,1.5619891378\\N,0,1.555911389,1.5418617434,1.5284360284\\C,0,0.0222876051,0.0222224816,1.5634629081\\C,0,1.5758112699,0.0205233829,1.5617974465\\H,0,2.1097663158,-0.6593333556,-0.6532172251\\H,0,-0.6397307543,2.1153556514,-0.653286676\\H,0,2.2394601165,2.2189383403,-0.5503681257\\H,0,-0.5109361611,2.2435726256,2.2237250392\\H,0,-0.640730055,-0.6346628997,2.1208471944\\H,0,2.2384717101,-0.531151438,2.2238224446\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-340.1784488\\CCSD(T)/GTBas1=-340.2629258\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-339.1853617\\MP2/GTMP2LargeXP=-340.5424637\\HF/GFHFB3=-339.1857856\\HF/GFHFB4=-339.2085863\\G4MP2=-340.7369816

**CN5+**

\\1,2\\N,0,0.0723558148,0.0765674077,0.08524554  
86\\N,0,1.5065829002,0.0286702083,0.0064472642\\N,0,-0.0536997746,1.5060285163,0.0065317785\\C,0,1.4639283357,1.5462355507,-0.0010225778\\C,0,-0.0706296585,1.5313888931,1.5755591594\\C,0,1.4872611329,1.5708090242,1.5623108596\\C,0,-0.022011664,-0.0231671072,1.6057750191\\C,0,1.5328798704,0.0130927848,1.575476604\\H,0,2.0261238872,2.1400305784,-0.7157746495\\H,0,-0.7787199405,2.1919835693,2.0642381408\\H,0,2.113941968,2.2326374295,2.1526572053\\H,0,-0.695745792,-0.734745541,2.072054109\\H,0,2.2311329203,-0.6579313141,2.0641015387\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-356.1216491\\CCSD(T)/GTBas1=-356.2218698\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-355.135976\\MP2/GTMP2LargeXP=-356.4975683\\HF/GFHFB3=-355.1366779\\HF/GFHFB4=-355.1605796\\G4MP2=-356.7210424

**CN6+**

\\1,2\\N,0,0.0501783681,0.0296484754,0.04994828  
17\\C,0,1.5845986557,0.0128194685,-0.0134950182\\N,0,0.0161942658,1.4676690731,0.0495529864\\C,0,1.5334224482,1.5513733637,0.0219677447\\C,0,0.038515594,1.515484824,1.5685369317\\N,0,1.5261703508,1.5453825671,1.5447461488\\C,0,0.0048066376,-0.0242514268,1.5841461877\\C,0,1.5652485298,0.0349200407,1.5482037555\\H,0,2.1136115605,-0.6622484854,-0.6787558049\\H,0,2.0457612803,2.3160665178,-0.5541410819\\H,0,-0.5840016152,2.254366

424,2.1048512371\H,0,-0.6384703572,-0.7268251856,2.10446352\H,0,2.2431  
283162,-0.5054056565,2.2059751113\Version=EM64L-G09RevA.02\State=2-A\  
MP2/GTBas1=-356.166707\CCSD(T)/GTBas1=-356.2550271\MP2/GTBas2=0.\MP2/G  
TBas3=0.\HF/GTMP2LargeXP=-355.1615307\MP2/GTMP2LargeXP=-356.5428569\HF  
/GFHFB3=-355.1621182\HF/GFHFB4=-355.1858472\G4MP2=-356.7527796

**CN9+**

\1,2\N,0,0.0895445798,0.0942709763,0.09829201  
03\N,0,1.5334390728,0.0123944378,0.0132871842\N,0,-0.0579637563,1.5323  
468138,0.0131861531\C,0,1.4802702392,1.5496479315,0.0494096627\C,0,-0.  
0934253561,1.4774904873,1.5507245516\C,0,1.4583913516,1.5274240434,1.6  
026275704\N,0,-0.0581239056,-0.0608662601,1.530651707\C,0,1.480352941,  
-0.025169635,1.5506006496\H,0,2.0477986031,2.1439902438,-0.6597156857\  
H,0,-0.8552511616,2.0107614314,2.1105755247\H,0,2.0561637033,2.1534029  
74,2.2589844511\H,0,2.0482036888,-0.7617934443,2.1101762209\Version=E  
M64L-G09RevA.02\State=2-A\MP2/GTBas1=-372.0948116\CCSD(T)/GTBas1=-372.  
1931153\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.0850742\MP2/G  
TMP2LargeXP=-372.4831444\HF/GFHFB3=-371.0858192\HF/GFHFB4=-371.1104907  
\G4MP2=-372.718228

**CN10+**

\1,2\N,0,-0.0125183323,0.0121014524,0.0114934  
534\C,0,1.4946373532,0.0663576876,0.0640549962\C,0,0.0878231514,1.5236  
870575,-0.0075771387\N,0,1.6016300764,1.5674859214,-0.0456350493\N,0,0  
.1160491245,1.5506235378,1.4957320803\C,0,1.618680867,1.5225412285,1.4  
68685009\C,0,0.0884767891,0.048079474,1.5232632605\N,0,1.6024902634,0.  
0109390694,1.5684297597\H,0,2.1020739502,-0.5871865262,-0.5676702212\H  
,0,-0.5466381305,2.1604115895,-0.6189022645\H,0,2.2527270078,2.1588056  
876,2.08094125\H,0,-0.5459321201,-0.5397461796,2.1818848647\Version=E  
M64L-G09RevA.02\State=2-A\MP2/GTBas1=-372.1524579\CCSD(T)/GTBas1=-372.  
247245\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.1479518\MP2/GT  
MP2LargeXP=-372.5403518\HF/GFHFB3=-371.1481552\HF/GFHFB4=-371.1726767\  
G4MP2=-372.7719684

**CN11+**

\1,2\N,0,0.030002736,-0.0091108474,0.01050374  
12\C,0,1.5347254462,0.0252242078,0.0087781417\N,0,0.0768152361,1.45613  
61643,0.062945435\N,0,1.5397700648,1.5301349434,-0.0160490937\C,0,0.02  
98008274,1.5286520206,1.5942052323\C,0,1.5741887449,1.51481384,1.52571  
33284\C,0,0.0725540155,-0.0161522168,1.5521202859\N,0,1.5810114524,0.0  
058931829,1.5205710954\H,0,2.1594529613,-0.598462496,-0.6250525198\H,0  
, -0.647327461,2.2017292738,2.1102912384\H,0,2.3137189903,2.1101111155,  
2.0544121877\H,0,-0.499013014,-0.7575691882,2.1038609274\Version=EM64  
L-G09RevA.02\State=2-A\MP2/GTBas1=-372.1306741\CCSD(T)/GTBas1=-372.228  
958\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.1099112\MP2/GTMP2  
LargeXP=-372.5197815\HF/GFHFB3=-371.1105769\HF/GFHFB4=-371.1351563\G4M  
P2=-372.7534487

**CN12+**

\1,2\C,0,-0.0033242157,0.0195213069,-0.003512  
9287\N,0,1.5182983274,0.0171405181,0.0408004979\C,0,0.0314654294,1.551  
4995022,-0.0036483697\N,0,1.5516414188,1.4848761387,0.0407418538\N,0,0  
.0139922202,1.5198558281,1.5181985659\C,0,1.5356288502,1.5174815935,1.  
5625857811\N,0,-0.0192552668,0.0521113763,1.5183463811\C,0,1.500924215  
1,-0.0144976345,1.5626494961\H,0,-0.5692879891,-0.7098362359,-0.575228  
3442\H,0,-0.5008238812,2.3056966581,-0.5754797638\H,0,2.1015801036,2.2  
468442022,2.1343071991\H,0,2.033260788,-0.7686932538,2.1344396316\Ver

sion=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-372.1642437\CCSD(T)/GTBas1=-372.2412332\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.1180623\MP2/GTMP2LargeXP=-372.5534024\HF/GFHFB3=-371.1188411\HF/GFHFB4=-371.1433902\G4MP2=-372.7646514

#### CN13<sup>+</sup>

\1,2\N,0,-0.0250837122,0.0093857986,0.0213095  
642\N,0,1.5360489672,0.0212732723,0.0087910859\N,0,-0.026905724,1.4810148038,0.057200328\C,0,1.485039898,1.5424616457,-0.0255896742\C,0,-0.0304089786,1.5303151338,1.5707405439\C,0,1.5429999984,1.5836450489,1.5162421819\C,0,0.0266668613,-0.0118398402,1.5427495535\N,0,1.5386036633,0.0696782972,1.4799042012\H,0,2.0025311125,2.1128885416,-0.7915948011\H,0,-0.6873110799,2.1878240701,2.1347893831\H,0,2.200464586,2.1530198586,2.1685660091\H,0,-0.4909455919,-0.7725666305,2.1200916244\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-372.1240576\CCSD(T)/GTBas1=-372.2050043\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-371.0725314\MP2/GTMP2LargeXP=-372.5120274\HF/GFHFB3=-371.0735025\HF/GFHFB4=-371.0980268\G4MP2=-372.7296201

#### CN14<sup>+</sup>

\1,2\C,0,-0.0008394886,-0.0005209493,-0.03235  
52927\C,0,1.5503669746,0.0038665587,0.0136919583\C,0,0.0456527287,1.5499924365,0.0137003296\N,0,1.5459478433,1.5048401089,0.0250534306\N,0,0.050665227,1.5403516248,1.5481552325\N,0,1.5940651681,1.5516735386,1.5298928778\N,0,0.0859836509,0.0839589618,1.4937633686\N,0,1.5408689037,0.0091590674,1.548145615\H,0,-0.6877050663,-0.6690119251,-0.5434941\H,0,2.2824396257,-0.5899120246,-0.5282284293\H,0,-0.5280455671,2.2979026022,-0.5282249906\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-388.0562217\CCSD(T)/GTBas1=-388.1570606\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-386.9979753\MP2/GTMP2LargeXP=-388.4564408\HF/GFHFB3=-386.999316\HF/GFHFB4=-387.0248842\G4MP2=-388.708154

#### CN15<sup>+</sup>

\1,2\C,0,0.0008524673,0.0245400103,0.00039483  
97\N,0,1.5199103512,0.0372106957,0.013650256\C,0,0.0253144162,1.5601764397,-0.0089024451\N,0,1.5511063424,1.4957475416,0.0048858444\N,0,0.0592776612,1.5286919501,1.5176150419\C,0,1.5633136283,1.478956351,1.5096218238\N,0,0.0358273184,0.069980367,1.5184804347\N,0,1.5665218447,-0.0334486671,1.5457466178\H,0,-0.5681280413,-0.7232038713,-0.5444844783\H,0,-0.5243991836,2.3124243572,-0.5673887446\H,0,2.1994031953,2.1123248257,2.1230808096\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-388.1133955\CCSD(T)/GTBas1=-388.1895842\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-387.0342488\MP2/GTMP2LargeXP=-388.5142975\HF/GFHFB3=-387.0352612\HF/GFHFB4=-387.0606966\G4MP2=-388.7392385

#### CN16<sup>+</sup>

\1,2\C,0,0.0131314072,0.0271928846,0.02671248  
81\N,0,1.5199319468,0.0352430721,0.0345080809\N,0,-0.0381738488,1.5417345185,-0.0264731512\C,0,1.476420397,1.5412905854,0.038759708\N,0,0.0156173295,1.4780321897,1.4523870982\N,0,1.4896753725,1.5817528414,1.5542176336\N,0,-0.0380582086,0.0007480506,1.5420500587\C,0,1.4765240076,0.0657878832,1.5400451187\H,0,-0.6020274449,-0.6122831946,-0.6016347765\H,0,2.099517955,2.1826584901,-0.5797837854\H,0,2.0996410866,-0.5415573209,2.1920115268\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-388.1031322\CCSD(T)/GTBas1=-388.2011341\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-387.0570018\MP2/GTMP2LargeXP=-388.5047053\HF/GFHFB3=-387.0576742\HF/GFHFB4=-387.0831325\G4MP2=-388.751684



**CN17\***

\\1,2\C,0,-0.007655103,0.0169002715,-0.0079727  
 316\N,0,1.5150167329,0.0350982656,0.0198240524\C,0,0.0212871909,1.5557  
 584304,-0.0077021793\N,0,1.5421899353,1.4803068235,0.0200873484\N,0,0.  
 0673383806,1.5077887696,1.5138784409\N,0,1.5886096431,1.5286778085,1.5  
 402366307\N,0,0.0401687109,0.0625776258,1.5136198237\N,0,1.5595617508,  
 -0.0155067996,1.5399734941\H,0,-0.5763687657,-0.7298019287,-0.55573717  
 14\H,0,-0.5189484757,2.3235007336,-0.5552077079\\Version=EM64L-G09RevA  
 .02\State=2-A\MP2/GTBas1=-404.0391288\CCSD(T)/GTBas1=-404.1155972\MP2/  
 GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-402.920716\MP2/GTMP2LargeXP=-  
 404.451894\HF/GFHFB3=-402.9224545\HF/GFHFB4=-402.9490738\G4MP2=-404.69  
 26838

**CN18\***

\\1,2\C,0,0.006758498,0.0072024775,0.040249169  
 \N,0,1.516173693,0.0448305219,0.0062317614\N,0,-0.0096948628,1.5170179  
 278,0.0066658157\C,0,1.5001032703,1.5550055027,0.0090590188\N,0,0.0162  
 348475,1.5213172654,1.4619410211\N,0,1.5416793627,1.5976537264,1.52209  
 74071\N,0,-0.0038787204,-0.0042810645,1.5543760127\N,0,1.5199987347,0.  
 0704667494,1.4615043659\H,0,-0.6076044183,-0.6294143681,-0.59243011\H,  
 0,2.1013295951,2.1783012615,-0.6489944618\\Version=EM64L-G09RevA.02\St  
 ate=2-A\MP2/GTBas1=-404.0603928\CCSD(T)/GTBas1=-404.1356903\MP2/GTBas2  
 =0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-402.9479127\MP2/GTMP2LargeXP=-404.4  
 731119\HF/GFHFB3=-402.9491735\HF/GFHFB4=-402.975636\G4MP2=-404.7119555

**CN19\***

\\1,2\C,0,0.0505417774,0.0151699364,0.01515488  
 39\N,0,1.5694456855,-0.040117361,-0.0390431437\N,0,0.0587633812,1.5167  
 432392,0.0110849191\N,0,1.5056317711,1.5020285327,-0.0027041746\N,0,-0.  
 0051222716,1.5780723163,1.5528631059\C,0,1.5137830587,1.5227869816,1.  
 4986624704\N,0,0.0586907354,0.0359259176,1.5165227621\N,0,1.5055605238  
 ,0.0212143629,1.5027396838\H,0,-0.6201974477,-0.5953503286,-0.58543497  
 11\H,0,2.1845027861,2.1333264029,2.0992544641\\Version=EM64L-G09RevA.0  
 2\State=2-A\MP2/GTBas1=-404.0584813\CCSD(T)/GTBas1=-404.1341939\MP2/GT  
 Bas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-402.944866\MP2/GTMP2LargeXP=-40  
 4.4714665\HF/GFHFB3=-402.9462138\HF/GFHFB4=-402.9725211\G4MP2=-404.711  
 3217

**2. Carbon-phosphorus cubanoids****CP1**

\\0,1\P,0,0.0010627181,0.0008715431,0.0007534707\C,0  
 ,1.9236812456,0.0094611404,0.0074073221\C,0,0.4771441001,1.8634767225,  
 0.0077109409\C,0,2.0083020314,1.5666301675,-0.1408149257\C,0,0.6511640  
 84,1.9066693781,1.5638869983\C,0,2.201403767,1.7173868188,1.4093525517  
 \C,0,0.4770380637,0.3721090293,1.8258786625\C,0,2.0077948697,0.1675849  
 366,1.5636973613\H,0,2.5598678416,-0.6729266,-0.5526593777\H,0,-0.0301  
 25198,2.6465088459,-0.5522593049\H,0,2.6240254982,2.0470298832,-0.9012  
 158052\H,0,0.1682447385,2.6622559777,2.1835826468\H,0,2.9680045684,2.3  
 155229546,1.9004449787\H,0,-0.0302883264,-0.0236547716,2.7034048147\H,  
 0,2.6231799981,-0.484726026,2.1833296657\\Version=EM64L-G09RevA.02\Sta  
 te=1-A\MP2/GTBas1=-610.6934476\CCSD(T)/GTBas1=-610.7962242\MP2/GTBas2=  
 0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-609.7954122\MP2/GTMP2LargeXP=-611.07  
 27997\HF/GFHFB3=-609.8004546\HF/GFHFB4=-609.8221602\G4MP2=-611.2805117

**CP2**

\\0,1\p,0,0.0108681083,-0.038621812,0.0139445171\C,0  
,1.9337735768,0.0004572556,0.0182396631\p,0,0.4218873064,2.2446622458,  
0.0139795482\C,0,2.2104528824,1.5374542884,0.0182494299\C,0,0.77223641  
89,1.796353034,1.8512011132\C,0,2.2896672752,1.5244910679,1.5812387578  
\C,0,0.4954979713,0.2593640068,1.8511883778\C,0,2.0124614712,-0.015107  
5671,1.5812332512\H,0,2.5207466263,-0.6690663286,-0.6094141018\H,0,2.9  
940654397,1.9602705007,-0.6093851037\H,0,0.4210456151,2.4234483062,2.6  
698360366\H,0,3.0846115516,2.0253769272,2.1342447962\H,0,-0.0523841742  
, -0.2058635426,2.6698073125\H,0,2.5827699308,-0.7618183823,2.134236402  
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-912.9704512\CCSD(T)/GT  
bas1=-913.0762029\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-912.11  
04967\MP2/GTMP2LargeXP=-913.3733464\HF/GFHFB3=-912.120513\HF/GFHFB4=-9  
12.1421505\G4MP2=-913.6037347

**CP3**

\\0,1\p,0,0.0204900838,0.0182196877,-0.0032391009\C,  
0,1.9329273953,0.0369130633,0.0099336529\C,0,0.261737045,1.9154699086,  
0.010166328\p,0,2.1261802766,1.8915225585,-0.4155674021\C,0,0.53791990  
85,1.9441245267,1.5507659261\C,0,2.1010678844,1.8689482102,1.497990980  
7\C,0,0.4543314437,0.4039429501,1.8204441579\C,0,1.993735789,0.3076720  
714,1.5505606322\H,0,2.5334145011,-0.7406850444,-0.4564545859\H,0,-0.4  
407193866,2.6024687795,-0.4560405919\H,0,0.0143056816,2.6701402842,2.1  
752048404\H,0,2.7494901121,2.4457134405,2.1550366003\H,0,-0.026195968,  
-0.023651375,2.6985533274\H,0,2.6539152334,-0.2969990613,2.1748452348\  
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-912.9696989\CCSD(T)/GT  
bas1=-913.0745072\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-912.112  
0611\MP2/GTMP2LargeXP=-913.3753014\HF/GFHFB3=-912.1216447\HF/GFHFB4=-9  
12.143547\G4MP2=-913.6051611

**CP4**

\\0,1\p,0,-0.0067444568,-0.0051263694,-0.0050588402\  
C,0,1.9243131091,0.0033662922,0.0023833944\C,0,0.5109517539,1.85532895  
08,0.0023717626\C,0,2.0125214852,1.5358069963,-0.2556306038\C,0,0.5987  
161277,1.922052412,1.5553883394\p,0,2.5297721334,1.9305364097,1.562838  
3802\C,0,0.5105181292,0.3896096997,1.8134110956\C,0,2.0120857076,0.070  
0802839,1.5553979336\H,0,2.5591673562,-0.6848404585,-0.5535123811\H,0,  
0.015097727,2.6489068343,-0.5545154681\H,0,2.5085846889,1.9137934996,-  
1.148260376\H,0,-0.0361608966,2.6102556035,2.1112606141\H,0,0.01444884  
78,0.0116369578,2.7060447629\H,0,2.5079282873,-0.7235071121,2.11228138  
64\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-912.9708984\CCSD(T)  
/GTbas1=-913.0755413\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-912.  
1079609\MP2/GTMP2LargeXP=-913.3740312\HF/GFHFB3=-912.117726\HF/GFHFB4=  
-912.139499\G4MP2=-913.603444

**CP5**

\\0,1\p,0,-0.055566333,-0.0518627859,0.0464327218\p,  
0,2.2611225704,0.0474002081,0.0037991107\p,0,0.2019606426,2.252610966,  
0.0039489798\C,0,2.0747216673,1.9373265969,0.2125749782\C,0,0.40251097  
06,1.8908033087,1.8762108201\C,0,1.9597529583,1.8298658895,1.767025519  
1\C,0,0.354779445,0.3311794351,1.8882260188\C,0,1.9140126227,0.2720944  
399,1.8760995704\H,0,2.7917091622,2.6068590606,-0.2606401309\H,0,-0.11  
71883303,2.4729630212,2.6366988684\H,0,2.609096287,2.4361589649,2.4013  
714398\H,0,-0.210516609,-0.1967267367,2.6576430852\H,0,2.4593049462,-0  
.2862723684,2.6365090185\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas  
1=-1215.2451249\CCSD(T)/GTbas1=-1215.3538616\MP2/GTbas2=0.\MP2/GTbas3=  
0.\HF/GTMP2LargeXP=-1214.4270633\MP2/GTMP2LargeXP=-1215.6751778\HF/GFH  
FB3=-1214.44194\HF/GFHFB4=-1214.4635284\G4MP2=-1215.9283296

**CP6**

\\0,1\p,0,0.0016777903,-0.0325941571,0.0056377332\C,  
0,1.9342948701,-0.0101432622,0.008094763\p,0,0.4754695816,2.233846732,  
0.0321302305\C,0,2.2377982114,1.512982063,-0.0972848825\C,0,0.72786004  
54,1.8055834004,1.8747017681\p,0,2.6380526635,1.6645108445,1.772473837  
9\C,0,0.5307866872,0.2618359778,1.8410949271\C,0,2.0097496293,-0.13357  
95114,1.5581902537\H,0,2.5101078076,-0.6911468194,-0.6194195308\H,0,2.  
9093036438,1.8731868302,-0.8745905384\H,0,0.2205559073,2.3942207698,2.  
6369481505\H,0,-0.0069161756,-0.2033871845,2.6678617127\H,0,2.44195933  
8,-1.0200156831,2.020661575\\Version=EM64L-G09RevA.02\State=1-A\MP2/GT  
Bas1=-1215.2445826\CCSD(T)/GTBas1=-1215.3521988\MP2/GTBas2=0.\MP2/GTBa  
s3=0.\HF/GTMP2LargeXP=-1214.4238212\MP2/GTMP2LargeXP=-1215.6743696\HF/  
GFHFB3=-1214.4384458\HF/GFHFB4=-1214.460227\G4MP2=-1215.9267087

**CP7**

\\0,1\p,0,0.0289312661,0.0220188157,0.0175208215\C,0  
,1.9344164772,0.0391347865,0.0316901254\C,0,0.221767142,1.9164896881,0  
.0067925755\p,0,2.1044973962,1.9110657039,-0.2803659227\C,0,0.40423472  
59,1.9603846094,1.5615833076\C,0,1.9681427763,2.0270460956,1.615435586  
3\C,0,0.2211556358,0.4350127503,1.8662421999\p,0,2.103539399,0.1532591  
696,1.9261931311\H,0,2.5088726639,-0.6826071536,-0.5433927465\H,0,-0.4  
617241474,2.5856762367,-0.511163582\H,0,-0.1740211578,2.6858151477,2.1  
394403154\H,0,2.4917641362,2.7726884628,2.2096585081\H,0,-0.4627763134  
,0.0799156874,2.6339656804\\Version=EM64L-G09RevA.02\State=1-A\MP2/GT  
Bas1=-1215.2438857\CCSD(T)/GTBas1=-1215.3506677\MP2/GTBas2=0.\MP2/GTBa  
s3=0.\HF/GTMP2LargeXP=-1214.4311906\MP2/GTMP2LargeXP=-1215.6791056\HF/  
FHFB3=-1214.4452996\HF/GFHFB4=-1214.4674826\G4MP2=-1215.9312913

**CP8**

\\0,1\p,0,-0.0213933378,-0.0212179181,0.0319039498\p  
,0,2.2929754584,-0.0215096075,0.0320292353\p,0,-0.0210919745,2.2931499  
253,0.0320619979\p,0,2.2932770879,2.2928584038,0.0322006695\C,0,0.3572  
335859,1.914456152,1.8763247404\C,0,1.9146036758,1.9142949996,1.876414  
5727\C,0,0.3570721717,0.3570874951,1.8762165333\C,0,1.9144418104,0.356  
9270225,1.8763030041\H,0,-0.1936743146,2.4654513541,2.6403510479\H,0,2  
.4656006852,2.4651026211,2.6405094116\H,0,-0.1940124548,-0.1938285088,  
2.6401722162\H,0,2.4652676064,-0.194171939,2.6403126214\\Version=EM64L  
-G09RevA.02\State=1-A\MP2/GTBas1=-1517.5132723\CCSD(T)/GTBas1=-1517.62  
65253\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.7416583\MP2/GT  
MP2LargeXP=-1517.973912\HF/GFHFB3=-1516.7619111\HF/GFHFB4=-1516.783216  
1\G4MP2=-1518.2510189

**CP9**

\\0,1\p,0,-0.0621111167,-0.0577258882,-0.0539143003\  
p,0,2.2548362926,0.0425868791,0.0398887616\p,0,0.2080515235,2.24536327  
12,0.0399293721\C,0,2.0811011715,1.9332540183,0.1838456721\C,0,0.46873  
4388,2.0521457762,1.9158439759\C,0,2.0099545222,1.8671366119,1.7427458  
091\p,0,0.2082514805,0.1937091524,2.2375155948\C,0,2.0811695589,0.3164  
915214,1.9159788556\H,0,2.7855702235,2.587935603,-0.327843312\H,0,0.05  
69953217,2.7894844472,2.6040165784\H,0,2.6860064813,2.4949992644,2.328  
7918262\H,0,2.7860401529,-0.1485806568,2.6042011667\\Version=EM64L-G09  
RevA.02\State=1-A\MP2/GTBas1=-1517.5168057\CCSD(T)/GTBas1=-1517.628601  
5\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.7453774\MP2/GTMP2L  
argeXP=-1517.9780331\HF/GFHFB3=-1516.7650097\HF/GFHFB4=-1516.7865963\G  
4MP2=-1518.2540237

**CP10**

\\0,1\p,0,0.0290385957,0.0263966267,0.0245135336\C,0  
,1.9268510757,0.0330151967,0.0308743276\C,0,0.1897364301,1.9176172357,  
0.0308531771\p,0,2.0809130893,1.9179806419,-0.1276070018\p,0,0.1870785  
272,2.0729753552,1.9223238691\C,0,2.0714025912,1.9090285227,1.77022777  
05\C,0,0.1897293819,0.1749844881,1.9097311823\p,0,2.0809237138,0.01738  
55379,1.9225119766\H,0,2.5038338828,-0.6428941651,-0.5961002651\H,0,-0  
.4373348687,2.5474914637,-0.5959605722\H,0,2.7486072865,2.5330413987,2  
.348910999\H,0,-0.4373797055,-0.4028223023,2.5848210034\\Version=EM64L  
-G09RevA.02\State=1-A\MP2/GTbas1=-1517.5164676\CCSD(T)/GTbas1=-1517.62  
51485\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1516.7541983\MP2/GT  
MP2LargeXP=-1517.9856943\HF/GFHFB3=-1516.7729018\HF/GFHFB4=-1516.79543  
68\G4MP2=-1518.2603451

**CP11**

\\0,1\p,0,0.0606030465,-0.0061097874,0.0243066942\C,  
0,1.9602621234,0.0154665173,0.0450596006\p,0,0.1050597388,2.310861776,  
0.0394251015\p,0,2.3772525793,1.8660621809,-0.0599541109\C,0,0.5377400  
509,1.8578545729,1.8701523961\C,0,2.09303966,1.8090138309,1.8209888024  
\C,0,0.2584055728,0.3263774797,1.8877140667\p,0,2.117479984,-0.0936916  
753,1.942273564\H,0,2.493896979,-0.6741894873,-0.6063969217\H,0,0.0799  
515046,2.4597936256,2.6582103705\H,0,2.6732943692,2.456148584,2.476766  
5535\H,0,-0.4661856085,-0.0809876172,2.5909538829\\Version=EM64L-G09Re  
vA.02\State=1-A\MP2/GTbas1=-1517.5159453\CCSD(T)/GTbas1=-1517.6266305\  
MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1516.7425038\MP2/GTMP2Lar  
geXP=-1517.9771654\HF/GFHFB3=-1516.7619563\HF/GFHFB4=-1516.7837732\G4M  
P2=-1518.2525678

**CP12**

\\0,1\C,0,0.0331199274,-0.0051331526,0.0356095251\p,  
0,1.9480992456,-0.0404646096,0.0271247959\C,0,-0.2444334523,1.52300039  
02,0.0354380488\p,0,1.5358137934,2.2294870733,0.026868033\p,0,-0.52856  
44341,1.854748757,1.9002912841\C,0,1.3864144029,1.8194179473,1.8918061  
535\p,0,-0.1162797418,-0.4152075242,1.9005476169\C,0,1.6639654322,0.29  
12840067,1.8919788333\H,0,-0.5122893579,-0.6120214055,-0.6867903376\H,  
0,-0.9683966663,1.8991727057,-0.6870696272\H,0,1.9318229588,2.42630408  
65,2.61420815\H,0,2.3879278921,-0.0848882747,2.6144875242\\Version=EM6  
4L-G09RevA.02\State=1-A\MP2/GTbas1=-1517.5126791\CCSD(T)/GTbas1=-1517.  
6235416\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1516.7356526\MP2/  
GTMP2LargeXP=-1517.9723446\HF/GFHFB3=-1516.7552453\HF/GFHFB4=-1516.776  
9831\G4MP2=-1518.247965

**CP13**

\\0,1\p,0,-0.0144762958,-0.0683831532,0.0798297141\p  
,0,2.2880789338,0.0774884245,-0.0711341814\p,0,0.1947997632,2.23747988  
16,-0.008609733\C,0,2.0656817662,1.9427680425,0.2761161571\C,0,0.35966  
03169,1.8905811118,1.8765887375\C,0,1.9135105796,1.9437020301,1.821700  
9196\C,0,0.2076626317,0.3459503353,1.9313924861\p,0,2.0785434092,0.072  
2614867,2.2363968338\H,0,2.7921101625,2.611398622,-0.1867379934\H,0,-0  
.1775773728,2.4890299343,2.6135051476\H,0,2.4505920277,2.701788465,2.3  
932420109\H,0,-0.5187859223,-0.0925651806,2.6162099012\\Version=EM64L-  
G09RevA.02\State=1-A\MP2/GTbas1=-1517.5178154\CCSD(T)/GTbas1=-1517.629  
295\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1516.7402998\MP2/GTMP  
2LargeXP=-1517.9753816\HF/GFHFB3=-1516.7601022\HF/GFHFB4=-1516.7816212  
\G4MP2=-1518.2510234

**CP14**

\\0,1\C,0,-0.0222399615,-0.0271291108,0.0209426555\C  
,0,1.5295996717,0.0236558575,0.0050180412\C,0,-0.2984536897,1.50076274  
74,0.003606552\P,0,1.5475783902,1.9154234938,-0.2328049054\P,0,-0.6128  
395876,1.8325522622,1.852102136\P,0,1.6747712775,2.0750539526,2.078446  
6788\P,0,-0.3808488392,-0.4691788536,1.8656118713\P,0,1.9182730425,-0.  
2126305186,1.8540636566\H,0,-0.5121538089,-0.6341687757,-0.7437669501\  
H,0,2.0730762936,-0.6122834783,-0.6948963333\H,0,-1.0336627886,1.89804  
24233,-0.6973234026\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-18  
19.7833591\CCSD(T)/GTBas1=-1819.8993961\MP2/GTBas2=0.\MP2/GTBas3=0.\HF  
/GTMP2LargeXP=-1819.0567172\MP2/GTMP2LargeXP=-1820.2753916\HF/GFHFB3=-  
1819.0817654\HF/GFHFB4=-1819.1030355\G4MP2=-1820.5751717

#### CP15

\\0,1\C,0,0.0046575941,-0.0162672527,0.0023755452\P,  
0,1.9187419498,-0.0865463013,-0.0122513295\C,0,-0.2575792886,1.5113043  
016,0.0402462243\P,0,1.5225029091,2.1834989526,0.1880446957\P,0,-0.671  
4515987,1.7647660486,1.8860081145\C,0,1.21881473,1.8858760886,2.040281  
04\P,0,-0.4195102335,-0.5328168738,1.797406392\P,0,1.7548268331,0.0795  
374003,2.2873938514\H,0,-0.4974392584,-0.5811307734,-0.7856781571\H,0,  
-0.9228180121,1.9272671749,-0.7167393628\H,0,1.6334543752,2.5998112347  
,2.7521129863\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1819.784  
3117\CCSD(T)/GTBas1=-1819.8990259\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2  
LargeXP=-1819.0552248\MP2/GTMP2LargeXP=-1820.2759815\HF/GFHFB3=-1819.0  
799043\HF/GFHFB4=-1819.10143\G4MP2=-1820.574915

#### CP16

\\0,1\C,0,0.0443250714,0.0174084417,0.0220798151\P,0  
,1.9419545121,0.0124824067,0.0158217866\P,0,-0.1073497595,1.9056927941  
,0.0210706497\C,0,1.7629267866,1.8765204894,0.3223016798\P,0,-0.421967  
9533,1.8253924755,2.3173724865\P,0,1.8934372276,1.7378187263,2.2068157  
556\P,0,-0.1066804688,-0.4262273945,1.8573817107\C,0,1.7628325913,-0.1  
26236945,1.8999164235\H,0,-0.5288889366,-0.5553312651,-0.7052412224\H,  
0,2.3896300669,2.6012553228,-0.1950445187\H,0,2.3886808624,-0.79917505  
18,2.4839254335\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1819.7  
841084\CCSD(T)/GTBas1=-1819.8980386\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM  
P2LargeXP=-1819.0643869\MP2/GTMP2LargeXP=-1820.2824232\HF/GFHFB3=-1819  
.0886175\HF/GFHFB4=-1819.1105249\G4MP2=-1820.5811435

#### CP17

\\0,1\C,0,0.0055069703,-0.0092497341,0.0048068895\P,  
0,1.9146511065,-0.0329832818,0.0065263061\C,0,-0.2842647293,1.51067397  
71,0.0046288195\P,0,1.4822358684,2.2351630972,0.0062816127\P,0,-0.8777  
639408,1.7854451169,1.7984095842\P,0,1.3349542926,2.2074599366,2.31179  
93123\P,0,-0.445333781,-0.4826935997,1.798686113\P,0,1.7674527837,-0.0  
60900784,2.312029285\H,0,-0.4758923521,-0.6001781059,-0.7773758144\H,0  
, -0.9492462182,1.8828633777,-0.7776921079\\Version=EM64L-G09RevA.02\St  
ate=1-A\MP2/GTBas1=-2122.0465227\CCSD(T)/GTBas1=-2122.1669271\MP2/GTBas  
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2121.369965\MP2/GTMP2LargeXP=-212  
2.5735585\HF/GFHFB3=-2121.4002728\HF/GFHFB4=-2121.421302\G4MP2=-2122.8  
973441

#### CP18

\\0,1\C,0,0.0289683307,0.0317606349,0.001263062\P,0,  
1.9227187335,0.0289645378,0.0405142679\P,0,-0.1275601326,1.9190355806,  
0.0403608096\C,0,1.7143308095,1.8600169843,0.4783012686\P,0,-0.5968501  
181,1.7599585603,2.3080081381\P,0,1.7095490477,1.8549823402,2.37191052  
01\P,0,-0.4417151115,-0.4786766124,1.7629984933\P,0,1.8020812867,-0.45

15242866,2.3081880133\H,0,-0.4720267914,-0.5117711511,-0.8004344308\H,  
0,2.3809039454,2.5830534118,0.0070898578\\Version=EM64L-G09RevA.02\Sta  
te=1-A\MP2/GTBas1=-2122.0479814\CCSD(T)/GTBas1=-2122.1671871\MP2/GTBas  
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2121.3750686\MP2/GTMP2LargeXP=-212  
2.5790094\HF/GFHFB3=-2121.4048871\HF/GFHFB4=-2121.4262269\G4MP2=-2122.  
9020676

### CP19

\\0,1\C,0,-0.0122839868,-0.0143245628,-0.0197181608\  
P,0,1.887882746,-0.0232365406,-0.0308808719\P,0,-0.4485679131,1.835294  
09,-0.0296795612\P,0,1.7679211038,2.2241040353,0.4965442406\P,0,-0.569  
6407033,1.6821896867,2.2728040435\C,0,1.3305291233,1.6732602394,2.2616  
57962\P,0,-0.449691647,-0.5651517918,1.745395418\P,0,1.7668128663,-0.1  
763550345,2.2716180955\H,0,-0.479148727,-0.6015490749,-0.813043092\H,0  
,1.7973871377,2.2604689533,3.0550019265\\Version=EM64L-G09RevA.02\Stat  
e=1-A\MP2/GTBas1=-2122.050248\CCSD(T)/GTBas1=-2122.1692074\MP2/GTBas2=  
0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2121.370672\MP2/GTMP2LargeXP=-2122.5  
763897\HF/GFHFB3=-2121.4004619\HF/GFHFB4=-2121.4217585\G4MP2=-2122.899  
1135

### CP20

\\0,1\C,0,-0.0052613325,-0.0060965938,-0.0088457778\  
P,0,1.8881680936,-0.0026636184,-0.0033608717\P,0,-0.448424211,1.835049  
4374,-0.0032326705\P,0,1.7902437661,2.27749609,0.3498154227\P,0,-0.788  
5906464,1.6493091132,2.2728576332\P,0,1.4820118655,1.8850803136,2.6011  
618309\P,0,-0.4500012338,-0.5720907266,1.7430357352\P,0,1.7888077201,-  
0.3768308059,2.27317669\H,0,-0.4629540215,-0.5880532096,-0.811807992\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2424.3074909\CCSD(T)/GT  
Bas1=-2424.4322677\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2423.6  
865159\MP2/GTMP2LargeXP=-2424.8745445\HF/GFHFB3=-2423.7219194\HF/GFHFB  
4=-2423.7427607\G4MP2=-2425.2223796

### CP1+

\\1,2\P,0,0.0872506048,0.0680772221,0.05573365  
79\C,0,1.9687623352,-0.0001921531,-0.0004128557\C,0,0.4783472137,1.909  
5641983,-0.0006256979\C,0,2.0015469108,1.5618116149,-0.1690037369\C,0,  
0.6222730424,1.9069964796,1.5645558852\C,0,2.1609810551,1.6859005096,1  
.383243194\C,0,0.4779107097,0.3727241381,1.8724963109\C,0,2.0012679523  
,0.1394221187,1.5645651925\H,0,2.6119989858,-0.6752325385,-0.554255643  
6\H,0,-0.0197794559,2.6977831922,-0.5544464\H,0,2.6047765582,2.0321484  
828,-0.940514039\H,0,0.1244142552,2.6535072421,2.1771116317\H,0,2.9272  
200084,2.2832361796,1.8736445112\H,0,-0.0206173963,-0.0160531026,2.753  
6697296\H,0,2.6041472206,-0.5254935837,2.17673826\\Version=EM64L-G09Re  
vA.02\State=2-A\MP2/GTBas1=-610.4221071\CCSD(T)/GTBas1=-610.5247194\MP  
2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-609.5419752\MP2/GTMP2LargeX  
P=-610.7892119\HF/GFHFB3=-609.546626\HF/GFHFB4=-609.5687405\G4MP2=-610  
.9983167

### CP2+

\\1,2\P,0,0.0607691221,-0.0114790867,0.0492852  
746\C,0,1.9892497387,0.005220543,-0.0193596021\P,0,0.4594419747,2.2021  
397625,0.0494202254\C,0,2.2608353763,1.5135018369,-0.0193685793\C,0,0.  
7453471578,1.7863289599,1.9120671151\C,0,2.2578603565,1.5163099473,1.5  
574842277\C,0,0.4737981319,0.278032298,1.9119802896\C,0,1.9855321735,0  
.0036116945,1.5574747295\H,0,2.5305348695,-0.7076042673,-0.6341440655\  
H,0,3.016676402,1.9927948969,-0.6342228204\H,0,0.4071278109,2.46257704  
83,2.6913985127\H,0,3.0457961676,2.0337851483,2.1025617151\H,0,-0.0789

388349,-0.2378573641,2.6913448668\H,0,2.5436695533,-0.7559614174,2.1026781108\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-912.7046733\CCSD(T)/GTBas1=-912.8047107\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-911.8463594\MP2/GTMP2LargeXP=-913.0958917\HF/GFHFB3=-911.8561133\HF/GFHFB4=-911.878169\G4MP2=-913.3221484

**CP3+**

\\1,2\P,0,0.062114977,0.0552514991,0.031316414  
7\C,0,1.9691896071,-0.0056640305,0.0016442887\C,0,0.2236774722,1.9564492957,0.0018838028\P,0,2.0937293774,1.8626442466,-0.3665057082\C,0,0.4997386758,1.9813860124,1.5251075019\C,0,2.0744053443,1.8452349058,1.5005522302\C,0,0.4804110324,0.4271472034,1.8126853864\C,0,2.0262963963,0.2654166375,1.5248916048\H,0,2.545148498,-0.7664077324,-0.5133448376\H,0,-0.4648950925,2.6171369553,-0.5129300873\H,0,-0.0048002731,2.6917417361,2.1758933977\H,0,2.6827589418,2.3863396953,2.2201384853\H,0,0.0516701641,0.0456071062,2.7353440086\H,0,2.6731548791,-0.3184835305,2.175523512\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-912.7077305\CCSD(T)/GTBas1=-912.8077876\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-911.8545664\MP2/GTMP2LargeXP=-913.1024194\HF/GFHFB3=-911.8637933\HF/GFHFB4=-911.8860748\G4MP2=-913.328261

**CP4+**

\\1,2\P,0,0.0499508752,0.0376243791,0.03008816  
45\C,0,1.964684746,0.0019833357,0.0016880127\C,0,0.520760042,1.8941673873,0.0019661702\C,0,2.00302098,1.5281044566,-0.2942036152\C,0,0.5583494199,1.9234354191,1.556089563\P,0,2.4730721594,1.8877932905,1.5276870689\C,0,0.5200216591,0.3973078026,1.8519798097\C,0,2.0022815416,0.0312475077,1.5558057519\H,0,2.6142048168,-0.6745490314,-0.545064303\H,0,0.0398503018,2.6989737332,-0.54534239\H,0,2.4842345548,1.8951155299,-1.1954449911\H,0,-0.091212053,2.5999511436,2.1028120298\H,0,0.0388049675,0.0303146659,2.7532274101\H,0,2.4831759889,-0.7735696197,2.1031113184\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-912.7278976\CCSD(T)/GTBas1=-912.8257254\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-911.8699436\MP2/GTMP2LargeXP=-913.1195647\HF/GFHFB3=-911.8793627\HF/GFHFB4=-911.9015493\G4MP2=-913.3422395

**CP5+**

\\1,2\P,0,-0.1249528739,-0.1166438858,0.055888  
8861\P,0,2.1810037243,0.1011573297,0.0187323977\P,0,0.2500975997,2.169038453,0.0188607969\C,0,2.1370078957,1.9954956789,0.2250849989\C,0,0.4177660779,1.8707170619,1.8556670297\C,0,1.9888517086,1.857036129,1.7628986018\C,0,0.3232784179,0.3017537883,1.8779791417\C,0,1.8950264294,0.2886815319,1.8555734294\H,0,2.8354813042,2.6477392936,-0.2900194872\H,0,-0.0908555283,2.4499891229,2.6240946639\H,0,2.6113541336,2.4382597641,2.4398930189\H,0,-0.2165671086,-0.2023928931,2.6773297002\H,0,2.4382082195,-0.2584313745,2.623916822\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1214.9760686\CCSD(T)/GTBas1=-1215.0830092\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1214.169698\MP2/GTMP2LargeXP=-1215.3970508\HF/GFHFB3=-1214.1840425\HF/GFHFB4=-1214.2061301\G4MP2=-1215.6490672

**CP6+**

\\1,2\P,0,0.0588579479,0.013439858,0.042584923  
4\C,0,1.9897927407,-0.005974485,-0.0085971128\P,0,0.4886749028,2.2508153873,0.0397208695\C,0,2.2521266945,1.5049644581,-0.1393486125\C,0,0.6905536469,1.8075668612,1.9000663051\P,0,2.5815035828,1.6291424097,1.7344274806\C,0,0.5305132687,0.2768065633,1.8972294234\C,0,1.9903961235,-0.1537462092,1.5463637098\H,0,2.562774934,-0.706544776,-0.6112132623\H

,0,2.9023852798,1.8933895228,-0.9176954689\H,0,0.1804705098,2.42084137  
67,2.6371170147\H,0,0.0129845777,-0.21243177,2.7188519926\H,0,2.389665  
791,-1.062969197,1.9869927375\\Version=EM64L-G09RevA.02\State=2-A\MP2/  
GTBas1=-1214.9964064\CCSD(T)/GTBas1=-1215.0973592\MP2/GTBas2=0.\MP2/GT  
Bas3=0.\HF/GTMP2LargeXP=-1214.1782408\MP2/GTMP2LargeXP=-1215.4160359\H  
F/GFHFB3=-1214.192567\HF/GFHFB4=-1214.2147548\G4MP2=-1215.6619303

**CP7+**

\\1,2\P,0,0.0805120475,0.0700485668,0.04806942  
32\C,0,1.9712731766,0.0191237309,-0.0065652597\C,0,0.2500513686,1.9150  
113652,0.0296109294\P,0,2.145237064,1.9059579447,-0.3251389688\C,0,0.3  
635096744,1.9470806686,1.6068110906\C,0,1.9433735041,2.0217177299,1.58  
8609142\C,0,0.1824159125,0.4332117051,1.9081585491\P,0,2.0656754741,0.  
1950911938,1.8755432784\H,0,2.5170363185,-0.7470917697,-0.5469498986\H  
,0,-0.3964119519,2.6282506305,-0.4765114961\H,0,-0.2008020623,2.689911  
0133,2.1687039861\H,0,2.449331813,2.8079367047,2.1442179047\H,0,-0.482  
4023392,0.0196505161,2.6590413197\\Version=EM64L-G09RevA.02\State=2-A\  
MP2/GTBas1=-1214.9730726\CCSD(T)/GTBas1=-1215.0776594\MP2/GTBas2=0.\MP  
2/GTBas3=0.\HF/GTMP2LargeXP=-1214.1667376\MP2/GTMP2LargeXP=-1215.39773  
77\HF/GFHFB3=-1214.1804763\HF/GFHFB4=-1214.2030117\G4MP2=-1215.6492126

**CP8+**

\\1,2\P,0,-0.1332270081,-0.133028141,0.0966381  
697\P,0,2.1611375331,0.1103584297,-0.0039131537\P,0,0.1107423165,2.161  
293522,-0.0038877367\P,0,2.4051028292,2.4046598715,0.0969570408\C,0,0.  
3717089215,1.9000233416,1.8373172264\C,0,1.935486605,1.935136104,1.898  
089364\C,0,0.3361885928,0.3362427428,1.8978892207\C,0,1.8999743759,0.3  
713628886,1.837298977\H,0,-0.2136380237,2.4854228467,2.5465246035\H,0,  
2.4382946045,2.437798598,2.7228620681\H,0,-0.1667131732,-0.1665349764,  
2.7225344204\H,0,2.4852424264,-0.2141352274,2.5464897999\\Version=EM64  
L-G09RevA.02\State=2-A\MP2/GTBas1=-1517.2477701\CCSD(T)/GTBas1=-1517.3  
587519\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.4845985\MP2/G  
TMP2LargeXP=-1517.6971867\HF/GFHFB3=-1516.5041329\HF/GFHFB4=-1516.5260  
256\G4MP2=-1517.9723522

**CP9+**

\\1,2\P,0,0.0611556208,0.0563612704,0.05192158  
67\P,0,2.3398073111,0.0309404751,0.0299457108\P,0,0.2024127975,2.33067  
18818,0.0296337118\C,0,2.0692120878,1.9224331379,0.1580039809\C,0,0.44  
12666877,2.0437107954,1.9072507773\C,0,1.9714411564,1.8310898412,1.709  
2669554\P,0,0.2032327909,0.1890339685,2.3209805831\C,0,2.0704165421,0.  
2895626763,1.9072955186\H,0,2.768847146,2.5727892328,-0.3646582858\H,0  
,0.0193660518,2.7765747797,2.5931750579\H,0,2.6475633552,2.4591958649,  
2.2949481331\H,0,2.7698784527,-0.185563924,2.59323627\\Version=EM64L-G  
09RevA.02\State=2-A\MP2/GTBas1=-1517.2362981\CCSD(T)/GTBas1=-1517.3515  
107\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.4790024\MP2/GTMP  
2LargeXP=-1517.6811662\HF/GFHFB3=-1516.4983922\HF/GFHFB4=-1516.5203643  
\G4MP2=-1517.962816

**CP10+**

\\1,2\P,0,0.0014439687,0.0140356011,0.01311516  
04\C,0,1.8916029052,0.0742757672,0.0690974873\C,0,0.1739292157,1.93349  
72901,-0.0039316596\P,0,2.096211575,1.9440865556,-0.142563782\P,0,0.27  
28117541,1.9718377257,1.8285058022\C,0,2.1068982752,1.9244331378,1.784  
3275527\C,0,0.172961178,0.1413906629,1.9281970603\P,0,2.0947499077,0.0  
047413804,1.9485234351\H,0,2.4696373036,-0.6030108168,-0.559216856\H,0  
, -0.4585866333,2.5674807529,-0.6177043262\H,0,2.7710129589,2.553461128



6,2.3691304287\H,0,-0.4592724089,-0.4220291855,2.607619697\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1517.2399639\CCSD(T)/GTBas1=-1517.3498965\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.4927709\MP2/GTMP2LargeXP=-1517.6990392\HF/GFHFB3=-1516.5111027\HF/GFHFB4=-1516.5340011\G4MP2=-1517.9760006

#### CP11<sup>+</sup>

\\1,2\p,0,0.0616108058,-0.0504751699,0.0171283  
033\C,0,1.9675630052,0.0046977333,0.008555304\p,0,0.164895599,2.2383425471,0.0760974223\p,0,2.4198659358,1.8554851257,-0.0685853277\C,0,0.5439218405,1.8536448239,1.9441810988\C,0,2.0859963269,1.8411149047,1.8264727962\C,0,0.228806377,0.3402518963,1.8939108905\p,0,2.0724861926,-0.0402848783,1.8918903665\H,0,2.5035634051,-0.6873661264,-0.6360662111\H,0,0.0852041623,2.4563458001,2.7263942802\H,0,2.6775929123,2.5096413073,2.4466495327\H,0,-0.5207065624,-0.0747979638,2.5628715442\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1517.2611735\CCSD(T)/GTBas1=-1517.3656215\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.4890152\MP2/GTMP2LargeXP=-1517.7133412\HF/GFHFB3=-1516.5081437\HF/GFHFB4=-1516.5303812\G4MP2=-1517.9830028

#### CP12<sup>+</sup>

\\1,2\C,0,-0.0117899704,0.0022155106,-0.012406  
6374\p,0,1.9125994818,-0.0227632352,0.0554832524\C,0,-0.2838860587,1.5003128479,-0.0125767443\p,0,1.5088063483,2.2004443619,0.0552311136\p,0,-0.4930671622,1.8370580138,1.8719310871\C,0,1.4313266132,1.812062377,1.9398236998\p,0,-0.0892767548,-0.3861519588,1.8721864049\C,0,1.703420417,0.3139656256,1.9399923224\H,0,-0.5288929344,-0.6498867531,-0.7126566541\H,0,-0.9972524568,1.9287714734,-0.7129443028\H,0,1.9484280907,2.4641649278,2.6400746427\H,0,2.4167843875,-0.1144931907,2.6403618168\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1517.265604\CCSD(T)/GTBas1=-1517.3692082\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.4878968\MP2/GTMP2LargeXP=-1517.71609\HF/GFHFB3=-1516.5073252\HF/GFHFB4=-1516.5294515\G4MP2=-1517.9846846

#### CP13<sup>+</sup>

\\1,2\p,0,-0.0178079361,-0.1189647598,0.096238  
4046\p,0,2.2914723567,0.0920413241,-0.1222794979\p,0,0.2352655561,2.1569171265,0.0298245234\C,0,2.1223529599,1.9509872564,0.279372464\C,0,0.3552800906,1.8794179592,1.9067254193\C,0,1.9178695492,1.9734023149,1.809452081\C,0,0.1509868125,0.3495147208,1.939513017\p,0,2.0380773673,0.1077619823,2.1544990955\H,0,2.8356832369,2.6267317184,-0.1877636366\H,0,-0.1562511099,2.4923159765,2.6460491055\H,0,2.4292559459,2.7344260059,2.3953148875\H,0,-0.5623848291,-0.0930516252,2.6315541368\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1517.2645591\CCSD(T)/GTBas1=-1517.3692475\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1516.4905562\MP2/GTMP2LargeXP=-1517.7155462\HF/GFHFB3=-1516.5098868\HF/GFHFB4=-1516.5319245\G4MP2=-1517.9845994

#### CP14<sup>+</sup>

\\1,2\C,0,-0.0206897398,-0.0252770639,-0.01416  
821\C,0,1.5327737738,-0.0167496322,-0.0003030899\C,0,-0.3385994807,1.4953755266,-0.0016976041\p,0,1.5094000968,1.8682699927,-0.1384260689\p,0,-0.6412554744,1.8976154213,1.8383675274\p,0,1.6577714583,2.0540947369,2.1378614534\p,0,-0.3007019549,-0.3699974668,1.8418553925\p,0,1.9878312226,-0.2267536047,1.8403707255\H,0,-0.5154403283,-0.6382581302,-0.767001927\H,0,2.0723694747,-0.6397323145,-0.7117336421\H,0,-1.0603590481,1.8915125349,-0.7141245567\\Version=EM64L-G09RevA.02\State=2-A\MP2/G

GTBas1=-1819.5259982\CCSD(T)/GTBas1=-1819.6352706\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1818.8027629\MP2/GTMP2LargeXP=-1820.0132344\HF/GFHFB3=-1818.8272081\HF/GFHFB4=-1818.8491132\G4MP2=-1820.3064591

#### CP15<sup>+</sup>

\1,2\C,0,-0.0524636283,0.0044961212,-0.066297  
2421\P,0,1.867374907,-0.1156263429,0.0573596957\C,0,-0.2893301704,1.5037657052,-0.0026444582\P,0,1.5098869224,2.1191107742,0.2132203125\P,0,-0.6297674255,1.7107447972,1.8691640963\C,0,1.2525016603,1.8899573446,2.0847975673\P,0,-0.3354181478,-0.5360447346,1.7621590894\P,0,1.8093280766,0.1107915798,2.3655458479\H,0,-0.5340173426,-0.5963410493,-0.8366946888\H,0,-0.9419926069,1.9871050893,-0.7267618313\H,0,1.6280977552,2.6573407153,2.7593516113\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1819.5287279\CCSD(T)/GTBas1=-1819.6376528\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1818.8027278\MP2/GTMP2LargeXP=-1820.0154605\HF/GFHFB3=-1818.8269993\HF/GFHFB4=-1818.8490574\G4MP2=-1820.3087943

#### CP16<sup>+</sup>

\1,2\C,0,0.0145427683,0.0148037754,0.01874618  
45\P,0,1.880394051,0.0599371805,0.0764114534\P,0,-0.1091533157,1.9179709906,-0.0445600505\C,0,1.763375789,1.9069037465,0.3240903075\P,0,-0.3418403606,1.7642214927,2.2397470882\P,0,1.9590803623,1.744828792,2.2155426993\P,0,-0.1092863532,-0.4927629568,1.8539832972\C,0,1.7631888815,-0.1317713066,1.9299334747\H,0,-0.5682978296,-0.5535998629,-0.7029276885\H,0,2.3836448219,2.6398808259,-0.1873876976\H,0,2.3832511851,-0.8008126774,2.5228209318\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1819.5234893\CCSD(T)/GTBas1=-1819.6325329\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1818.8026421\MP2/GTMP2LargeXP=-1820.0124223\HF/GFHFB3=-1818.8264653\HF/GFHFB4=-1818.8488296\G4MP2=-1820.3068545

#### CP17<sup>+</sup>

\1,2\C,0,-0.0425360393,-0.0045457363,-0.05730  
48462\P,0,1.870222616,-0.0150900613,0.0631766387\C,0,-0.327250341,1.4885816962,-0.0574657924\P,0,1.4474618292,2.2021086471,0.0630765589\P,0,-0.8082904907,1.7723907073,1.7759169878\P,0,1.3825441434,2.2158338314,2.3766590207\P,0,-0.3854464931,-0.4447843761,1.7762152111\P,0,1.8148724149,-0.0512119341,2.3768038206\H,0,-0.4956440172,-0.6437288193,-0.8143102248\H,0,-0.9836336222,1.916046045,-0.8146673744\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-2121.7866992\CCSD(T)/GTBas1=-2121.8996445\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2121.1132568\MP2/GTMP2LargeXP=-2122.312975\HF/GFHFB3=-2121.1430324\HF/GFHFB4=-2121.1647519\G4MP2=-2122.6296677

#### CP18<sup>+</sup>

\1,2\C,0,0.0129165746,0.0143459689,-0.0470145  
312\P,0,1.8846543187,0.0202325609,0.2084737126\P,0,-0.1331876986,1.8804115483,0.2083019817\C,0,1.7413565424,1.8893278362,0.4422236641\P,0,-0.3594878552,1.4978878077,2.4737950467\P,0,1.8930924705,2.054075635,2.2967934352\P,0,-0.5933775665,-0.6432077911,1.5929983913\P,0,1.5215909243,-0.2362104695,2.473954776\H,0,-0.3958118125,-0.4291050624,-0.954075147\H,0,2.3486541022,2.5480419661,-0.1772513295\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-2121.7889059\CCSD(T)/GTBas1=-2121.9023834\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2121.1158648\MP2/GTMP2LargeXP=-2122.3207686\HF/GFHFB3=-2121.144747\HF/GFHFB4=-2121.1668432\G4MP2=-2122.6383145

#### CP19<sup>+</sup>

\\1,2\C,0,-0.062430171,0.0082279092,-0.0815769  
574\P,0,1.8423351683,-0.0113074384,0.0265287895\P,0,-0.4981371458,1.84  
28562923,-0.0929774206\P,0,1.7062973306,2.1894256693,0.5223911391\P,0,  
-0.5241016658,1.6701893753,2.2154256853\C,0,1.3806583569,1.650743208,2  
.3235089336\P,0,-0.3880243733,-0.5305377137,1.7195317362\P,0,1.8163805  
156,-0.1838854372,2.3349479285\H,0,-0.5004736458,-0.6252480496,-0.8530  
971094\H,0,1.8186956303,2.2842361847,3.0950172752\\Version=EM64L-G09Re  
vA.02\State=2-A\MP2/GTbas1=-2121.7902522\CCSD(T)/GTbas1=-2121.901602\M  
P2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-2121.1111162\MP2/GTMP2Larg  
eXP=-2122.3131326\HF/GFHFB3=-2121.1402837\HF/GFHFB4=-2121.1622121\G4MP  
2=-2122.6285912

### 3. Carbon-silicon cubanoids

#### CSi1

\\0,1\Si,0,-0.0368690381,-0.0318966074,-0.028339961  
2\C,0,1.8676756237,0.0164055753,0.0141293252\C,0,0.2489441983,1.851915  
5812,0.0151778303\C,0,1.811720757,1.5984826621,-0.0492295306\C,0,0.352  
5631977,1.7816725073,1.5947455497\C,0,1.911362915,1.6856797529,1.50930  
54164\C,0,0.2487187092,0.2194841999,1.8389909537\C,0,1.8113450021,0.12  
70749518,1.5937341789\H,0,-1.0021801807,-0.8838244457,-0.7902443723\H,  
0,2.6810311166,-0.5199932077,-0.4662969849\H,0,-0.1822126614,2.7259756  
201,-0.4645428677\H,0,2.434308261,2.1479746973,-0.754913583\H,0,-0.205  
7833188,2.4790648543,2.2188399573\H,0,2.6143370225,2.3055331188,2.0645  
362127\H,0,-0.1821498634,-0.1605481065,2.7609026935\H,0,2.4339882592,-  
0.5139011536,2.2175051821\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTba  
s1=-559.4397121\CCSD(T)/GTbas1=-559.5404312\MP2/GTbas2=0.\MP2/GTbas3=0  
=-558.5717515\HF/GFHFB4=-558.5938396\G4MP2=-560.0179533

#### CSi2

\\0,1\Si,0,-0.0195178489,-0.1490611566,-0.000470781  
1\C,0,1.9064180071,-0.0114129931,0.0259671905\Si,0,0.2692160588,2.1753  
332962,-0.0012932363\C,0,2.1029256086,1.5706078067,0.0253681556\C,0,0.  
5371993018,1.7657902424,1.8666887962\C,0,2.0776529443,1.5541375384,1.6  
023170474\C,0,0.3407357243,0.183766505,1.867234048\C,0,1.8861519565,0.

#### CSi3

\\0,1\Si,0,-0.0628888535,-0.069213007,0.0053397581\  
C,0,1.842251997,0.0395591241,0.0097405524\C,0,-0.1532586266,1.83687628  
36,0.0101947149\Si,0,1.7386040624,1.9309750916,-0.2208616609\C,0,0.120  
869022,1.7691092032,1.5942602106\C,0,1.6952712814,1.8823933995,1.67017  
27384\C,0,0.1914893214,0.2127380956,1.8589956937\C,0,1.7466765547,0.30  
47739241,1.5938792062\H,0,-0.9078676795,-1.0072205835,-0.7912571043\H,  
0,2.5859344862,-0.6696354052,-0.3376461645\H,0,-0.9361762338,2.5026900  
088,-0.3368362286\H,0,2.4825372514,2.7572724663,-1.2169576487\H,0,-0.5  
124118782,2.4090313845,2.2092998844\H,0,2.1657953548,2.4045642807,2.49  
82611372\H,0,-0.1796956594,-0.1996250036,2.79278565\H,0,2.4492695997,-

0.2584892628,2.2086292611\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTBa  
s1=-810.4737432\\CCSD(T)/GTBas1=-810.574499\\MP2/GTBas2=0.\\MP2/GTBas3=0.  
\\HF/GTMP2LargeXP=-809.668331\\MP2/GTMP2LargeXP=-810.8799169\\HF/GFHFB3=-  
809.6750526\\HF/GFHFB4=-809.6977164\\G4MP2=-811.0900728

#### CSi4

\\0,1\\Si,0,-0.0662012441,-0.0584965164,-0.053303246  
\\C,0,1.836767923,0.0020956544,0.0018318082\\C,0,0.2262026038,1.82327359  
96,0.0017026259\\C,0,1.7848946705,1.5790324113,-0.2165756174\\C,0,0.1730  
689264,1.7764027021,1.5928496119\\Si,0,2.076048247,1.8369977068,1.64798  
49567\\C,0,0.2249852991,0.199485778,1.8112703622\\C,0,1.7836569821,-0.04  
47784499,1.5929757986\\H,0,-1.0315809127,-0.9129201912,-0.8191225133\\H,  
0,2.6544950484,-0.5309757683,-0.4755686435\\H,0,-0.2033887722,2.6995595  
463,-0.4760643294\\H,0,2.214620219,1.959191428,-1.1393902158\\H,0,-0.644  
6650324,2.3094124197,2.070303691\\H,0,3.0415561824,2.6914457956,2.41360  
75664\\H,0,-0.2047991429,-0.1806591512,2.7340666732\\H,0,2.2131390026,-0  
.9210669649,2.0708314713\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTBa  
s1=-810.4600392\\CCSD(T)/GTBas1=-810.5607403\\MP2/GTBas2=0.\\MP2/GTBas3=0.  
\\HF/GTMP2LargeXP=-809.6525037\\MP2/GTMP2LargeXP=-810.8666531\\HF/GFHFB3=-  
-809.659319\\HF/GFHFB4=-809.681922\\G4MP2=-811.0766213

#### CSi5

\\0,1\\Si,0,-0.1363891359,-0.1239788276,0.02558827\\S  
i,0,2.220130658,-0.0133144433,0.0072014325\\Si,0,0.1977522766,2.2113466  
053,0.0070682355\\C,0,2.0962949434,1.9056695084,0.0976720047\\C,0,0.4130  
286861,1.8942457461,1.8834318142\\C,0,1.9682218123,1.789358625,1.684907  
2893\\C,0,0.3388183958,0.3081467523,1.8885764804\\C,0,1.9247878391,0.231  
2532948,1.8835286949\\H,0,-1.2075541599,-1.0977707521,-0.3307604344\\H,0  
,3.3551533637,-0.7153201154,-0.6623097577\\H,0,-0.3929725266,3.40794721  
68,-0.6626538011\\H,0,2.8414576232,2.5831348121,-0.3140041707\\H,0,0.003  
7702613,2.4226988293,2.7423088275\\H,0,2.6481318702,2.4074709575,2.2737  
534862\\H,0,-0.1843256277,-0.1673660758,2.7190227434\\H,0,2.4118937203,-  
0.2263221337,2.7424688852\\Version=EM64L-G09RevA.02\\State=1-A\\MP2/GTBa  
s1=-1061.4791196\\CCSD(T)/GTBas1=-1061.5860614\\MP2/GTBas2=0.\\MP2/GTBas3  
=0.\\HF/GTMP2LargeXP=-1060.7308249\\MP2/GTMP2LargeXP=-1061.8964865\\HF/GF  
HFB3=-1060.7418875\\HF/GFHFB4=-1060.7640056\\G4MP2=-1062.1236124

#### CSi6

\\0,1\\Si,0,-0.0453793365,-0.1783801689,-0.019327535  
3\\C,0,1.8828225552,-0.0183934221,0.0080496958\\Si,0,0.2559783251,2.1335  
74015,-0.0246952214\\C,0,2.0949256893,1.5682778655,-0.1629372892\\C,0,0.  
3749285994,1.796354795,1.8708202797\\Si,0,2.2735673619,1.6785632552,1.7  
328065769\\C,0,0.3313131836,0.1873647677,1.8431076274\\C,0,1.8633186577,  
-0.1554773796,1.5918927636\\H,0,-0.830128697,-1.3333842824,-0.555031522  
5\\H,0,2.6240546093,-0.6142378723,-0.5217083106\\H,0,-0.2081338764,3.445  
0320503,-0.5629500221\\H,0,2.7657669526,1.8695293511,-0.9620080629\\H,0,  
-0.2589156628,2.2711818094,2.6138469065\\H,0,3.2874049086,2.4632796329,  
2.502149896\\H,0,-0.1248646237,-0.2492391505,2.7298831799\\H,0,2.2368413  
538,-1.0855452662,2.0119010384\\Version=EM64L-G09RevA.02\\State=1-A\\MP2  
/GTBas1=-1061.4835591\\CCSD(T)/GTBas1=-1061.5875851\\MP2/GTBas2=0.\\MP2/G  
TBas3=0.\\HF/GTMP2LargeXP=-1060.7386414\\MP2/GTMP2LargeXP=-1061.9088476\\  
HF/GFHFB3=-1060.7492081\\HF/GFHFB4=-1060.7717804\\G4MP2=-1062.1337454

#### CSi7

\\0,1\\Si,0,-0.0902574243,-0.0446046421,-0.041684055  
1\\C,0,1.8243838362,0.055050532,0.0513185659\\C,0,-0.2248458364,1.848865  
0152,-0.0089507701\\Si,0,1.6698607742,1.9680646968,-0.0016706491\\C,0,-0

.1166225027,1.7213152798,1.5903561958\C,0,1.4331463121,2.0362915249,1.8812308369\C,0,-0.2249020007,0.1367126844,1.8432021486\Si,0,1.6696872443,0.1541505727,1.9624432025\H,0,-0.7878651689,-1.0115648211,-0.9352556523\H,0,2.5293368999,-0.5507388491,-0.5082221976\H,0,-0.9799410753,2.5171488725,-0.4079727195\H,0,2.5521703919,2.808114044,-0.8596915881\H,0,-0.8255417378,2.3293519059,2.152532103\H,0,1.6589661866,2.8155135516,2.6008257495\H,0,-0.98008754,-0.2083545853,2.5408255976\H,0,2.5520116408,-0.6347157823,2.8676132319\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1061.5195905\CCSD(T)/GTBas1=-1061.6204764\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1060.7836857\MP2/GTMP2LargeXP=-1061.952941\HF/GFHFB3=-1060.7935623\HF/GFHFB4=-1060.8167938\G4MP2=-1062.1753119

#### CSi8

\\0,1\Si,0,-0.10623754,-0.1065069413,0.0336234066\Si,0,2.2680708615,-0.1052494414,0.035457604\Si,0,-0.1074779639,2.2678159533,0.0350483021\Si,0,2.2668270535,2.2690710391,0.0368848459\C,0,0.2878017937,1.8702494523,1.9016304798\C,0,1.868929939,1.8712150463,1.902856226\C,0,0.2887672057,0.2891222608,1.9006827933\C,0,1.8698926579,0.290088185,1.9018976074\H,0,-1.111312156,-1.1126054929,-0.4163816708\H,0,3.2749891496,-1.1102489329,-0.4128818785\H,0,-1.1136530147,3.2733378585,-0.4137846972\H,0,3.2725735422,3.2757307432,-0.410356058\H,0,-0.2152103007,2.3718928519,2.7294310327\H,0,2.3704138696,2.3730947139,2.7314400845\H,0,-0.2140012538,-0.2137514255,2.7278845506\H,0,2.3716261562,-0.2125558704,2.7298673715\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1312.4902323\CCSD(T)/GTBas1=-1312.6029731\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1311.8015228\MP2/GTMP2LargeXP=-1312.9202815\HF/GFHFB3=-1311.8167942\HF/GFHFB4=-1311.8385093\G4MP2=-1313.1639568

#### CSi9

\\0,1\Si,0,-0.1203515554,-0.1007630205,-0.0868548586\Si,0,2.2669990111,-0.0125887933,-0.0117569277\Si,0,0.3718977736,2.2359224265,-0.0107798219\C,0,2.2557751204,1.9013341936,0.000245868\C,0,0.6568664947,2.1780245882,1.8800475474\C,0,2.1894899947,1.8448437071,1.5921986531\Si,0,0.3724952162,0.3157723949,2.2136379415\C,0,2.2561471635,0.2777675813,1.8796540868\H,0,-1.1162848402,-0.9371352414,-0.8079444932\H,0,3.2894605264,-0.8343106692,-0.7219553895\H,0,-0.2643901589,3.3834848618,-0.7203297\H,0,3.0089684168,2.536368218,-0.4605085096\H,0,0.4281619126,2.982957957,2.5747356618\H,0,2.9196279087,2.4592435499,2.1225614095\H,0,-0.2626906934,-0.2190258672,3.4529340461\H,0,3.0097277093,-0.0849958869,2.5749144861\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1312.5164676\CCSD(T)/GTBas1=-1312.625722\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1311.8339866\MP2/GTMP2LargeXP=-1312.9554581\HF/GFHFB3=-1311.8483683\HF/GFHFB4=-1311.8706856\G4MP2=-1313.1961499

#### CSi10

\\0,1\Si,0,-0.0531070891,-0.0607402229,-0.0717159674\C,0,1.8573524686,0.0223591459,0.0258514785\C,0,-0.2276176116,1.8435027627,0.0258339357\Si,0,1.6763951294,1.9190442667,0.2114935359\Si,0,-0.3159595959,1.6479004046,1.9283457682\C,0,1.5815994828,1.8110307794,2.1213958118\C,0,-0.2285138815,-0.2618985008,1.8239681992\Si,0,1.675815312,-0.0913966794,1.9287600767\H,0,-0.7865988899,-0.9004930531,-1.0562965477\H,0,2.5678228731,-0.5106282968,-0.5968509125\H,0,-0.8509561002,2.4762926446,-0.596766506\H,0,2.5314693495,2.8985559144,-0.5110542406\H,0,-1.2917910535,2.3774197996,2.7817192417\H,0,2.1171138784,2.4244391138,2.8380399491\H,0,-0.8515934551,-0.9749461199,2.3530915059\H,0,2.5297691829,-0.9611419589,2.7813846714\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1312.5791623\CCSD(T)/GTBas1=-1312.6805603\MP2/GTBas2=0.\M

P2/GTbas3=0.\HF/GTMP2LargeXP=-1311.9158722\MP2/GTMP2LargeXP=-1313.0405  
245\HF/GFHFB3=-1311.9291427\HF/GFHFB4=-1311.9528439\G4MP2=-1313.275594  
7

### CSi11

\0,1\Si,0,-0.0285817727,-0.0908019831,-0.030665348  
1\C,0,1.8979808152,0.0056488695,0.0714650542\Si,0,-0.1748563878,2.2552  
136898,0.0133760578\Si,0,2.1442500404,1.9172678679,0.1995648235\C,0,0.  
1213907091,1.7189650668,1.8946107615\C,0,1.7198130466,1.8271729403,2.0  
661560094\C,0,-0.1207251332,0.1261934737,1.8711358359\Si,0,1.757677250  
4,-0.0613386211,1.9797948947\H,0,-0.6307206652,-1.2478553625,-0.752700  
4835\H,0,2.5238682653,-0.5967228022,-0.5816775594\H,0,-1.130937818,3.3  
335812469,-0.3692252349\H,0,3.4162585382,2.492313615,-0.3238794787\H,0  
, -0.4229551261,2.2158426522,2.6981624458\H,0,2.0691720091,2.51713455,2  
.8279286841\H,0,-0.9161695523,-0.2418454892,2.511613569\H,0,2.55653578  
08,-1.0194697141,2.7972399686\Version=EM64L-G09RevA.02\State=1-A\MP2/  
GTbas1=-1312.521499\CCSD(T)/GTbas1=-1312.6282996\MP2/GTbas2=0.\MP2/GT  
bas3=0.\HF/GTMP2LargeXP=-1311.8426032\MP2/GTMP2LargeXP=-1312.9676474\HF  
/GFHFB3=-1311.856811\HF/GFHFB4=-1311.8794531\G4MP2=-1313.2066353

### CSi12

\0,1\C,0,0.0449531353,-0.0204999778,0.0382844146\Si,  
i,0,1.9735043546,-0.1436183973,-0.0338017719\C,0,-0.1454529494,1.58693  
32633,0.040281937\Si,0,1.7021915472,2.1526572934,-0.0304089398\Si,0,-0  
.1611583955,1.9296162755,1.9432595768\C,0,1.7673613059,1.8064240186,1.  
8710641361\Si,0,0.1099280567,-0.3666867162,1.9397100973\C,0,1.95761926  
21,0.1989744143,1.86913181\H,0,-0.6255541575,-0.5271100648,-0.65225180  
3\H,0,2.6664607068,-1.3289000701,-0.6196928551\H,0,-0.9160224778,1.924  
913338,-0.6489156023\H,0,2.1062969625,3.4692505074,-0.6062977989\H,0,-  
0.8545752696,3.1148564921,2.5287023121\H,0,2.438070001,2.3130112752,2.  
5614262535\H,0,-0.2937154492,-1.6832394525,2.5160034129\H,0,2.72799336  
71,-0.1390821989,2.5585048206\Version=EM64L-G09RevA.02\State=1-A\MP2/  
GTbas1=-1312.5009337\CCSD(T)/GTbas1=-1312.6083272\MP2/GTbas2=0.\MP2/GT  
Bas3=0.\HF/GTMP2LargeXP=-1311.8180255\MP2/GTMP2LargeXP=-1312.9460397\H  
F/GFHFB3=-1311.8325435\HF/GFHFB4=-1311.8549442\G4MP2=-1313.1860546

### CSi13

\0,1\Si,0,-0.0947365287,-0.122695009,0.0226774487\  
Si,0,2.2683005629,0.0157796193,-0.1237940061\Si,0,0.1515403149,2.21185  
42931,-0.0145502609\C,0,2.0488508432,1.9377631114,0.1712491287\C,0,0.2  
963158751,1.9028537847,1.8693669795\C,0,1.8733990481,2.0040216407,1.76  
22209493\C,0,0.1224583082,0.3110865382,1.9184229489\Si,0,2.0196682968,  
0.1476034954,2.2070736137\H,0,-1.067350293,-1.1743071688,-0.3862425634  
\H,0,3.242413888,-0.4672347627,-1.1420676301\H,0,-0.4320966648,3.39964  
15614,-0.708525641\H,0,2.8125981744,2.5943160226,-0.2445861182\H,0,-0.  
1715691895,2.4297611255,2.6995783125\H,0,2.3399343438,2.8707278615,2.2  
280141137\H,0,-0.6415421729,-0.0568629932,2.6026795241\H,0,2.602715193  
5,-0.45790912,3.4425832005\Version=EM64L-G09RevA.02\State=1-A\MP2/GT  
bas1=-1312.499438\CCSD(T)/GTbas1=-1312.6089882\MP2/GTbas2=0.\MP2/GTbas3  
=0.\HF/GTMP2LargeXP=-1311.8137035\MP2/GTMP2LargeXP=-1312.9372421\HF/GF  
HFB3=-1311.8284223\HF/GFHFB4=-1311.8505607\G4MP2=-1313.1783342

### CSi14

\0,1\C,0,-0.0363195486,-0.0483444278,0.0173475498\  
C,0,1.5618467162,0.0125343421,-0.0027410175\C,0,-0.4048750482,1.507945  
6042,-0.0024887055\Si,0,1.4519156536,1.9089836444,-0.1991940104\Si,0,-  
0.6758364487,1.817384008,1.8928026195\Si,0,1.6748893955,2.2017666561,2

.1488606536\Si,0,-0.4041325609,-0.5324350121,1.8751481158\Si,0,1.93282  
96476,-0.1661452322,1.8924379277\H,0,-0.4602423245,-0.6057442024,-0.81  
94341656\H,0,2.0535761276,-0.6650899116,-0.6995899247\H,0,-1.189447307  
3,1.8007393268,-0.6991140727\H,0,2.0300535109,2.6693453416,-1.34648249  
73\H,0,-1.7609389522,2.730300914,2.3525595265\H,0,2.3870489684,3.13825  
88322,3.0582818589\H,0,-1.273166079,-1.6753421848,2.2807525508\H,0,3.1  
026982497,-0.9677576984,2.351853591\Version=EM64L-G09RevA.02\State=1-  
A\MP2/GTbas1=-1563.5237398\CCSD(T)/GTbas1=-1563.6384375\MP2/GTbas2=0.\  
MP2/GTbas3=0.\HF/GTMP2LargeXP=-1562.9003097\MP2/GTMP2LargeXP=-1563.976  
7062\HF/GFHFB3=-1562.9189627\HF/GFHFB4=-1562.9407971\G4MP2=-1564.23357  
26

### CSi15

\0,1\C,0,-0.0013787992,-0.0203149326,-0.0057008587  
\Si,0,1.955605204,-0.1442394254,-0.1227987102\C,0,-0.2523931137,1.5744  
10598,0.0469027017\Si,0,1.5721398469,2.1305940079,0.2289101175\Si,0,-0  
.4855609553,1.750247258,1.9406108345\C,0,1.4361401798,1.8009754043,2.1  
27106839\Si,0,-0.3982181337,-0.5793087201,1.8351759852\Si,0,1.88042876  
67,-0.0953297573,2.2398681405\H,0,-0.5740023392,-0.5010350271,-0.80096  
035\H,0,2.5847246277,-1.0659516348,-1.1098665073\H,0,-0.9467587242,1.9  
364529654,-0.707330047\H,0,2.0682442419,3.4631540436,-0.2221921079\H,0  
, -1.2844452363,2.8434090374,2.5667961212\H,0,1.927065518,2.4410817209,  
2.8594655945\H,0,-1.2519332228,-1.7751210729,2.0818485105\H,0,2.841642  
1395,-0.4826244655,3.3092637365\Version=EM64L-G09RevA.02\State=1-A\MP  
2/GTbas1=-1563.5309728\CCSD(T)/GTbas1=-1563.6432409\MP2/GTbas2=0.\MP2/  
GTbas3=0.\HF/GTMP2LargeXP=-1562.9108163\MP2/GTMP2LargeXP=-1563.9909254  
\HF/GFHFB3=-1562.9293043\HF/GFHFB4=-1562.9513947\G4MP2=-1564.2461374

### CSi16

\0,1\C,0,0.0527827901,0.0019050225,0.0029144472\Si  
,0,1.9530401144,-0.0826941248,-0.0889940408\Si,0,0.1927906953,1.919786  
972,-0.0645375709\C,0,2.1137843481,1.8150597317,-0.0632405329\Si,0,0.0  
711729883,2.1442323178,2.3081790528\Si,0,2.3706456362,1.7092999422,1.8  
406539445\Si,0,0.1927383181,-0.2057252466,1.910476036\C,0,2.1138431539  
, -0.1970216434,1.8051197377\H,0,-0.6811629448,-0.5430659948,-0.5840940  
805\H,0,2.6951469975,-0.9608991174,-1.0342860644\H,0,-0.4859176002,2.6  
512455634,-1.1704559468\H,0,2.7268278367,2.4538644343,-0.6927902112\H,  
0,-0.669550518,3.0216740061,3.2523128081\H,0,3.6269278246,2.2538955907  
, 2.4271198348\H,0,-0.4861720002,-1.362304698,2.5586904328\H,0,2.726702  
3601,-0.8723527557,2.3955321535\Version=EM64L-G09RevA.02\State=1-A\MP  
2/GTbas1=-1563.5744252\CCSD(T)/GTbas1=-1563.6836992\MP2/GTbas2=0.\MP2/  
GTbas3=0.\HF/GTMP2LargeXP=-1562.9645819\MP2/GTMP2LargeXP=-1564.0432106  
\HF/GFHFB3=-1562.9823525\HF/GFHFB4=-1563.0051223\G4MP2=-1564.2958396

### CSi17

\0,1\C,0,0.0016994003,-0.0293700597,-0.0030164286\  
Si,0,1.9409431781,-0.1137627472,-0.0878449867\C,0,-0.2380003631,1.5602  
227435,-0.0014426364\Si,0,1.5900974861,2.2128848423,-0.0855306268\Si,0  
, -0.7072239232,1.864525063,1.8592600669\Si,0,1.6070305769,2.2434132357  
, 2.3004135839\Si,0,-0.3563894212,-0.4621199013,1.8569522205\Si,0,1.966  
8260072,-0.1425989306,2.2980364028\H,0,-0.5724208395,-0.5463868468,-0.  
773799874\H,0,2.6117332468,-1.0806290025,-1.0037629274\H,0,-0.93928162  
01,1.886442702,-0.7713857214\H,0,1.9457379973,3.3362353534,-0.99947694  
11\H,0,-1.8456159676,2.761532629,2.2101712758\H,0,2.2711400667,3.17494  
75287,3.2520021919\H,0,-1.1795872893,-1.6555805042,2.2058001707\H,0,2.  
8764114645,-0.8386561053,3.2480242297\Version=EM64L-G09RevA.02\State=  
1-A\MP2/GTbas1=-1814.5417261\CCSD(T)/GTbas1=-1814.6614146\MP2/GTbas2=0

.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1813.9801745\MP2/GTMP2LargeXP=-1815.0  
105401\HF/GFHFB3=-1814.0029349\HF/GFHFB4=-1814.0243874\G4MP2=-1815.282  
9946

### CSi18

\\0,1\C,0,0.0304473892,0.0272936496,-0.0159724325\S  
i,0,1.9455372623,-0.0435537596,-0.0837987748\Si,0,0.130278911,1.941077  
1544,-0.0841677386\C,0,2.0305699896,1.8567605426,0.1586626218\Si,0,-0.  
2608559627,2.1463787451,2.2433189752\Si,0,2.1178959086,1.9369930374,2.  
0948106664\Si,0,-0.2399811734,-0.2196933374,1.8889098407\Si,0,2.114790  
1192,-0.4509272446,2.2438067358\H,0,-0.6080896795,-0.556879718,-0.6767  
880301\H,0,2.6093635616,-0.6561384025,-1.2694727099\H,0,-0.4206735998,  
2.6565475902,-1.2700431223\H,0,2.7265402255,2.4932123621,-0.3855952511  
\H,0,-1.1083638647,2.9887351563,3.127713018\H,0,3.135076659,2.86750167  
94,2.6601647948\H,0,-1.3024129581,-1.191396745,2.2725246628\H,0,2.8782  
772121,-1.3698107101,3.1285267438\\Version=EM64L-G09RevA.02\State=1-A\  
MP2/GTBas1=-1814.5721067\CCSD(T)/GTBas1=-1814.6889789\MP2/GTBas2=0.\MP  
2/GTBas3=0.\HF/GTMP2LargeXP=-1814.0172404\MP2/GTMP2LargeXP=-1815.04912  
78\HF/GFHFB3=-1814.0395119\HF/GFHFB4=-1814.0613881\G4MP2=-1815.3192683

### CSi19

\\0,1\C,0,-0.0280693958,-0.0336887199,-0.0400417057  
\Si,0,1.9248871773,-0.0935291069,-0.1154780247\Si,0,-0.4068700237,1.88  
30041263,-0.1142680612\Si,0,1.8842182143,2.221907251,0.295423165\Si,0,  
-0.4446410077,1.8368920309,2.2379129065\C,0,1.508231842,1.7770087558,2.  
.1624505059\Si,0,-0.4040369023,-0.4785712542,1.8269433833\Si,0,1.88706  
47821,-0.139708842,2.2366627836\H,0,-0.5462911282,-0.6441323432,-0.783  
6521527\H,0,2.5322115094,-0.9560576805,-1.1664868218\H,0,-1.3571740463  
,2.3413624286,-1.1651183524\H,0,2.8339027844,3.342334711,0.0496115077\  
H,0,-1.0520337609,2.6994389501,3.2888642539\H,0,2.0266938115,2.3872657  
123,2.9060468952\H,0,-1.3540322012,-1.5987078504,2.0728885814\H,0,2.83  
78383451,-0.597718169,3.2872411359\\Version=EM64L-G09RevA.02\State=1-A\  
\MP2/GTBas1=-1814.5520047\CCSD(T)/GTBas1=-1814.6692747\MP2/GTBas2=0.\M  
P2/GTBas3=0.\HF/GTMP2LargeXP=-1813.9942781\MP2/GTMP2LargeXP=-1815.0280  
384\HF/GFHFB3=-1814.0168948\HF/GFHFB4=-1814.038549\G4MP2=-1815.2987644

### CSi20

\\0,1\C,0,-0.0078460559,-0.0069257977,-0.0078211713  
\Si,0,1.9272610173,-0.0752378783,-0.087946405\Si,0,-0.335683464,1.9014  
109302,-0.0881015143\Si,0,2.0067416384,2.2992416907,0.024476888\Si,0,-  
0.6012690298,1.9463548863,2.2755934433\Si,0,1.7983883051,2.0613490111,  
2.4101681196\Si,0,-0.3357743942,-0.3817459294,1.8650855652\Si,0,2.0066  
471599,-0.3325287553,2.2751489109\H,0,-0.5470697454,-0.6243630371,-0.7  
296666842\H,0,2.517477511,-0.9646144418,-1.1282836804\H,0,-1.296368726  
2,2.3664457254,-1.1286645249\H,0,2.8736907136,3.2917525906,-0.66573199  
42\H,0,-1.5461474054,2.6930782095,3.1489059144\H,0,2.5333685646,2.9031  
941171,3.3950093637\H,0,-1.2966400006,-1.4817410493,2.1634474464\H,0,2  
.8738239116,-1.167970272,3.1486803227\\Version=EM64L-G09RevA.02\State=  
1-A\MP2/GTBas1=-2065.5756073\CCSD(T)/GTBas1=-2065.6997921\MP2/GTBas2=0  
.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2065.0787971\MP2/GTMP2LargeXP=-2066.0  
624189\HF/GFHFB3=-2065.1054776\HF/GFHFB4=-2065.1266221\G4MP2=-2066.349  
7071

### CSi1+

\\1,2\Si,0,0.0309763339,-0.2331111805,0.05238  
73386\C,0,1.8818713033,-0.0135577134,0.0361979842\C,0,0.3319676759,1.9  
687835502,0.082024852\C,0,1.8026035216,1.5727931592,-0.0774448813\C,0,



0.320475475,1.7552021591,1.5975247881\C,0,1.8971552961,1.6797803461,1.4978855171\C,0,0.2727685735,0.1845506112,1.85317839\C,0,1.8386910609,0.1264514683,1.6140444772\H,0,-1.0532121628,-0.6666049933,-0.8635858161\H,0,2.6911295705,-0.5182642308,-0.4786908466\H,0,-0.1803934709,2.7607481729,-0.457834042\H,0,2.4133431693,2.0798195015,-0.8199688154\H,0,-0.2788834059,2.4100035528,2.2247363147\H,0,2.5535305108,2.3852291194,2.0018945854\H,0,-0.1862927312,-0.1667089296,2.7700198997\H,0,2.4710692797,-0.4960145932,2.2419302542\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-559.1554752\CCSD(T)/GTBas1=-559.2593621\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-558.3115881\MP2/GTMP2LargeXP=-559.5180764\HF/GFHFB3=-558.3152952\HF/GFHFB4=-558.3375731\G4MP2=-559.7211534

### CSi2<sup>+</sup>

\\1,2\Si,0,0.0426152516,-0.3201363393,0.0705172499\C,0,1.9069230234,-0.004578538,0.0051425161\Si,0,0.3737638976,2.3286990322,0.0712047502\C,0,2.1044846723,1.568296433,0.0075379678\C,0,0.5197230807,1.7658176133,1.8710787613\C,0,2.0671612392,1.5598476878,1.5927694773\C,0,0.3210876344,0.1930632713,1.8700734348\C,0,1.8713697379,0.0079240029,1.5907848145\H,0,-0.8171641636,-1.3601139998,-0.5499761403\H,0,2.6375582489,-0.5914626534,-0.5445909407\H,0,-0.2196174625,3.5345948468,-0.5610223653\H,0,2.9578187001,1.9573482792,-0.5409659726\H,0,0.1640016749,2.3056529053,2.7442572991\H,0,2.8075552637,2.1169313676,2.1633592222\H,0,-0.1575334048,-0.243011296,2.742554589\H,0,2.4486526063,-0.7189726131,2.1586753367\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-810.1856336\CCSD(T)/GTBas1=-810.2891887\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-809.3981329\MP2/GTMP2LargeXP=-810.5697653\HF/GFHFB3=-809.4050432\HF/GFHFB4=-809.427771\G4MP2=-810.7829394

### CSi3<sup>+</sup>

\\1,2\Si,0,-0.055551333,-0.0610912418,-0.0441743146\C,0,1.8367241635,0.0375904542,-0.0514831012\C,0,-0.154666427,1.8311722083,-0.0510146781\Si,0,1.7258010636,1.9167833774,-0.2678842798\C,0,0.0697812681,1.8057251331,1.5112078278\C,0,1.6291379163,1.8089915745,1.7252527159\C,0,0.2628485961,0.2919672288,1.8968184053\C,0,1.7883889768,0.2578321562,1.5108066586\H,0,-0.9779312522,-1.0850537819,-0.5828633779\H,0,2.5681561717,-0.6643321836,-0.4335206534\H,0,-0.9290882258,2.4855272988,-0.4327644868\H,0,2.574931768,2.8597019006,-1.0290374521\H,0,-0.5606516081,2.4430343987,2.1259280327\H,0,2.0153638707,2.2375633662,2.645284893\H,0,-0.0149495247,-0.016739737,2.9002279948\H,0,2.4881045761,-0.3028721524,2.1252158157\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-810.2060607\CCSD(T)/GTBas1=-810.3045015\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-809.4136554\MP2/GTMP2LargeXP=-810.595269\HF/GFHFB3=-809.4203664\HF/GFHFB4=-809.4432034\G4MP2=-810.8041737

### CSi4<sup>+</sup>

\\1,2\Si,0,-0.1264263424,0.0001674584,-0.0399620816\C,0,1.9086973239,0.0581673302,0.105280296\C,0,0.1742860649,1.8586304614,0.0474352889\C,0,1.6621075315,1.5183859837,-0.2747814871\C,0,0.1645736729,1.7812156282,1.6244231442\Si,0,2.0587939456,1.7845956591,1.7385803295\C,0,0.2003780264,0.195693565,1.8234013533\C,0,1.7501292617,-0.0658363983,1.6568542688\H,0,-0.8043228907,-0.8836802561,-1.0215431691\H,0,2.7430155792,-0.4418211295,-0.3768110142\H,0,-0.2332987418,2.7355121394,-0.4406535376\H,0,2.0860250063,1.8646194339,-1.2127044328\H,0,0,-0.609083265,2.3377744095,2.142480266\H,0,3.1958631316,2.6398812261,2.1642395259\H,0,-0.2800718184,-0.2105679973,2.7072266103\H,0,2.1881335143,-0.9447375138,2.1139346394\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-810.196823\CCSD(T)/GTBas1=-810.298155\MP2/GTBas2=0.\MP2/GT

as3=0.\HF/GTMP2LargeXP=-809.4061745\MP2/GTMP2LargeXP=-810.5854103\HF/G  
FHFB3=-809.4131922\HF/GFHFB4=-809.4358754\G4MP2=-810.7970808

**CSi5+**

\\1,2\Si,0,-0.1861865806,-0.1684736518,0.1809  
181828\Si,0,2.2709208193,0.1177929812,-0.0194892999\Si,0,0.3327305972,  
2.2498164135,-0.0191170779\C,0,2.1922859205,1.9930699846,0.1495309718\  
C,0,0.39024051,1.8558668419,1.8685132375\C,0,1.9670362943,1.7880763566  
,1.7125776411\C,0,0.3121743096,0.2848182563,1.9641529956\C,0,1.8833793  
854,0.2119747511,1.8682392982\H,0,-1.2278307913,-1.1192857909,-0.28460  
07203\H,0,3.1897236663,-0.6762144378,-0.8690580081\H,0,-0.369997314,3.  
2395860446,-0.8693730216\H,0,2.9519946177,2.6839059122,-0.2035458394\H  
,0,-0.0934113858,2.4487396678,2.6422172363\H,0,2.6099943258,2.37158304  
28,2.3710664118\H,0,-0.1522379874,-0.1372577357,2.8523256505\H,0,2.427  
3836131,-0.3267986362,2.6414423415\\Version=EM64L-G09RevA.02\State=2-A  
\MP2/GTbas1=-1061.2165497\CCSD(T)/GTbas1=-1061.3231207\MP2/GTbas2=0.\MP  
P2/GTbas3=0.\HF/GTMP2LargeXP=-1060.4886432\MP2/GTMP2LargeXP=-1061.6203  
795\HF/GFHFB3=-1060.4994371\HF/GFHFB4=-1060.5219423\G4MP2=-1061.847964  
6

**CSi6+**

\\1,2\Si,0,-0.0257766274,-0.2139618715,0.0020  
317645\C,0,1.9140794389,0.0697231666,-0.0308207471\Si,0,0.2768016639,2  
.1865690593,-0.0130237155\C,0,2.1063629348,1.6383859125,-0.1607456842\  
C,0,0.3865758839,1.8660946255,1.8726850555\Si,0,2.2646165874,1.7213111  
452,1.7204665164\C,0,0.3079853998,0.2822073191,1.8683734453\C,0,1.7359  
089648,-0.2058271513,1.489836611\H,0,-0.5927480784,-1.544920072,-0.330  
5332084\H,0,2.6467950436,-0.544310824,-0.5470313751\H,0,-0.3388827473,  
3.3637094355,-0.6655108919\H,0,2.792727133,1.9617516695,-0.9357391895\  
H,0,-0.2185946993,2.3612976624,2.6242506714\H,0,3.363496166,2.19266235  
13,2.5965234335\H,0,-0.137697287,-0.1748904837,2.7474506479\H,0,2.0418  
502234,-1.1813019442,1.8575866664\\Version=EM64L-G09RevA.02\State=2-A\  
MP2/GTbas1=-1061.2312213\CCSD(T)/GTbas1=-1061.3343344\MP2/GTbas2=0.\MP  
P2/GTbas3=0.\HF/GTMP2LargeXP=-1060.4982441\MP2/GTMP2LargeXP=-1061.63995  
19\HF/GFHFB3=-1060.5088127\HF/GFHFB4=-1060.5315834\G4MP2=-1061.8645972

**CSi8+**

\\1,2\Si,0,-0.158308654,-0.0599483844,0.03908  
13665\Si,0,2.2159327125,-0.2549725825,0.1588763657\Si,0,-0.1880950823,  
2.3021168624,0.0573994587\Si,0,2.1476643492,2.3918135599,0.0399200129\  
C,0,0.3172369518,1.8696755513,1.8986805637\C,0,1.8970380094,1.80682226  
51,1.8746917409\C,0,0.2761054983,0.2816289877,1.9080001107\C,0,1.85798  
72441,0.2347339227,1.952448817\H,0,-1.0436949765,-1.0979724636,-0.5394  
843152\H,0,3.4177100218,-0.9345312572,-0.3920926183\H,0,-1.1851716451,  
3.2954939792,-0.3975404195\H,0,3.2994864406,3.1632083392,-0.4948523071  
\H,0,-0.1263499048,2.4125655739,2.7341222163\H,0,2.4736423196,2.325549  
8283,2.6423664782\H,0,-0.2585479413,-0.2242068016,2.711460614\H,0,2.32  
93646568,-0.2212773805,2.8202219154\\Version=EM64L-G09RevA.02\State=2-  
A\MP2/GTbas1=-1312.2178091\CCSD(T)/GTbas1=-1312.331853\MP2/GTbas2=0.\MP  
P2/GTbas3=0.\HF/GTMP2LargeXP=-1311.5541772\MP2/GTMP2LargeXP=-1312.6348  
347\HF/GFHFB3=-1311.5691087\HF/GFHFB4=-1311.5912852\G4MP2=-1312.881142  
5

**CSi9+**

\\1,2\Si,0,-0.0124448902,-0.1928071756,-0.168  
4521292\Si,0,2.3293116877,-0.0357704087,-0.0312822493\Si,0,0.391893829  
5,2.2993617116,0.126403715\C,0,2.2298669796,1.8788681681,-0.0042791421

\C,0,0.7413563691,2.2786344154,1.9668871064\C,0,2.238500057,1.85094208  
63,1.5971613842\Si,0,0.3939376184,0.4616617102,2.2581273546\C,0,2.2307  
410249,0.2708149132,1.8589599884\H,0,-1.1171244347,-0.9449650969,-0.81  
42673495\H,0,3.402670689,-0.804843088,-0.6943636095\H,0,-0.5032997639,  
3.1836634854,-0.6549173694\H,0,2.9244604514,2.5215239961,-0.5428933422  
\H,0,0.5646101938,3.0897551668,2.6657661925\H,0,3.0231598914,2.4233185  
808,2.0911097466\H,0,-0.5020542033,-0.1854707997,3.2441469848\H,0,2.92  
63145003,-0.1677876649,2.5726927186\\Version=EM64L-G09RevA.02\State=2-  
A\MP2/GTbas1=-1312.2462802\CCSD(T)/GTbas1=-1312.3560011\MP2/GTbas2=0.\  
MP2/GTbas3=0.\HF/GTMP2LargeXP=-1311.5873902\MP2/GTMP2LargeXP=-1312.672  
6755\HF/GFHFB3=-1311.6014892\HF/GFHFB4=-1311.6242343\G4MP2=-1312.91478  
38

#### CSi10<sup>+</sup>

\\1,2\Si,0,-0.1312663406,-0.1517035255,0.0123  
117194\C,0,1.7845328817,0.0927015735,-0.01810937\C,0,-0.1478796519,1.7  
807406323,-0.0182960866\Si,0,1.7414755747,1.9948625277,0.3199916667\Si  
,0,-0.3051572615,1.6312489951,1.9689864309\C,0,1.5771326937,1.80684718  
72,2.1828432042\C,0,-0.2331848328,-0.2677668815,1.8853708611\Si,0,1.65  
83687026,-0.0817776754,1.9694034539\H,0,-0.8675771564,-0.9917239818,-0  
.9508881014\H,0,2.4019393551,-0.3324934298,-0.8068436708\H,0,-0.653766  
4131,2.3329105436,-0.80777458\H,0,2.5968108544,2.9706591742,-0.3812471  
335\H,0,-1.3496130476,2.4494497244,2.6180678574\H,0,2.0888388434,2.394  
0754314,2.9374759026\H,0,-0.8390717763,-0.9630296058,2.4560299957\H,0,  
2.6096175746,-1.0057006897,2.6198778503\\Version=EM64L-G09RevA.02\Stat  
e=2-A\MP2/GTbas1=-1312.2971391\CCSD(T)/GTbas1=-1312.4001813\MP2/GTbas2  
=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1311.6506446\MP2/GTMP2LargeXP=-1312  
.7407979\HF/GFHFB3=-1311.6639567\HF/GFHFB4=-1311.6877495\G4MP2=-1312.9  
784527

#### CSi11<sup>+</sup>

\\1,2\Si,0,0.0861383263,-0.1239816692,-0.0456  
583508\C,0,1.9720397191,-0.0755500937,0.0892957821\Si,0,-0.2396419785,  
2.3081001096,0.1683634643\Si,0,2.1711254992,1.803734992,0.1762863027\C  
,0,0.0832056169,1.7534979935,1.9720478713\C,0,1.6646982301,1.847040148  
,2.0344921389\C,0,-0.1333277672,0.1885204628,1.843048519\Si,0,1.775426  
2136,-0.0823869926,1.9955508116\H,0,-0.6070742043,-1.142584706,-0.8656  
081664\H,0,2.6142137553,-0.6996316412,-0.524872653\H,0,-1.1658435478,3  
.3587160777,-0.328526048\H,0,3.3220097032,2.4912290925,-0.4507990394\H  
,0,-0.4126442569,2.1911970479,2.8360691053\H,0,2.0830973485,2.57985139  
69,2.7194671605\H,0,-0.9692214205,-0.2353240738,2.3934507937\H,0,2.537  
798763,-1.0111281445,2.8602923082\\Version=EM64L-G09RevA.02\State=2-A\  
MP2/GTbas1=-1312.2693895\CCSD(T)/GTbas1=-1312.3755735\MP2/GTbas2=0.\MP  
2/GTbas3=0.\HF/GTMP2LargeXP=-1311.6066921\MP2/GTMP2LargeXP=-1312.70056  
12\HF/GFHFB3=-1311.6208057\HF/GFHFB4=-1311.6436943\G4MP2=-1312.9393388

#### CSi12<sup>+</sup>

\\1,2\C,0,0.0403486673,-0.0087680785,0.035177  
1426\Si,0,1.9562331046,-0.2084284125,0.0023111937\C,0,-0.1550281551,1.  
5897474112,0.0317384098\Si,0,1.6602416954,2.2102319916,-0.0039789855\  
Si,0,-0.1434002965,1.9944222874,1.9075859668\C,0,1.7722092702,1.7948700  
559,1.8739866688\Si,0,0.151548894,-0.4243536296,1.9128175109\C,0,1.967  
1624121,0.1962985266,1.8779200544\H,0,-0.6254985001,-0.5240685692,-0.6  
526624229\H,0,2.6599928357,-1.363662626,-0.6051482056\H,0,-0.925101254  
,1.9291377028,-0.6558152377\H,0,2.0888090715,3.5009109569,-0.595023162  
6\H,0,-0.8487648517,3.1490544238,2.5143190599\H,0,2.4391669368,2.31023  
99699,2.5606924079\H,0,-0.2762297546,-1.7150081943,2.5044765723\H,0,2.

7362099246,-0.1431238161,2.5666030274\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1312.2535691\\CCSD(T)/GTBas1=-1312.3568866\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1311.574129\\MP2/GTMP2LargeXP=-1312.6847783\\HF/GFHFB3=-1311.588512\\HF/GFHFB4=-1311.6111439\\G4MP2=-1312.921618

**CSi13+**

\\1,2\\Si,0,-0.1149903838,-0.1521516425,0.1579  
614238\\Si,0,2.2870155367,0.1486310315,-0.1625128633\\Si,0,0.2487496258,  
2.2499396738,-0.0536549653\\C,0,2.1163219296,2.018861246,0.1726649222\\C  
,0,0.2935408229,1.8772068638,1.8581264569\\C,0,1.8769843427,1.991091993  
,1.7378353316\\C,0,0.0553550784,0.3181415687,1.9992230791\\Si,0,1.922754  
8174,0.1113537401,2.2477674107\\H,0,-0.9443403858,-1.2842785203,-0.3203  
423803\\H,0,3.1186732104,-0.4084260884,-1.2563786734\\H,0,-0.4168538606,  
3.3010592699,-0.8634674184\\H,0,2.8759255908,2.7056966713,-0.1928687167  
\\H,0,-0.1833604206,2.4807367709,2.6290147806\\H,0,2.3517002902,2.804582  
6992,2.2844820981\\H,0,-0.704446542,0.0028208844,2.7103132762\\H,0,2.587  
8703478,-0.6188661616,3.3559362383\\Version=EM64L-G09RevA.02\\State=2-A  
\\MP2/GTBas1=-1312.2491311\\CCSD(T)/GTBas1=-1312.3572992\\MP2/GTBas2=0.\\M  
P2/GTBas3=0.\\HF/GTMP2LargeXP=-1311.5792987\\MP2/GTMP2LargeXP=-1312.6731  
401\\HF/GFHFB3=-1311.5937926\\HF/GFHFB4=-1311.6162437\\G4MP2=-1312.913259  
6

**CSi14+**

\\1,2\\C,0,0.0527062441,0.0653804797,-0.126602  
8509\\C,0,1.5713126769,0.0287065682,-0.0130759572\\C,0,-0.3917761074,1.5  
175167098,-0.0101025899\\Si,0,1.4863395266,1.9540320866,-0.2058554725\\S  
i,0,-0.6668363076,1.8298647094,1.8825678732\\Si,0,1.6817368161,2.211014  
792,2.161430487\\Si,0,-0.3847575641,-0.5038112588,2.0801684834\\Si,0,1.9  
413423359,-0.1541704337,1.8792761833\\H,0,-0.454438971,-0.6019101322,-0  
.8250819154\\H,0,2.0672847045,-0.6893780942,-0.6649532284\\H,0,-1.218716  
8708,1.8012468288,-0.660051032\\H,0,1.9979260599,2.631718343,-1.4213475  
532\\H,0,-1.830971081,2.6580568302,2.2704300824\\H,0,2.3615542585,3.1025  
346014,3.1268749515\\H,0,-1.2695924223,-1.6671450754,2.3553317051\\H,0,3  
.0467867016,-1.0572569546,2.2719908336\\Version=EM64L-G09RevA.02\\State  
=2-A\\MP2/GTBas1=-1563.25581\\CCSD(T)/GTBas1=-1563.3754892\\MP2/GTBas2=0.  
\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1562.6598017\\MP2/GTMP2LargeXP=-1563.69  
26658\\HF/GFHFB3=-1562.678569\\HF/GFHFB4=-1562.7005762\\G4MP2=-1563.95578  
3

**CSi15+**

\\1,2\\C,0,-0.0761330036,-0.0404386809,-0.1000  
333084\\Si,0,1.8320214381,-0.1998408759,-0.1647352151\\C,0,-0.2314240929  
,1.5410510189,0.0647034299\\Si,0,1.5946039534,2.1528840465,0.292799881\\  
Si,0,-0.4323592827,1.7782033236,1.9789023294\\C,0,1.4592045897,1.902891  
2156,2.1775139903\\Si,0,-0.4070902616,-0.6137147577,1.6978896411\\Si,0,1  
.8691315349,0.037081465,2.2556794469\\H,0,-0.6734113408,-0.4560527815,-  
0.9103714822\\H,0,2.5441601174,-1.2028565773,-0.9932875286\\H,0,-0.91331  
0713,1.9906404709,-0.6551522474\\H,0,2.1737843523,3.3996140641,-0.26107  
8022\\H,0,-1.325114075,2.752936579,2.6493144355\\H,0,1.9441011727,2.5511  
049691,2.9044400406\\H,0,-1.1038886794,-1.8771158045,2.0413660262\\H,0,2  
.8170242905,-0.439987675,3.2891485829\\Version=EM64L-G09RevA.02\\State=  
2-A\\MP2/GTBas1=-1563.2892661\\CCSD(T)/GTBas1=-1563.3994864\\MP2/GTBas2=0  
.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1562.6841394\\MP2/GTMP2LargeXP=-1563.7  
367868\\HF/GFHFB3=-1562.7023675\\HF/GFHFB4=-1562.7247681\\G4MP2=-1563.989  
8051

**CSi16\***

\\1,2\C,0,0.0467359091,0.0371225934,0.0304587  
191\Si,0,1.9660848192,-0.135308681,-0.1081676284\Si,0,0.3159222532,1.9  
092419672,-0.1219106506\C,0,2.1906736853,1.7661956832,-0.1559646954\Si  
,0,-0.0053138032,2.015399643,2.3937637506\Si,0,2.4067967419,1.70983050  
87,1.7136944394\Si,0,0.1768818607,-0.2727376231,1.9214125738\C,0,2.090  
8473263,-0.1604740785,1.8181697766\H,0,-0.7480003021,-0.4342833833,-0.  
5442952631\H,0,2.6703170494,-1.0591904815,-1.0209073606\H,0,-0.4530911  
004,2.8224852569,-0.9960307846\H,0,2.8218830555,2.3591456094,-0.810288  
5643\H,0,-0.6970867755,2.9920875168,3.2718786729\H,0,3.474209587,2.441  
627322,2.4309678029\H,0,-0.4514962824,-1.4763206942,2.5028881602\H,0,2  
.7082359761,-0.767921159,2.4769310516\\Version=EM64L-G09RevA.02\State=  
2-A\MP2/GTbas1=-1563.3107237\CCSD(T)/GTbas1=-1563.420623\MP2/GTbas2=0.  
\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1562.7227729\MP2/GTMP2LargeXP=-1563.76  
64876\HF/GFHFB3=-1562.74033\HF/GFHFB4=-1562.7634888\G4MP2=-1564.020208  
9

**CSi18\***

\\1,2\C,0,0.0271605535,0.0243249816,-0.081721  
6097\Si,0,1.9302960955,-0.021634519,-0.1300290093\Si,0,0.1505967204,1.  
9240598315,-0.1302877034\C,0,2.0407109245,1.8661050146,0.09240892\Si,0  
, -0.1939462523,2.0637602128,2.3215403216\Si,0,2.177585159,1.9915525146  
,2.0021221123\Si,0,-0.2915412382,-0.2668964861,1.7882402269\Si,0,2.038  
3656453,-0.3769139264,2.3221095801\H,0,-0.5904917587,-0.5407724083,-0.  
7784610521\H,0,2.6939574893,-0.7578990993,-1.1642111711\H,0,-0.5144282  
859,2.7497636961,-1.1650584662\H,0,2.7195988095,2.4869922096,-0.490470  
6857\H,0,-0.9590387638,2.8054864547,3.3517978754\H,0,3.1864776583,2.91  
42118448,2.5688324706\H,0,-1.3460050506,-1.2313036738,2.1732491048\H,0  
,2.7091022942,-1.2047366473,3.3525390859\\Version=EM64L-G09RevA.02\Sta  
te=2-A\MP2/GTbas1=-1814.3183322\CCSD(T)/GTbas1=-1814.4322334\MP2/GTbas  
2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1813.774519\MP2/GTMP2LargeXP=-1814  
.7852719\HF/GFHFB3=-1813.7965146\HF/GFHFB4=-1813.8187903\G4MP2=-1815.0  
529123

**CSi19\***

\\1,2\C,0,-0.0846387413,-0.1006136667,-0.1217  
135881\Si,0,1.8339546159,-0.1169834341,-0.1436108368\Si,0,-0.415019020  
7,1.7895110215,-0.142716434\Si,0,1.8928150327,2.2319982532,0.393628263  
4\Si,0,-0.3537721426,1.8604253566,2.2659590485\C,0,1.5647905139,1.8440  
494033,2.2440649384\Si,0,-0.4125863114,-0.4886422803,1.7287072654\Si,0  
,1.8951879119,-0.0460859062,2.2650973641\H,0,-0.6019130027,-0.71058830  
69,-0.8637753137\H,0,2.5318991751,-0.9469376459,-1.1538234471\H,0,-1.3  
480875841,2.3433533743,-1.1523278756\H,0,2.8245003364,3.3310014098,0.0  
456850107\H,0,-1.0517178569,2.6899274971,3.2765414591\H,0,2.0821824689  
,2.453980124,2.986080119\H,0,-1.3443170423,-1.5875887736,2.0767076945\  
H,0,2.8286216472,-0.599706426,3.2744963322\\Version=EM64L-G09RevA.02\St  
ate=2-A\MP2/GTbas1=-1814.3214025\CCSD(T)/GTbas1=-1814.4341599\MP2/GTB  
as2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1813.7769188\MP2/GTMP2LargeXP=-1  
814.788517\HF/GFHFB3=-1813.7991281\HF/GFHFB4=-1813.8211565\G4MP2=-1815  
.054314

**CSi20\***

\\0,1\C,0,-0.0078460559,-0.0069257977,-0.0078211713  
\Si,0,1.9272610173,-0.0752378783,-0.087946405\Si,0,-0.335683464,1.9014  
109302,-0.0881015143\Si,0,2.0067416384,2.2992416907,0.024476888\Si,0,-  
0.6012690298,1.9463548863,2.2755934433\Si,0,1.7983883051,2.0613490111,  
2.4101681196\Si,0,-0.3357743942,-0.3817459294,1.8650855652\Si,0,2.0066

471599,-0.3325287553,2.2751489109\H,0,-0.5470697454,-0.6243630371,-0.7  
296666842\H,0,2.517477511,-0.9646144418,-1.1282836804\H,0,-1.296368726  
2,2.3664457254,-1.1286645249\H,0,2.8736907136,3.2917525906,-0.66573199  
42\H,0,-1.5461474054,2.6930782095,3.1489059144\H,0,2.5333685646,2.9031  
941171,3.3950093637\H,0,-1.2966400006,-1.4817410493,2.1634474464\H,0,2  
.8738239116,-1.167970272,3.1486803227\\Version=EM64L-G09RevA.02\State=  
1-A\MP2/GTBas1=-2065.5756073\CCSD(T)/GTBas1=-2065.6997921\MP2/GTBas2=0  
\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2065.0787971\MP2/GTMP2LargeXP=-2066.0  
624189\HF/GFHFB3=-2065.1054776\HF/GFHFB4=-2065.1266221\G4MP2=-2066.349  
7071

#### 4. Nitrogen-phosphorus cubanoids

##### NP1

\\0,1\P,0,0.0600435619,0.0463840455,0.0376836565\N,0,1  
.891067269,-0.0150959752,-0.012212438\N,0,0.4659249968,1.8327816868,-0  
.0124902801\N,0,1.9450107247,1.500031465,-0.1611054378\N,0,0.635749377  
,1.8438690245,1.5013963356\N,0,2.1200953297,1.6349795354,1.3312611861\  
N,0,0.4654909941,0.3592894677,1.797202232\N,0,1.9447177467,0.146260750  
3,1.5015647459\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-722.593  
299\CCSD(T)/GTBas1=-722.6817405\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La  
rgeXP=-721.4936263\MP2/GTMP2LargeXP=-723.0537378\HF/GFHFB3=-721.500574  
7\HF/GFHFB4=-721.5284065\G4MP2=-723.3424217

##### NP2

\\0,1\P,0,0.0224358442,-0.0206965002,0.021491222\N,0,1  
.8794381936,-0.0132332729,-0.0065569327\N,0,0.502311267,2.234730112,0.  
0208928831\N,0,2.195427819,1.4719298657,-0.0069889918\N,0,0.7785462276  
,1.7739080968,1.7986847434\N,0,2.2248261869,1.4549054528,1.5029393868\  
N,0,0.4625292727,0.2887465995,1.7991088769\N,0,1.913385189,-0.00879035  
37,1.5033288123\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1008.8  
799423\CCSD(T)/GTBas1=-1008.973737\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP  
2LargeXP=-1007.8534579\MP2/GTMP2LargeXP=-1009.3551453\HF/GFHFB3=-1007.  
8650609\HF/GFHFB4=-1007.8919531\G4MP2=-1009.6555013

##### NP3

\\0,1\P,0,0.095701093,0.084209169,0.0215179192\N,0,1.8  
990336263,-0.0085834223,-0.0445218808\N,0,0.2360738469,1.8844780381,-0  
.0440914023\N,0,2.0131713304,1.7686982545,-0.3498535833\N,0,0.52831485  
16,1.8900845567,1.4902385838\N,0,2.0345616789,1.7870782934,1.459372969  
1\N,0,0.4629473315,0.4064229373,1.7637595376\N,0,1.9425962414,0.280112  
1733,1.4898778566\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1008  
.9286247\CCSD(T)/GTBas1=-1009.014897\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GT  
MP2LargeXP=-1007.9179265\MP2/GTMP2LargeXP=-1009.4177594\HF/GFHFB3=-100  
7.9288462\HF/GFHFB4=-1007.9566508\G4MP2=-1009.7117923

##### NP4

\\0,1\P,0,0.078728833,0.0596503217,0.0477247294\N,0,1.  
9009427383,-0.0224867649,-0.0178584729\N,0,0.4961992882,1.8353208338,-  
0.0178263972\N,0,1.9540215361,1.4777892292,-0.305098252\N,0,0.54810632  
63,1.8747829286,1.5093420139\N,0,2.3703241181,1.7926557958,1.443740323  
9\N,0,0.4950281588,0.3745077434,1.7965658441\N,0,1.9528490012,0.016979  
9124,1.5093102108\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1008  
.917469\CCSD(T)/GTBas1=-1009.0050346\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GT  
MP2LargeXP=-1007.8974065\MP2/GTMP2LargeXP=-1009.3977576\HF/GFHFB3=-100  
7.9081659\HF/GFHFB4=-1007.9359127\G4MP2=-1009.6928919

**NP5**

\\0,1\p,0,-0.1085671374,-0.0987660249,0.0398236429\p,0  
,2.2107975347,0.1317810558,-0.0131120336\p,0,0.3408688095,2.1882845069  
, -0.013169409\N,0,2.12263939,1.9300180891,0.1981533711\N,0,0.448544343  
4,1.8479452699,1.7692119147\N,0,1.951244566,1.7742157241,1.6987367423\  
N,0,0.3747203283,0.3407241182,1.8164990787\N,0,1.8821521654,0.27129726  
09,1.7692566928\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-1295.1  
831119\CCSD(T)/GTbas1=-1295.2790951\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTM  
P2LargeXP=-1294.2372792\MP2/GTMP2LargeXP=-1295.6834202\HF/GFHFB3=-1294  
.2533583\HF/GFHFB4=-1294.2795769\G4MP2=-1295.992474

**NP6**

\\0,1\p,0,0.0365275509,-0.0119082683,0.0296332329\N,0,  
1.895364013,-0.0308375761,-0.0198071426\p,0,0.5831106236,2.2063352097,  
0.0543497246\N,0,2.2393926345,1.4656406077,-0.1386109419\N,0,0.7230083  
084,1.817308257,1.8314888364\p,0,2.4968299297,1.5264224471,1.648696586  
9\N,0,0.4893830036,0.2952314777,1.8068761948\N,0,1.8958839363,-0.16379  
21548,1.487873509\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-1295  
.2154166\CCSD(T)/GTbas1=-1295.307009\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GT  
MP2LargeXP=-1294.2742452\MP2/GTMP2LargeXP=-1295.7180854\HF/GFHFB3=-129  
4.2897952\HF/GFHFB4=-1294.3167054\G4MP2=-1296.0236808

**NP7**

\\0,1\p,0,0.0930470331,0.0694694162,0.053894089\N,0,1.  
8987102832,-0.0013314967,-0.0000557941\N,0,0.2005422132,1.8550959253,-  
0.0291423008\p,0,1.9794870903,1.7900005426,-0.2264035308\N,0,0.3787379  
905,1.907818454,1.4977233682\N,0,1.9142777975,1.9773068692,1.553426708  
9\N,0,0.198981351,0.4123242893,1.8080772215\p,0,1.9777162412,0.2037160  
001,1.7938802381\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-1295.  
2802995\CCSD(T)/GTbas1=-1295.3651891\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GT  
MP2LargeXP=-1294.3646\MP2/GTMP2LargeXP=-1295.8025298\HF/GFHFB3=-1294.3  
79597\HF/GFHFB4=-1294.4075086\G4MP2=-1296.1018381

**NP9**

\\0,1\p,0,-0.1518703065,-0.1370101979,-0.1242223892\p,  
0,2.1764596279,0.0932719709,0.0842035292\p,0,0.3179378973,2.1545769154  
,0.0848679091\N,0,2.086671038,1.8810043127,0.1667909345\N,0,0.56110093  
73,2.0414902851,1.8564988902\N,0,2.0536354111,1.8509962046,1.681078154  
5\p,0,0.3208496049,0.2882236732,2.1370821497\N,0,2.0888157901,0.346746  
836,1.8562008221\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-1581.  
5070265\CCSD(T)/GTbas1=-1581.603272\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTM  
P2LargeXP=-1580.6471372\MP2/GTMP2LargeXP=-1582.0384104\HF/GFHFB3=-1580  
.6676652\HF/GFHFB4=-1580.6934293\G4MP2=-1582.3540931

**NP10**

\\0,1\p,0,0.0740139636,0.0690802567,0.0645211458\N,0,1  
.8653409091,0.0185780446,0.0174527798\N,0,0.1544232796,1.8593282136,0.  
0166313416\p,0,1.9447102847,1.8077863853,-0.0606171253\p,0,0.202841481  
1,1.9351649521,1.8071366595\N,0,1.9919257867,1.8528709039,1.7308531929  
\N,0,0.153687789,0.1437282665,1.8540425897\p,0,1.9441565061,0.06266297  
73,1.808079416\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-1581.65  
0246\CCSD(T)/GTbas1=-1581.733332\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2L  
argeXP=-1580.8345237\MP2/GTMP2LargeXP=-1582.2087641\HF/GFHFB3=-1580.85  
37327\HF/GFHFB4=-1580.8818148\G4MP2=-1582.5125226

**NP11**

\\0,1\p,0,0.1171418061,0.0281764664,0.0348280983\N,0,1

.9211309411,-0.0303517057,0.0181024076\N,0,0.0824687137,2.3325239903,0.0108286718\N,0,2.306325401,1.7313881537,-0.0591954003\N,0,0.5291664184,1.8569943218,1.7972935297\N,0,2.0539200062,1.7804484034,1.7210439707\N,0,0.2264899677,0.3586882085,1.7995296945\N,0,1.9750567458,-0.0002678386,1.8186690276\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1581.5331908\CCSD(T)/GTBas1=-1581.6277443\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1580.6783069\MP2/GTMP2LargeXP=-1582.065228\HF/GFHFB3=-1580.6984783\HF/GFHFB4=-1580.7248056\G4MP2=-1582.3800921

**NP12**

\0,1\N,0,-0.0052633744,-0.0414255219,-0.0146764492\N,0,1.8267032964,-0.0193813806,0.0610246396\N,0,-0.3277601036,1.4570029293,-0.0155120034\N,0,1.3510020505,2.1907115823,0.0597674316\N,0,-0.4893906115,1.7955214985,1.779336389\N,0,1.3425784131,1.8176247044,1.8550692283\N,0,-0.0136068287,-0.4145589805,1.7806201948\N,0,1.6651371581,0.3192051685,1.8558705692\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1581.511251\CCSD(T)/GTBas1=-1581.6056626\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1580.6439084\MP2/GTMP2LargeXP=-1582.036128\HF/GFHFB3=-1580.6643639\HF/GFHFB4=-1580.6903882\G4MP2=-1582.3510211

**NP13**

\0,1\N,0,-0.0159127013,-0.1404630054,0.1680938444\N,0,2.2927651068,0.1590396624,-0.1508584027\N,0,0.3629857735,2.1323747531,-0.0404502964\N,0,2.1131520361,1.940326233,0.2951670923\N,0,0.3793608627,1.9098297264,1.7835490942\N,0,1.8959886511,1.9059103701,1.7883784379\N,0,0.1627715943,0.4220424275,1.9161929676\N,0,1.9129886767,0.1005398329,2.1306272628\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1581.4835242\CCSD(T)/GTBas1=-1581.5818548\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1580.6127082\MP2/GTMP2LargeXP=-1582.0073734\HF/GFHFB3=-1580.6333908\HF/GFHFB4=-1580.6589158\G4MP2=-1582.3254562

**NP14**

\0,1\N,0,-0.0476161995,-0.059792061,-0.0829963263\N,0,1.4428718446,0.0254303027,0.1184236485\N,0,-0.3068417724,1.4107421187,0.1174755456\N,0,1.4173286502,1.7909116457,-0.3136487855\N,0,-0.4268753182,1.6266834237,1.8499771817\N,0,1.8613168222,2.3544390424,1.7984894096\N,0,-0.5460709248,-0.689054024,1.5467164054\N,0,1.679286898,-0.0409604481,1.8510629209\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1867.7799696\CCSD(T)/GTBas1=-1867.8764066\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1866.9573274\MP2/GTMP2LargeXP=-1868.3257835\HF/GFHFB3=-1866.9825133\HF/GFHFB4=-1867.0070039\G4MP2=-1868.6476508

**NP15**

\0,1\N,0,-0.0514912138,0.0003789436,-0.0717357567\N,0,1.7762911652,-0.1360605343,0.016225941\N,0,-0.3045290807,1.5010093885,0.0322854875\N,0,1.3738992394,2.1099699423,0.3024450371\N,0,-0.6915407417,1.6586481652,1.7890729093\N,0,1.0672777081,1.8763431979,2.0521397171\N,0,-0.4393977009,-0.6202066207,1.6109820303\N,0,1.6303906244,0.1637175175,2.3145846344\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1867.7982488\CCSD(T)/GTBas1=-1867.8990701\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1867.0115319\MP2/GTMP2LargeXP=-1868.3485528\HF/GFHFB3=-1867.0369419\HF/GFHFB4=-1867.0618655\G4MP2=-1868.6756

**NP16**

\0,1\N,0,0.0561093723,0.0013443516,0.0026928436\N,0,1.8360921029,0.0344726412,0.0445820465\N,0,-0.0486722992,1.7895196876,0.078580435\N,0,1.7282253984,1.7910935837,0.3157600315\N,0,-0.480404205



7, 1.7919911946, 2.3611836202\ P, 0, 1.8191172338, 1.5923101596, 2.0951426241  
\ P, 0, -0.0470742329, -0.4056759913, 1.7458155625\ N, 0, 1.7299066305, -0.1753  
55627, 1.8094428365\ \Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-186  
7.873199\CCSD(T)/GTBas1=-1867.9681897\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/G  
TMP2LargeXP=-1867.1081874\MP2/GTMP2LargeXP=-1868.4395548\HF/GFHFB3=-18  
67.1328666\HF/GFHFB4=-1867.1587985\G4MP2=-1868.7606538

**NP17**

\ \0, 1\N, 0, -0.0120703934, -0.0279485897, -0.0258154527\ P,  
0, 1.7879068824, -0.0399473999, 0.0282595324\ N, 0, -0.3417235152, 1.42507192  
6, -0.0264693654\ P, 0, 1.2767930945, 2.2126624849, 0.0268256296\ P, 0, -0.9941  
172164, 1.6982811471, 1.6295579359\ P, 0, 1.1616577905, 2.1966148392, 2.35124  
60109\ P, 0, -0.4829778679, -0.554322945, 1.6307492896\ P, 0, 1.6763312255, -0.  
0722114627, 2.3526464198\ \Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1  
=-2154.0358965\CCSD(T)/GTBas1=-2154.14939\MP2/GTBas2=0.\MP2/GTBas3=0.\  
HF/GTMP2LargeXP=-2153.3198326\MP2/GTMP2LargeXP=-2154.5985928\HF/GFHFB3  
=-2153.3507295\HF/GFHFB4=-2153.3739313\G4MP2=-2154.9436813

**NP18**

\ \0, 1\N, 0, 0.0318190378, 0.033545772, 0.0860992524\ P, 0, 1.  
8370585895, 0.0312863554, 0.0451491598\ P, 0, -0.0762999278, 1.835548525, 0.0  
451926192\ N, 0, 1.6253868833, 1.7234557859, 0.6387158616\ P, 0, -0.8455193884  
, 1.874649009, 2.1437948369\ P, 0, 1.4933818897, 1.5834263521, 2.3564503935\ P  
, 0, -0.3809829611, -0.4042544628, 1.7064622417\ P, 0, 1.9212558771, -0.734357  
3366, 2.1437356349\ \Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2154  
.1084083\CCSD(T)/GTBas1=-2154.2108552\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/G  
TMP2LargeXP=-2153.3807564\MP2/GTMP2LargeXP=-2154.6853003\HF/GFHFB3=-21  
53.410591\HF/GFHFB4=-2153.4345733\G4MP2=-2155.0190805

**NP19**

\ \0, 1\N, 0, -0.0330431209, -0.0439699045, -0.0635968339\ P,  
0, 1.764116372, -0.0274934846, -0.0411429605\ P, 0, -0.4995803479, 1.69165824  
49, -0.040831698\ P, 0, 1.657121889, 2.1814367524, 0.6748074779\ P, 0, -0.60541  
00022, 1.5526767754, 2.2770569352\ N, 0, 1.1917454742, 1.5691775581, 2.299475  
5269\ P, 0, -0.4984122219, -0.6562317943, 1.5610856332\ P, 0, 1.6582619577, -0.  
1664541474, 2.2767459192\ \Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1  
=-2154.0796604\CCSD(T)/GTBas1=-2154.187979\MP2/GTBas2=0.\MP2/GTBas3=0.  
\HF/GTMP2LargeXP=-2153.3707909\MP2/GTMP2LargeXP=-2154.6513164\HF/GFHFB  
3=-2153.401332\HF/GFHFB4=-2153.4250938\G4MP2=-2154.9916357

**NP20**

\ \0, 1\N, 0, -0.0007234285, -0.0020687014, -0.0013026356\ P,  
0, 1.7654690734, 0.0065339185, 0.0090202496\ P, 0, -0.517897143, 1.6869548948  
, 0.009151998\ P, 0, 1.6802314769, 2.2823822701, 0.4500953814\ P, 0, -1.0206173  
506, 1.4443465034, 2.2603914822\ P, 0, 1.2477567214, 1.6948343493, 2.64676785  
82\ P, 0, -0.5144180829, -0.7007210678, 1.5372383154\ P, 0, 1.6839987332, -0.54  
52621671, 2.260337351\ \Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2  
440.330487\CCSD(T)/GTBas1=-2440.4500471\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/  
/GTMP2LargeXP=-2439.690365\MP2/GTMP2LargeXP=-2440.917562\HF/GFHFB3=-24  
39.7260721\HF/GFHFB4=-2439.7482482\G4MP2=-2441.2743971

**NP2<sup>+</sup>**

\ \1, 2\ P, 0, -0.0230888466, -0.043813009, -0.01037557  
81\ N, 0, 1.8523741078, 0.0454747099, 0.0386858852\ P, 0, 0.4701167139, 2.27439  
01625, -0.0109972801\ N, 0, 2.1468537222, 1.4293804607, 0.0382605057\ N, 0, 0.8  
027662587, 1.7158097044, 1.7511176047\ N, 0, 2.2707921139, 1.4662612164, 1.53  
71254047\ N, 0, 0.5083021522, 0.3318989914, 1.7515557164\ N, 0, 1.950783778, -0

.0379022364,1.5375277415\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1008.5970573\\CCSD(T)/GTBas1=-1008.6804821\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1007.5607397\\MP2/GTMP2LargeXP=-1009.0607798\\HF/GFHFB3=-1007.5718888\\HF/GFHFB4=-1007.5996158\\G4MP2=-1009.350716

### NP3<sup>+</sup>

\\1,2\\P,0,0.0168301571,0.0149131951,0.0156826954  
\\N,0,1.8522938121,0.0580779004,0.0164647286\\N,0,0.2961121845,1.8295697151,0.0168706014\\P,0,2.087526614,1.8340241897,-0.3853639213\\N,0,0.5470057563,1.8548214681,1.4268337247\\N,0,2.0587592467,1.8083694682,1.4782426409\\N,0,0.4437624834,0.3895884749,1.7910311571\\N,0,1.9101097458,0.3031355885,1.4265383732\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1008.6345742\\CCSD(T)/GTBas1=-1008.7151567\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1007.6150332\\MP2/GTMP2LargeXP=-1009.1038522\\HF/GFHFB3=-1007.6255202\\HF/GFHFB4=-1007.6540064\\G4MP2=-1009.3922537

### NP5<sup>+</sup>

\\1,2\\P,0,-0.1217501435,-0.110763974,0.002625346  
5\\P,0,2.2475286884,0.0919195767,-0.0096919568\\P,0,0.3046779615,2.2286227649,-0.0097462336\\N,0,2.0331164031,1.8486201515,0.2127108402\\N,0,0.459717513,1.8289286424,1.8170045794\\N,0,1.9790693363,1.7995125818,1.7279692433\\N,0,0.45577743,0.4144295519,1.7074945959\\N,0,1.8642628112,0.2842307049,1.8170335852\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1294.8967772\\CCSD(T)/GTBas1=-1295.0019712\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1293.9698801\\MP2/GTMP2LargeXP=-1295.3827276\\HF/GFHFB3=-1293.9854568\\HF/GFHFB4=-1294.0125145\\G4MP2=-1295.7007196

### NP6<sup>+</sup>

\\1,2\\P,0,-0.0026332338,-0.0326487624,0.00319224  
75\\N,0,1.8599406222,0.0358699654,0.0216534425\\P,0,0.5290896965,2.245677974,0.0057056316\\N,0,2.1849815401,1.4165301227,-0.0760476169\\N,0,0.759254923,1.747216602,1.7763713968\\P,0,2.5715346621,1.5370855279,1.7042678967\\N,0,0.5304583197,0.344279513,1.7489331072\\N,0,1.9268734701,-0.1896109427,1.5164238947\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1294.9560809\\CCSD(T)/GTBas1=-1295.0388577\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1294.0027428\\MP2/GTMP2LargeXP=-1295.4397353\\HF/GFHFB3=-1294.0178292\\HF/GFHFB4=-1294.0453506\\G4MP2=-1295.7357468

### NP7<sup>+</sup>

\\1,2\\P,0,0.0508700684,0.0323520993,0.0247798451  
\\N,0,1.848187065,0.0613792451,0.0489187217\\N,0,0.1896469913,1.8729151727,0.005128162\\P,0,2.0148951793,1.8234087044,-0.2666705721\\N,0,0.4579590603,1.8080712366,1.4194915826\\N,0,1.8792734226,1.9937902005,1.5663640533\\N,0,0.1878536334,0.4499466565,1.8176706696\\P,0,2.0128145797,0.1725366849,1.8357175378\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1294.9860005\\CCSD(T)/GTBas1=-1295.0811051\\MP2/GTBas2=0.\\MP2/GTBas3=0.\\HF/GTMP2LargeXP=-1294.084089\\MP2/GTMP2LargeXP=-1295.4876113\\HF/GFHFB3=-1294.0986706\\HF/GFHFB4=-1294.1270765\\G4MP2=-1295.7963906

### NP9<sup>+</sup>

\\1,2\\P,0,-0.0733728958,-0.0664277452,-0.0593539  
242\\P,0,2.2654827248,0.0576320675,0.0508498268\\P,0,0.2908574034,2.2470223962,0.0511787064\\N,0,2.0849262205,1.8795186494,0.1735169874\\N,0,0.5672860832,2.0383988855,1.8534527046\\N,0,1.9381612639,1.746444293,1.5865607881\\P,0,0.2932103057,0.2639915964,2.2327386901\\N,0,2.0870488942,0.3527198571,1.8535562208\\Version=EM64L-G09RevA.02\\State=2-A\\MP2/GTBas1=-1581.2144727\\CCSD(T)/GTBas1=-1581.3220794\\MP2/GTBas2=0.\\MP2/GTBas3=0

.\HF/GTMP2LargeXP=-1580.3781127\MP2/GTMP2LargeXP=-1581.7289082\HF/GFHF  
B3=-1580.3986401\HF/GFHF4=-1580.4249984\G4MP2=-1582.0558577

**NP11+**

\\1,2\N,0,0.0853462156,0.009416534,0.0137708057\  
N,0,1.859744506,0.0510529159,0.0635557158\N,0,0.0652714279,2.353961232  
8,-0.0013780059\N,0,2.3311388409,1.7566626451,-0.0826865632\N,0,0.5984  
913419,1.7612944206,1.677755432\N,0,2.0192744151,1.7790893439,1.763531  
1951\N,0,0.2385427659,0.3936654837,1.8400139894\N,0,2.0138904866,-0.04  
7542576,1.8665374312\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-1  
581.264669\CCSD(T)/GTBas1=-1581.3684451\MP2/GTBas2=0.\MP2/GTBas3=0.\HF  
/GTMP2LargeXP=-1580.4256612\MP2/GTMP2LargeXP=-1581.7767242\HF/GFHF3=-  
1580.4453496\HF/GFHF4=-1580.4722455\G4MP2=-1582.0997055

**NP12+**

\\1,2\N,0,0.0355172628,0.0246265666,0.0441248505  
\N,0,1.8825184336,-0.0306357033,0.0134286624\N,0,-0.2634077857,1.41359  
10487,0.0433964287\N,0,1.3971666557,2.2238933316,0.0120945049\N,0,-0.5  
451577688,1.80681475,1.8269567228\N,0,1.3018248376,1.7515460702,1.7962  
543408\N,0,-0.0598223516,-0.447717885,1.8282770762\N,0,1.6007607163,0.  
3625818211,1.7969674138\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1  
=-1581.2734868\CCSD(T)/GTBas1=-1581.3604639\MP2/GTBas2=0.\MP2/GTBas3=0  
.\HF/GTMP2LargeXP=-1580.3955139\MP2/GTMP2LargeXP=-1581.7774516\HF/GFHF  
B3=-1580.4154562\HF/GFHF4=-1580.4419795\G4MP2=-1582.0833931

**NP13+**

\\1,2\N,0,-0.0546827548,-0.0679225647,0.08645552  
97\N,0,2.3320289199,0.0821568609,-0.0732947895\N,0,0.2871323927,2.2496  
165603,-0.0125947394\N,0,1.9924999176,1.7899337904,0.3094147456\N,0,0.  
3608607405,1.8687480876,1.8254250567\N,0,1.9144083373,1.9446764707,1.7  
442444115\N,0,0.2832489939,0.426381532,1.765361656\N,0,1.9886034528,0.  
1360092628,2.2456881293\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1  
=-1581.2355765\CCSD(T)/GTBas1=-1581.3258897\MP2/GTBas2=0.\MP2/GTBas3=0  
.\HF/GTMP2LargeXP=-1580.3504706\MP2/GTMP2LargeXP=-1581.7360463\HF/GFHF  
B3=-1580.3704343\HF/GFHF4=-1580.3967322\G4MP2=-1582.0455109

**NP14+**

\\1,2\N,0,0.0318964778,0.0407927835,0.1057249096  
\N,0,1.4281102052,0.0236516846,-0.0474094671\N,0,-0.3051146737,1.39559  
69289,-0.0480942905\N,0,1.4387868707,1.8178896569,-0.3543629229\N,0,-0  
.6678279636,1.818073167,1.7218804922\N,0,1.6290822011,2.0603973998,1.9  
748592304\N,0,-0.402762245,-0.5072524529,1.8096091695\N,0,1.9212291275  
, -0.2307491679,1.7232928789\Version=EM64L-G09RevA.02\State=2-A\MP2/GT  
Bas1=-1867.4944909\CCSD(T)/GTBas1=-1867.6103336\MP2/GTBas2=0.\MP2/GTBas  
3=0.\HF/GTMP2LargeXP=-1866.7260766\MP2/GTMP2LargeXP=-1868.022152\HF/G  
FHF3=-1866.7516283\HF/GFHF4=-1866.776662\G4MP2=-1868.3629408

**NP15+**

\\1,2\N,0,0.0496107122,0.0520964469,0.0844331518  
\N,0,1.8558703477,-0.0812207765,-0.069174056\N,0,-0.2827589591,1.41411  
61886,0.0361465285\N,0,1.394725796,2.1758480012,0.2682918469\N,0,-0.74  
71069988,1.7078395241,1.809891777\N,0,1.0420585758,1.7624382235,1.9825  
304289\N,0,-0.5552806151,-0.6080804719,1.6662722149\N,0,1.6037811412,0  
.1307628642,2.267608108\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1  
=-1867.5504271\CCSD(T)/GTBas1=-1867.6577795\MP2/GTBas2=0.\MP2/GTBas3=0  
.\HF/GTMP2LargeXP=-1866.7706247\MP2/GTMP2LargeXP=-1868.077871\HF/GFHF  
3=-1866.7954023\HF/GFHF4=-1866.8209596\G4MP2=-1868.4100929

**NP17<sup>+</sup>**

\\1,2\N,0,0.0374229248,0.0414184229,0.066632696\  
 P,0,1.8463541897,-0.041124704,-0.0356055476\N,0,-0.2671213061,1.383899  
 8442,0.0659521737\P,0,1.3289992158,2.2389131213,-0.0369950323\P,0,-1.0  
 751653251,1.6943863568,1.6596708234\N,0,1.1271540851,2.165594525,2.292  
 5236774\N,0,-0.5577936884,-0.585647868,1.6610015348\N,0,1.6319499042,-  
 0.0592396983,2.2938196744\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas  
 s1=-2153.7887007\CCSD(T)/GTBas1=-2153.9042332\MP2/GTBas2=0.\MP2/GTBas3  
 =0.\HF/GTMP2LargeXP=-2153.0810868\MP2/GTMP2LargeXP=-2154.3355398\HF/GF  
 HFB3=-2153.1115805\HF/GFHFB4=-2153.1355008\G4MP2=-2154.6816608

**NP18<sup>+</sup>**

\\1,2\N,0,0.0475102589,0.0501814268,0.0673693853  
 \P,0,1.8613566046,0.0151871937,0.0242729616\N,0,-0.093797064,1.8588552  
 718,0.0243176673\N,0,1.6171416572,1.7147165018,0.611663356\N,0,-0.8147  
 293146,1.8164637083,2.2329588355\N,0,1.5016504117,1.5922025628,2.31133  
 51091\N,0,-0.3743958697,-0.3972680362,1.6607848871\N,0,1.8613633159,-0  
 .7070386288,2.232897798\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1  
 =-2153.8431802\CCSD(T)/GTBas1=-2153.9475207\MP2/GTBas2=0.\MP2/GTBas3=0  
 .\HF/GTMP2LargeXP=-2153.1349277\MP2/GTMP2LargeXP=-2154.4046375\HF/GFH  
 B3=-2153.164283\HF/GFHFB4=-2153.1888372\G4MP2=-2154.739762

**NP19<sup>+</sup>**

\\1,2\N,0,0.0338575052,0.0443707246,0.065714464\  
 P,0,1.7990409271,-0.0353972126,-0.0527413893\N,0,-0.5170111265,1.72329  
 90132,-0.0528814758\N,0,1.6743165118,2.2039659412,0.6497844361\N,0,-0.  
 64035407,1.5606087227,2.2886144574\N,0,1.1248360554,1.480815931,2.1701  
 92936\N,0,-0.5156030705,-0.6787441067,1.5861668731\N,0,1.6757172675,-0  
 .1981190135,2.2887496985\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas  
 1=-2153.8540186\CCSD(T)/GTBas1=-2153.9543167\MP2/GTBas2=0.\MP2/GTBas3=  
 0.\HF/GTMP2LargeXP=-2153.1260781\MP2/GTMP2LargeXP=-2154.4032646\HF/GFH  
 FB3=-2153.1556699\HF/GFHFB4=-2153.1801454\G4MP2=-2154.7341855

**NP20<sup>+</sup>**

\\1,2\N,0,0.0466267632,0.0620874811,0.0990963221  
 \P,0,1.7936529218,0.0086252658,0.0115285825\N,0,-0.5243861823,1.714102  
 5182,0.0116634112\N,0,1.6984433708,2.3074945046,0.4164473583\N,0,-1.06  
 53019175,1.4498793389,2.2686068386\N,0,1.1936123605,1.6211170843,2.531  
 9884554\N,0,-0.5212301627,-0.7097491023,1.563786191\N,0,1.7023828461,-  
 0.5865570906,2.2685828409\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas  
 s1=-2440.0861577\CCSD(T)/GTBas1=-2440.1975653\MP2/GTBas2=0.\MP2/GTBas3  
 =0.\HF/GTMP2LargeXP=-2439.4364532\MP2/GTMP2LargeXP=-2440.661936\HF/GFH  
 FB3=-2439.4712662\HF/GFHFB4=-2439.494201\G4MP2=-2441.0099152

**5. Silicon-nitrogen cubanoids****SiN1**

\\0,1\N,0,0.0559196886,0.072166821,0.0970689227\Si,  
 0,1.8350818236,-0.0418035782,-0.0538556038\Si,0,-0.4378308664,1.785429  
 1483,-0.0535225399\Si,0,1.8603850127,2.3166901966,0.1420567415\Si,0,-0  
 .8891631027,1.7110287896,2.2689743446\Si,0,1.508366582,1.8780857628,2.  
 4894311663\Si,0,-0.4373113885,-0.5426303532,1.7033786963\Si,0,1.860779  
 6631,-0.5000171904,2.2677690002\H,0,2.339288061,-0.8867151581,-1.17320  
 66469\H,0,-1.3716449331,2.0955077276,-1.17281822\H,0,2.7264257303,3.39  
 42781198,-0.4080292009\H,0,-1.8798609281,2.3795705322,3.1552377386\H,0  
 ,2.1566628842,2.685112337,3.5581494738\H,0,-1.3706208838,-1.7044904246

,1.6950897397\H,0,2.7271226572,-1.3237127305,3.1537763877\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2081.6551814\CCSD(T)/GTBas1=-2081.7703916\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2081.1428436\MP2/GTMP2LargeXP=-2082.1618367\HF/GFHFB3=-2081.1690214\HF/GFHFB4=-2081.1916353\G4MP2=-2082.4508256

#### SiN2

\\0,1\N,0,0.0797619312,-0.0375867589,0.0892291586\Si,0,1.8796695863,-0.0942557277,-0.0478942304\N,0,-0.2045175562,1.4951288743,0.0838572453\Si,0,1.4547811387,2.1937952169,-0.0567613208\Si,0,-0.7527611859,1.7907832104,1.778912615\Si,0,1.5191344555,2.2711775595,2.3270667797\Si,0,-0.3276359151,-0.4972238269,1.7875961443\Si,0,1.9642144829,-0.1244585548,2.336348682\H,0,2.4369292061,-1.0896925194,-1.0040546619\H,0,1.6180223859,3.3153570727,-1.0217285655\H,0,-1.9466862475,2.664576565,1.9424313927\H,0,2.1749073451,3.1775162569,3.3147137071\H,0,-1.1277764432,-1.7404692223,1.9602022382\H,0,2.9003568162,-0.7274481455,3.3297808157\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1846.60095\CCSD(T)/GTBas1=-1846.7087868\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1846.0015592\MP2/GTMP2LargeXP=-1847.1046093\HF/GFHFB3=-1846.024082\HF/GFHFB4=-1846.0476628\G4MP2=-1847.3896741

#### SiN3

\\0,1\N,0,0.0220826022,0.0202131559,0.0365965128\Si,0,1.8159800571,-0.0008375277,-0.0166953534\Si,0,0.0858611709,1.8131268448,-0.0161880067\N,0,1.8574994667,1.770726291,0.2681929574\Si,0,-0.4200473283,2.0442050898,2.2472687361\Si,0,1.9647020372,1.8725816036,2.0509408367\Si,0,-0.3164690209,-0.30311153,1.7631340211\Si,0,2.0234308727,-0.5176355058,2.2466168124\H,0,2.4245853284,-0.4709988697,-1.2862956128\H,0,-0.3552822731,2.4435861657,-1.2855450667\H,0,-1.3255679804,2.8847849952,3.070334611\H,0,2.9666299632,2.828107896,2.5912033753\H,0,-1.3725278619,-1.3104331469,2.0438731986\H,0,2.8200229661,-1.4620154618,3.0697629783\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1846.7210511\CCSD(T)/GTBas1=-1846.8218024\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1846.1335591\MP2/GTMP2LargeXP=-1847.2342154\HF/GFHFB3=-1846.1549838\HF/GFHFB4=-1846.1796786\G4MP2=-1847.5104745

#### SiN4

\\0,1\N,0,0.0194871898,-0.4208763209,-1.4820692479\Si,0,1.4707262276,-0.9135632651,-0.506404909\Si,0,0.0037562219,1.3965616769,-1.5077992696\Si,0,1.4434078552,1.2665928088,0.3231367574\Si,0,-1.4708546976,1.2407309313,0.293107555\N,0,-0.0194276553,0.7478522643,1.2686919749\Si,0,-1.4434023439,-0.9394214687,-0.5362743728\Si,0,-0.0033830151,-1.0695517367,1.2945296635\H,0,2.4459121712,-1.8023781305,-1.1913186744\H,0,2.3870578743,2.1730447028,1.0288651619\H,0,-2.4459803426,2.1292600206,0.9784895676\H,0,-2.3870562877,-1.8453325158,-1.2427211225\H,0,-0.0123200905,-1.7015746732,2.6401371972\H,0,0.0117968928,2.0283357061,-2.8535302812\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1846.6854839\CCSD(T)/GTBas1=-1846.7864893\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1846.0958601\MP2/GTMP2LargeXP=-1847.2016881\HF/GFHFB3=-1846.1175833\HF/GFHFB4=-1846.142001\G4MP2=-1847.4786311

#### SiN5

\\0,1\N,0,-0.0187048149,-0.0238160271,0.1206083358\N,0,1.5328015359,0.0278176594,0.0821132956\N,0,-0.3060727839,1.5015706353,0.0833941623\Si,0,1.4172579055,1.7680337723,-0.2403891386\Si,0,-0.4940651998,1.9440942954,1.8191281463\Si,0,1.8787923216,2.3423633308,2.0144801614\Si,0,-0.3086078111,-0.3869637247,1.9199062685\Si,0,2.006816

6717,-0.06012998,1.8175153171\H,0,1.8526171093,2.3127225786,-1.5522962  
714\H,0,-1.5742890754,2.9107436227,2.1546671532\H,0,2.6724094224,3.331  
2496509,2.8061989314\H,0,-1.215017958,-1.5184075158,2.2543358099\H,0,3  
.1857626768,-0.9038782978,2.1522378285\\Version=EM64L-G09RevA.02\State  
=1-A\MP2/GTbas1=-1611.5917064\CCSD(T)/GTbas1=-1611.6907379\MP2/GTbas2=  
0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1610.9030156\MP2/GTMP2LargeXP=-1612.  
0914539\HF/GFHFB3=-1610.9215279\HF/GFHFB4=-1610.9464142\G4MP2=-1612.37  
02876

#### SiN6

\\0,1\N,0,0.0701184774,-0.0516899688,0.0693681045\Si,  
i,0,1.8905118584,-0.12932854,-0.0769596314\N,0,-0.3069047446,1.4883142  
832,0.0519185045\Si,0,1.3928876176,2.0557691006,0.3227537045\Si,0,-0.5  
190533256,1.6049628891,1.84804095\N,0,1.2762232243,1.6752819518,2.0916  
166419\Si,0,-0.3775470179,-0.6640976268,1.7324472865\Si,0,1.8271105888  
, -0.0251151663,2.2795952889\H,0,2.4311489044,-1.0126035946,-1.14294474  
5\H,0,1.6980652899,3.4694765134,-0.018067188\H,0,-1.2899517462,2.76495  
39591,2.3657270927\H,0,-1.2350372674,-1.8769687808,1.7818600013\H,0,2.  
7807281408,-0.29835502,3.3942439896\\Version=EM64L-G09RevA.02\State=1-  
A\MP2/GTbas1=-1611.6587313\CCSD(T)/GTbas1=-1611.751181\MP2/GTbas2=0.\M  
P2/GTbas3=0.\HF/GTMP2LargeXP=-1610.9793735\MP2/GTMP2LargeXP=-1612.1701  
492\HF/GFHFB3=-1610.9973162\HF/GFHFB4=-1611.0228737\G4MP2=-1612.441522  
5

#### SiN7

\\0,1\N,0,0.034986551,0.0114935166,0.0123290945\Si,  
0,1.809879295,-0.0190858425,-0.0220502185\Si,0,0.1635914722,1.81012462  
93,-0.0183239338\N,0,1.9654233415,1.7490813067,0.0276794556\Si,0,-0.05  
53588037,2.0338252757,2.3264324969\Si,0,2.2069524628,1.5783899437,1.80  
7171767\Si,0,0.1625523076,-0.260147104,1.7912143276\N,0,1.9645162646,-  
0.2076434557,1.7368761807\H,0,2.5660393243,-0.8526629913,-0.9734501999  
\H,0,-0.4531207364,2.5073774427,-1.1693739159\H,0,-0.8153854313,2.8725  
368044,3.2830099056\H,0,3.4950610256,2.0585585612,2.356354743\H,0,-0.4  
560370732,-1.4943480868,2.3258302971\\Version=EM64L-G09RevA.02\State=1  
-A\MP2/GTbas1=-1611.799761\CCSD(T)/GTbas1=-1611.8850771\MP2/GTbas2=0.\  
MP2/GTbas3=0.\HF/GTMP2LargeXP=-1611.138009\MP2/GTMP2LargeXP=-1612.3181  
424\HF/GFHFB3=-1611.1547755\HF/GFHFB4=-1611.1816659\G4MP2=-1612.580427  
2

#### SiN8

\\0,1\N,0,-0.0256301094,-0.0257651177,0.1568343756\  
N,0,1.4909623874,-0.0254500369,0.1574229089\N,0,-0.0260006693,1.490863  
7378,0.1585641664\N,0,1.4906806152,1.4911873778,0.1591532594\Si,0,-0.4  
531888158,1.9158439014,1.9035950256\Si,0,1.9170276707,1.9155897272,1.9  
045256392\Si,0,-0.453480972,-0.4544514229,1.9007274323\Si,0,1.91687500  
24,-0.4546906432,1.9016715118\H,0,-1.4930686048,2.9556871918,2.1699688  
383\H,0,2.9567351295,2.9553814684,2.171774129\H,0,-1.4937423991,-1.494  
6930761,2.1640472887\H,0,2.9569307652,-1.4949031075,2.1659154246\\Vers  
ion=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-1376.4838737\CCSD(T)/GTbas1  
=-1376.5821387\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1375.69469  
86\MP2/GTMP2LargeXP=-1376.9655994\HF/GFHFB3=-1375.7106063\HF/GFHFB4=-1  
375.7356257\G4MP2=-1377.2478246

#### SiN9

\\0,1\N,0,0.0039803122,0.0034306601,0.0065480229\N,  
0,1.5462653449,0.0219180556,0.0298381262\N,0,-0.2668959366,1.521806615  
3,0.028461421\Si,0,1.4931288819,1.8041222095,0.0661456965\Si,0,-0.6228

179157,1.4020202938,1.7713975779\Si,0,1.6098992151,1.9482609473,2.4573  
935768\N,0,-0.2661648994,-0.3222155387,1.4898935592\Si,0,1.4940908886,  
-0.3482879915,1.7727141429\H,0,2.141832315,2.5856266783,-1.0137467619\  
H,0,-1.9521705031,1.8085770306,2.2860339977\H,0,2.2930465996,2.7742013  
966,3.4987127519\H,0,2.1426056976,-1.5772603568,2.2890078889\\Version=  
EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1376.6135637\CCSD(T)/GTBas1=-13  
76.7023106\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1375.8372644\M  
P2/GTMP2LargeXP=-1377.1113386\HF/GFHFB3=-1375.8517025\HF/GFHFB4=-1375.  
8780747\G4MP2=-1377.3817282

#### SiN10

\\0,1\N,0,0.0252772051,0.0219838231,0.0216850173\Si  
,0,1.8177037811,-0.0025077945,-0.0021894782\Si,0,0.1802999344,1.808327  
8799,-0.0021752115\N,0,1.9664650365,1.7775051662,-0.1550533604\N,0,0.2  
09373355,1.9573318925,1.7845370232\Si,0,1.9886559524,1.797155701,1.637  
7030585\Si,0,0.1814215209,0.1647803473,1.8019675527\N,0,1.9668448044,0  
.0104365656,1.7850855883\H,0,2.5815335023,-0.9315279475,-0.8473532023\  
H,0,-0.6674648777,2.6604411869,-0.8483749333\H,0,2.919152481,2.6392113  
337,2.4031265297\H,0,-0.6653626957,-0.5993381541,2.7293414161\\Version  
=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1376.8847989\CCSD(T)/GTBas1=-1  
376.9542684\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1376.1491487\  
MP2/GTMP2LargeXP=-1377.4072006\HF/GFHFB3=-1376.1614034\HF/GFHFB4=-1376  
.190509\G4MP2=-1377.6552702

#### SiN11

\\0,1\N,0,0.0056758059,-0.0667819028,0.0799184606\Si  
,0,1.7586929872,0.0547997961,-0.0258023832\N,0,0.0677980112,1.5158143  
233,0.1566257422\N,0,1.61007632,1.8084353373,-0.0669792051\Si,0,-0.242  
7296834,1.9234651789,1.9690028746\Si,0,2.040459864,1.8070508646,1.6995  
240407\Si,0,0.2111500196,-0.3310185352,1.867012632\N,0,1.9737852233,0.  
0113095236,1.7682642367\H,0,2.6238940019,-0.7544187214,-0.9065029386\  
H,0,-1.3445824432,2.8856428917,2.2165163905\H,0,3.3010568439,2.47604262  
06,2.113635892\H,0,-0.2167769505,-1.6354413768,2.4357842577\\Version=E  
M64L-G09RevA.02\State=1-A\MP2/GTBas1=-1376.6614998\CCSD(T)/GTBas1=-137  
6.7450106\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1375.8942933\M  
P2/GTMP2LargeXP=-1377.1683292\HF/GFHFB3=-1375.9082778\HF/GFHFB4=-1375.9  
352364\G4MP2=-1377.4335208

#### SiN12

\\0,1\Si,0,0.0380066323,-0.1108026324,0.0263283909\  
N,0,1.865306397,-0.0883918682,-0.0070898247\Si,0,0.375537117,2.0911446  
304,0.058514343\N,0,2.1124900923,1.5233753871,0.0161864357\N,0,0.26837  
66289,1.7792891463,1.8562274459\Si,0,2.0957896047,1.8016704171,1.82252  
85306\N,0,0.0210259102,0.1675323071,1.8327878898\Si,0,1.7578716639,-0.  
4002281949,1.7907261152\H,0,-0.6467305044,-1.3209095327,-0.4915425267\  
H,0,0.0875919807,3.4649105275,-0.4223875103\H,0,2.7799023909,3.0118412  
038,2.3410739659\H,0,2.0466320863,-1.7741313911,2.2707467448\\Version=  
EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1376.6039747\CCSD(T)/GTBas1=-13  
76.6886599\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1375.8308379\M  
P2/GTMP2LargeXP=-1377.1097919\HF/GFHFB3=-1375.8454804\HF/GFHFB4=-1375.  
8718528\G4MP2=-1377.3772746

#### SiN13

\\0,1\N,0,-0.0142527966,0.035004063,0.0570847737\N,  
0,1.4944467663,0.0642483047,0.022394222\N,0,-0.333070126,1.5922191588,  
0.0553111679\Si,0,1.338317356,1.7920313038,-0.5128374913\Si,0,-0.45351  
35635,2.1285878772,1.7825161822\Si,0,1.9291539063,2.2150604801,1.67713

77416\Si,0,0.1401654448,-0.0997406902,1.8609915349\N,0,1.8112208334,0.4114708231,1.5408377921\H,0,1.5717216575,2.1255455819,-1.94274355\H,0,-1.6015577637,3.0169077307,2.1274373621\H,0,3.0756379456,2.7516020243,2.4669383318\H,0,-0.0921696601,-1.4190366574,2.5058319332\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1376.5754727\CCSD(T)/GTBas1=-1376.6646029\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1375.7961305\MP2/GTMP2LargeXP=-1377.0740499\HF/GFHFB3=-1375.8107039\HF/GFHFB4=-1375.8369454\G4MP2=-1377.3460935

#### SiN15

\\0,1\Si,0,0.0514835368,-0.0812493264,0.052421194\N,0,1.8745904679,0.0157312063,-0.0749535982\Si,0,0.3526617209,2.1626251844,0.0103648087\N,0,2.0745653196,1.6401650859,-0.2526933342\N,0,0.4995449033,1.8904645625,1.8023961535\Si,0,2.228497733,1.6023332734,1.5162205452\N,0,0.4271500837,0.2456080129,1.8135030596\N,0,1.8611166473,-0.1312854498,1.4456020872\H,0,-0.6383993698,-1.3401183794,-0.3224466924\H,0,-0.1195077771,3.4714570177,-0.5110859762\H,0,3.3294967344,2.2214688126,2.2846717529\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1141.5596073\CCSD(T)/GTBas1=-1141.6396569\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1140.6897146\MP2/GTMP2LargeXP=-1142.0538599\HF/GFHFB3=-1140.7006509\HF/GFHFB4=-1140.728041\G4MP2=-1142.3202565

#### SiN16

\\0,1\Si,0,0.0039351594,0.0293443489,0.0249065444\N,0,1.8023871348,0.0060450887,0.0040819209\N,0,-0.0818299204,1.8022622535,-0.0864737047\Si,0,1.6969484149,1.7992170165,-0.0915672168\N,0,0.0540691274,1.7764886959,1.4912656399\N,0,1.611347857,1.9958349479,1.6741046072\N,0,-0.0804532469,0.2275839049,1.7904854894\Si,0,1.6983834937,0.2226304406,1.7863966395\H,0,-0.8214561231,-0.9056378039,-0.7599986374\H,0,2.5400164787,2.6074932522,-0.9902123638\H,0,2.5418516244,-0.5228621452,2.7374110814\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1141.69026\CCSD(T)/GTBas1=-1141.7632466\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1140.8349326\MP2/GTMP2LargeXP=-1142.194032\HF/GFHFB3=-1140.8448665\HF/GFHFB4=-1140.8733812\G4MP2=-1142.4510046

#### SiN17

\\0,1\Si,0,0.0407012771,-0.1115538944,0.0462203223\N,0,1.8714855467,-0.0267433795,-0.07376215\Si,0,0.3945135416,2.1544363707,0.0448259216\N,0,2.1119136412,1.5147453828,-0.0749033144\N,0,0.698877018,1.7372769561,1.8073901341\N,0,2.1467695804,1.4683939592,1.4412976336\N,0,0.4579520532,0.1958494905,1.8081461901\N,0,1.9186931379,0.0093908489,1.4425427408\H,0,-0.7304683773,-1.3104888626,-0.3889170832\H,0,0.0275625812,3.5304931283,-0.3948403949\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-906.4235472\CCSD(T)/GTBas1=-906.5087954\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-905.4485257\MP2/GTMP2LargeXP=-906.8929451\HF/GFHFB3=-905.4572061\HF/GFHFB4=-905.484248\G4MP2=-907.1667768

#### SiN19

\\0,1\Si,0,0.1074492667,0.0868642789,0.074714043\N,0,1.8868447684,-0.0409388137,-0.0321332846\N,0,0.3507736124,1.8544485181,-0.0324836887\N,0,1.8574889513,1.5052726794,-0.3252842726\N,0,0.3203892521,1.8303809059,1.5412348458\Si,0,2.0997776471,1.7024803608,1.4344827999\N,0,0.3497269656,0.2840295246,1.8344765607\N,0,1.8565051929,-0.0651079624,1.5416528356\H,0,-0.9090155356,-0.7378656477,-0.6191619515\H,0,3.1162598789,2.5272361561,2.1283021125\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-906.4972365\CCSD(T)/GTBas1=-906.5735506\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-905.5277571\MP2/GTMP2LargeXP=-906



.9794323\HF/GFHFB3=-905.5352017\HF/GFHFB4=-905.5633459\G4MP2=-907.2454  
827

### SiN20

\0,1\Si,0,0.1171053398,0.0895459746,0.0735202111\N  
,0,1.904423431,-0.0531796652,-0.0437348456\N,0,0.423204315,1.855912480  
2,-0.0439494478\N,0,1.916483928,1.485284118,-0.1768604231\N,0,0.598457  
0516,1.8252640236,1.4901089925\N,0,2.0687310032,1.6036133761,1.3084548  
377\N,0,0.4240237708,0.3283224535,1.8275829241\N,0,1.9173514475,0.1246  
504761,1.4903647879\H,0,-0.9295802868,-0.7219132369,-0.588087037\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-671.3858218\CCSD(T)/GTbas1=  
-671.4677788\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-670.3110116\  
MP2/GTMP2LargeXP=-671.8459174\HF/GFHFB3=-670.3162533\HF/GFHFB4=-670.34  
42576\G4MP2=-672.1189262

### SiN1+

\1,2\N,0,-0.0041050305,-0.0033161648,-0.0026  
675211\Si,0,1.7584513284,-0.0734218506,-0.0961138844\Si,0,-0.451571420  
5,1.7031837739,-0.0951390728\Si,0,1.8687887197,2.326701485,0.242373605  
8\Si,0,-0.7995224247,1.739098872,2.3060184715\Si,0,1.55984054,1.941869  
0661,2.5737483341\Si,0,-0.4516334679,-0.5603184898,1.6125718767\Si,0,1  
.8689101617,-0.4063474758,2.304787197\H,0,2.3315866779,-0.8970808305,-  
1.1866385894\H,0,-1.380121609,2.0855577043,-1.1848585075\H,0,2.7069694  
464,3.3713456152,-0.3942498927\H,0,-1.8569407522,2.3648193688,3.136268  
0368\H,0,2.2047338853,2.7440435178,3.6354552443\H,0,-1.3793372079,-1.7  
138026218,1.6822436044\H,0,2.7075511534,-1.3038319698,3.1357010972\Ve  
rsion=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-2081.3995715\CCSD(T)/GTba  
s1=-2081.5118232\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-2080.903  
0062\MP2/GTMP2LargeXP=-2081.8984785\HF/GFHFB3=-2080.928844\HF/GFHFB4=-  
2080.9519442\G4MP2=-2082.1851232

### SiN2+

\1,2\N,0,0.1448075678,0.0612963508,0.1891993  
377\Si,0,1.982385333,-0.0852484208,-0.072570077\N,0,-0.108985258,1.427  
0203514,0.1838173311\Si,0,1.5535734133,2.2220510202,-0.0817509877\Si,0  
, -0.7985800699,1.7926585323,1.874230525\Si,0,1.5037415383,2.26157519,2  
.3064118757\Si,0,-0.369737671,-0.5146409051,1.8833736767\Si,0,1.946683  
5697,-0.1216069417,2.3158920675\H,0,2.4039473237,-1.1079412312,-1.0537  
500928\H,0,1.5807019585,3.3203508363,-1.0713631757\H,0,-1.9896215649,2  
.6685634642,1.8975595839\H,0,2.1226567081,3.2093032114,3.2587491262\H,  
0,-1.1665889381,-1.7597653279,1.9153526702\H,0,2.8634160895,-0.7764161  
3,3.2745481392\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-1846.37  
81475\CCSD(T)/GTbas1=-1846.4896216\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP  
2LargeXP=-1845.8012888\MP2/GTMP2LargeXP=-1846.8575017\HF/GFHFB3=-1845.  
8237425\HF/GFHFB4=-1845.8477836\G4MP2=-1847.1448997

### SiN5+

\1,2\N,0,0.0974091573,0.1208481502,0.2979199  
43\N,0,1.4983577894,0.0492363139,0.0729975388\N,0,-0.2776006125,1.4726  
768328,0.0745600993\Si,0,1.4699711593,1.833976234,-0.2976658808\Si,0,-  
0.5471848647,1.9634501579,1.8438423492\Si,0,1.8326638592,2.2843205507,  
1.9917580649\Si,0,-0.3020376781,-0.3789936704,2.0772420383\Si,0,2.0372  
063545,-0.1079613692,1.8416647106\H,0,1.8674498555,2.331496671,-1.6277  
338052\H,0,-1.649687912,2.9131809396,2.0952691\H,0,2.622839406,3.26927  
42472,2.7598771058\H,0,-1.2234912852,-1.5284037754,2.2089023334\H,0,3.  
2038047713,-0.9777012824,2.0932664026\Version=EM64L-G09RevA.02\State=  
2-A\MP2/GTbas1=-1611.3527276\CCSD(T)/GTbas1=-1611.4596487\MP2/GTbas2=0

.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1610.6972178\MPS2/GTMP2LargeXP=-1611.8318142\HF/GFHFB3=-1610.7156317\HF/GFHFB4=-1610.740954\G4MP2=-1612.117387

**SiN6+**

\\1,2\N,0,0.0725355686,-0.0136667694,0.083630  
7362\Si,0,1.9446125611,-0.1243447321,-0.1179956501\N,0,-0.2100784632,1.3599120105,0.135318915\Si,0,1.485527477,2.0894788872,0.3264352319\Si,0,-0.5418231268,1.6114868896,1.9437819335\N,0,1.25816912,1.7047854156,2.077701174\Si,0,-0.4275253857,-0.6836151409,1.7743894777\Si,0,1.7951309076,-0.0156015825,2.2423531115\H,0,2.4550931608,-1.0177749237,-1.1757168814\H,0,1.6584102413,3.504325229,-0.050051573\H,0,-1.3226574462,2.8014354352,2.3281498495\H,0,-1.26885675,-1.895765365,1.7951855545\H,0,2.7397621356,-0.3200553535,3.3364181205\\Version=EM64L-G09RevA.02\State=2-A\MPS2/GTBas1=-1611.419194\CCSD(T)/GTBas1=-1611.5164446\MPS2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1610.7613929\MPS2/GTMP2LargeXP=-1611.9068904\HF/GFHFB3=-1610.7792595\HF/GFHFB4=-1610.8050521\G4MP2=-1612.1819644

**SiN7+**

\\1,2\N,0,0.0885339424,-0.0734761083,-0.08615  
45792\Si,0,1.8753733086,-0.0357031387,-0.0422163383\Si,0,0.149494,1.7011355539,-0.080854365\N,0,1.9148493722,1.7580218663,0.0589904654\Si,0,0.027569242,2.079268882,2.3791725123\Si,0,2.2469893633,1.605792461,1.8399606238\Si,0,0.1493957034,-0.3085512865,1.6724506224\N,0,1.914013847,-0.1792278529,1.7485388439\H,0,2.7213532467,-0.8225411353,-0.9433069931\H,0,-0.6241556222,2.5163888192,-1.0293967284\H,0,-0.819089157,2.878634289,3.2925467292\H,0,3.5715918786,2.0236380989,2.3206997518\H,0,-0.6268191251,-1.3558804487,2.3532694554\\Version=EM64L-G09RevA.02\State=2-A\MPS2/GTBas1=-1611.5063427\CCSD(T)/GTBas1=-1611.5942871\MPS2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1610.8691738\MPS2/GTMP2LargeXP=-1612.014492\HF/GFHFB3=-1610.8856299\HF/GFHFB4=-1610.9130013\G4MP2=-1612.2806712

**SiN8+**

\\1,2\N,0,0.0143034786,0.0138932374,0.1713284  
603\N,0,1.4513828561,0.0145402313,0.1718718385\N,0,0.0136040922,1.450988566,0.1730484187\N,0,1.4507445799,1.4516622562,0.1735902376\Si,0,-0.4544799943,1.9169834618,1.9466558859\Si,0,1.9182418931,1.9167989921,1.9475717908\Si,0,-0.4546760576,-0.4557584341,1.9437280674\Si,0,1.918087313,-0.4559312855,1.9446479259\H,0,-1.4926675168,2.9552602893,2.1123851316\H,0,2.9564933294,2.954865622,2.1142058828\H,0,-1.493177218,-1.4941642529,2.1066682507\H,0,2.9562432445,-1.4945386836,2.1084981098\\Version=EM64L-G09RevA.02\State=2-A\MPS2/GTBas1=-1376.2742118\CCSD(T)/GTBas1=-1376.3630374\MPS2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-1375.490552\MPS2/GTMP2LargeXP=-1376.7406382\HF/GFHFB3=-1375.5058999\HF/GFHFB4=-1375.5317857\G4MP2=-1377.0111316

**SiN9+**

\\1,2\N,0,0.1143226669,0.136831013,0.17547458  
19\N,0,1.536548979,0.0348625678,0.045691491\N,0,-0.2526918635,1.5140200069,0.0441684775\Si,0,1.5451072346,1.8669017263,0.0175410039\Si,0,-0.6924957273,1.4424665984,1.8216558858\Si,0,1.5752307134,1.9051568864,2.4037719699\N,0,-0.2517191187,-0.3044693842,1.4872812619\Si,0,1.5462709729,-0.4099047146,1.8227908886\H,0,2.147168592,2.5927759417,-1.1131544506\H,0,-2.0497420051,1.7963270476,2.2694916008\H,0,2.2499059623,2.7228232383,3.4346846175\H,0,2.1488935933,-1.6755909277,2.2730026718\\Vers

ion=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-1376.3427217\CCSD(T)/GTbas1=-1376.439734\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1375.6053962\MP2/GTMP2LargeXP=-1376.8226571\HF/GFHFB3=-1375.6198146\HF/GFHFB4=-1375.646614\G4MP2=-1377.1006985

#### SiN10<sup>+</sup>

\1,2\N,0,0.0156990489,0.0895469965,0.0831070  
829\Si,0,1.8653004316,0.0024828872,0.0029279015\Si,0,0.1972411027,1.8796471572,-0.0833065878\N,0,1.9743968826,1.7768023916,-0.1543077889\N,0,0.1863662935,1.8915227595,1.7242331143\Si,0,2.0345831662,1.7880863003,1.6291448774\Si,0,0.1982350816,0.0907060498,1.8808888438\N,0,1.9754130596,0.0111334277,1.7838746798\H,0,2.4975090743,-0.9722340258,-0.8866521253\H,0,-0.6443275393,2.726820885,-0.9255408445\H,0,2.8455654186,2.6880812006,2.4498289627\H,0,-0.6420820203,-0.6687960295,2.8041018842\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-1376.5636905\CCSD(T)/GTbas1=-1376.6415233\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1375.8514793\MP2/GTMP2LargeXP=-1377.0695647\HF/GFHFB3=-1375.8636092\HF/GFHFB4=-1375.8927737\G4MP2=-1377.3270488

#### SiN11<sup>+</sup>

\1,2\N,0,0.0214027034,0.025148914,0.08088153  
69\Si,0,1.8131266006,0.0064497524,-0.0484357592\N,0,0.1444474454,1.4543817628,0.2096531907\N,0,1.5221450748,1.7791902714,-0.0565259405\Si,0,-0.2705649188,1.9514129983,2.0216059119\Si,0,2.0354975643,1.8257883326,1.7369129252\Si,0,0.1947986819,-0.3255779286,1.9054458075\N,0,1.9586230777,0.0224460904,1.7448110676\H,0,2.6648023403,-0.7916732796,-0.9349491612\H,0,-1.3745874535,2.9109187029,2.2114721147\H,0,3.3108513959,2.4886034209,2.0558407868\H,0,-0.232042512,-1.6521890375,2.3802875195\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-1376.4062058\CCSD(T)/GTbas1=-1376.4996357\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1375.6705884\MP2/GTMP2LargeXP=-1376.8926278\HF/GFHFB3=-1375.6843041\HF/GFHFB4=-1375.7116105\G4MP2=-1377.1665286

#### SiN12<sup>+</sup>

\1,2\Si,0,-0.0145685944,-0.1165191757,-0.025  
8173361\N,0,1.8271620957,-0.0058075593,0.0435416156\Si,0,0.327050777,2.1139020124,0.0070754575\N,0,2.0514237571,1.4546002622,0.0645093637\N,0,0.3064308829,1.6967379354,1.805539211\Si,0,2.1481926044,1.8074032388,1.8748404311\N,0,0.0821383723,0.2362870803,1.7845600874\Si,0,1.8064578252,-0.4229815275,1.8420622781\H,0,-0.6485009955,-1.3627525724,-0.4896010486\H,0,0.096366325,3.5055882823,-0.4172608076\H,0,2.7822707781,3.0535735549,2.338592555\H,0,2.0373761721,-1.8147315313,2.2660581928\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-1376.3940977\CCSD(T)/GTbas1=-1376.4705744\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1375.6155574\MP2/GTMP2LargeXP=-1376.8787624\HF/GFHFB3=-1375.6299032\HF/GFHFB4=-1375.6564568\G4MP2=-1377.1361828

#### SiN13<sup>+</sup>

\1,2\N,0,-0.0131880195,0.1709213276,0.164897  
8447\N,0,1.4916040467,0.0624571206,-0.0138246232\N,0,-0.2862774148,1.5408227375,0.0457363532\Si,0,1.4230549356,1.8167650419,-0.6001858385\Si,0,-0.4850028638,2.125473794,1.8122536477\Si,0,1.9308715457,2.1629347162,1.618456379\Si,0,0.1535068938,-0.1240093597,1.9816492184\N,0,1.8168627365,0.3534728299,1.4743752667\H,0,1.5861682948,2.1871096316,-2.017992765\H,0,-1.6109837396,3.0373027035,2.1173987879\H,0,2.9651505517,2.737654516,2.504215902\H,0,-0.105666967,-1.4570050591,2.553919827\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-1376.3131187\CCSD(T)/GTbas1=-

-1376.4104323\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-1375.559003  
6\MP2/GTMP2LargeXP=-1376.7903616\HF/GFHFB3=-1375.5735205\HF/GFHFB4=-13  
75.600046\G4MP2=-1377.0698722

#### SiN15<sup>+</sup>

\1,2\Si,0,-0.0110592197,-0.1143010396,0.0083  
256803\N,0,1.8266724414,0.0898126797,-0.0459897778\Si,0,0.2887217979,2  
.1615587983,-0.038449427\N,0,2.0308864371,1.5364984148,-0.195709029\N,  
0,0.5302904634,1.7747344326,1.7621928499\Si,0,2.3117940189,1.604878832  
2,1.5797398115\N,0,0.4507261745,0.308266371,1.7490625903\N,0,1.8924136  
712,-0.1432979833,1.4710813969\H,0,-0.6697388535,-1.3836566213,-0.3407  
540404\H,0,-0.0708666112,3.5226019553,-0.4801998137\H,0,3.3613596801,2  
.3401041605,2.2946997589\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas  
1=-1141.322768\CCSD(T)/GTbas1=-1141.3936666\MP2/GTbas2=0.\MP2/GTbas3=0  
\HF/GTMP2LargeXP=-1140.4478903\MP2/GTMP2LargeXP=-1141.7978655\HF/GFHFB  
B3=-1140.4584694\HF/GFHFB4=-1140.4861791\G4MP2=-1142.0535

#### SiN16<sup>+</sup>

\1,2\Si,0,-0.0347302787,0.0010850531,0.00054  
71408\N,0,1.7742656985,0.0346061516,0.028751055\N,0,-0.0865452073,1.81  
23331653,-0.0147593382\Si,0,1.7221766544,1.8372443327,-0.119855393\N,0  
,0.1315720438,1.6974017717,1.4252675625\N,0,1.5392653939,1.9977780452,  
1.6756086365\N,0,-0.0852363101,0.2983689299,1.7867361942\Si,0,1.723711  
237,0.2014017176,1.8294973993\H,0,-0.8477364578,-0.9311037554,-0.78238  
16952\H,0,2.5628509001,2.6324447248,-1.0164729132\H,0,2.5656063261,-0.  
5431601365,2.7674613513\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1  
=-1141.3981974\CCSD(T)/GTbas1=-1141.4827193\MP2/GTbas2=0.\MP2/GTbas3=0  
\HF/GTMP2LargeXP=-1140.5794849\MP2/GTMP2LargeXP=-1141.8854344\HF/GFHFB  
B3=-1140.5889881\HF/GFHFB4=-1140.6179641\G4MP2=-1142.1529286

#### SiN17<sup>+</sup>

\1,2\Si,0,-0.0195404757,-0.1243966597,0.0026  
698159\N,0,1.8485361176,0.0371397329,-0.0202203924\Si,0,0.3412513727,2  
.1849160943,0.0009393711\N,0,2.0708872074,1.4609687246,-0.0213346608\N  
,0,0.7320801604,1.671760213,1.7616933516\N,0,2.1971950992,1.4806865151  
,1.4776969701\N,0,0.5095598197,0.2479928318,1.7626779021\N,0,1.9629518  
766,-0.0175757911,1.4790258016\H,0,-0.7383692612,-1.3540675924,-0.3895  
168084\H,0,0.0334480833,3.5743759315,-0.3956313508\Version=EM64L-G09R  
evA.02\State=2-A\MP2/GTbas1=-906.1712757\CCSD(T)/GTbas1=-906.2457331\MP  
P2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-905.1876479\MP2/GTMP2Large  
XP=-906.6268299\HF/GFHFB3=-905.1959987\HF/GFHFB4=-905.2236441\G4MP2=-9  
06.8889234

#### SiN19<sup>+</sup>

\1,2\Si,0,0.0470848761,0.0367147441,-0.02427  
19015\N,0,1.8731390995,0.0072110806,-0.0779854145\N,0,0.3958211379,1.8  
288284543,-0.0785272611\N,0,1.7990333179,1.4581873229,-0.2103785451\N,  
0,0.3341311667,1.7822550217,1.5869671293\Si,0,2.1601744128,1.752661583  
1,1.5333716601\N,0,0.4082213713,0.331211265,1.7194577999\N,0,1.8114037  
333,-0.0394337638,1.5876505811\H,0,-0.9945751432,-0.8059623052,-0.6255  
694013\H,0,3.2017660277,2.5951265974,2.1350853531\Version=EM64L-G09Re  
vA.02\State=2-A\MP2/GTbas1=-906.2235699\CCSD(T)/GTbas1=-906.2932816\MP  
2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-905.2536228\MP2/GTMP2LargeX  
P=-906.688833\HF/GFHFB3=-905.2607554\HF/GFHFB4=-905.2894402\G4MP2=-906  
.9480435

## 6. Silicon-phosphorus cubanoids

### SiP1

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\0,1\Si,0,-2.1083436256,-0.1349256733,-0.093234436
5\Si,0,-0.6104161358,-0.5685431166,-1.917260954\Si,0,-0.7765426648,1.7
598117859,0.4441400097\Si,0,0.6451637791,1.417679928,-1.4307979367\P,0
,0.5999813996,0.5579842282,1.8850891984\Si,0,1.9700079599,0.1182566553
,0.0561570751\Si,0,-0.6166138698,-1.3410186971,1.3117362283\Si,0,0.817
1740827,-1.8836966612,-0.5060282772\H,0,-3.5938267296,-0.230488547,-0.
1613682282\H,0,-1.0451905988,-0.9738259791,-3.2828253567\H,0,-1.258169
4892,3.0673727684,0.9709488536\H,0,1.0987599338,2.4152435529,-2.440563
7732\H,0,3.430947204,0.2646147786,0.3080763561\H,0,-0.9853234326,-2.22
61626732,2.4518373151\H,0,1.3916121871,-3.2111223496,-0.8645360736\Ve
rsion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2367.8635886\CCSD(T)/GTBa
s1=-2367.9909678\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2367.411
6682\MP2/GTMP2LargeXP=-2368.3778786\HF/GFHFB3=-2367.4437053\HF/GFHFB4=
-2367.4642604\G4MP2=-2368.6857965
```

### SiP2

```
\0,1\P,0,-1.5859931058,1.1102250018,-0.7875647888\
Si,0,-1.4404608659,-1.2124735371,-0.7867936941\P,0,0.7406415846,1.2700
558125,-0.787716241\Si,0,0.9140970335,-1.0507255422,-0.7869476324\Si,0
,0.7637853053,1.1395565332,1.5357608414\Si,0,0.9510616879,-1.233564429
9,1.5867796724\Si,0,-1.5907723948,0.9778081837,1.5359141198\Si,0,-1.45
17673272,-1.3986284646,1.5869365838\H,0,-2.3212061465,-1.9445891598,-1
.7410489472\H,0,1.8865586544,-1.6555353535,-1.7413229314\H,0,1.6277212
616,2.116143913,2.2583951207\H,0,1.867830027,-2.058897484,2.4243849475
\H,0,-2.5800403716,1.8270902057,2.2586710817\H,0,-2.2469553425,-2.3415
656788,2.4246518676\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-24
19.1153705\CCSD(T)/GTBas1=-2419.2419396\MP2/GTBas2=0.\MP2/GTBas3=0.\HF
/GTMP2LargeXP=-2418.6477998\MP2/GTMP2LargeXP=-2419.6434451\HF/GFHFB3=-
2418.6810406\HF/GFHFB4=-2418.7015999\G4MP2=-2419.9591922
```

### SiP3

```
\0,1\P,0,-1.4950702428,1.1137995976,-0.7313312604\
Si,0,-1.557867337,-1.1984211621,-0.7839641299\Si,0,0.7730741131,0.6600
877392,-0.7837353909\P,0,0.7003120366,-1.6396125624,-1.026966627\Si,0,
1.0739107901,0.6485456866,1.5577421844\Si,0,0.7482411825,-1.7000116916
,1.3066654779\Si,0,-1.3000412405,0.868910485,1.5824920002\Si,0,-1.6138
929139,-1.4944964903,1.5574785313\H,0,-2.4534266656,-1.8023370378,-1.8
097789093\H,0,1.5613872471,1.3987587952,-1.8093885862\H,0,2.0757502538
,1.3566477207,2.4024488913\H,0,1.6030116601,-2.7721352326,1.8884225547
\H,0,-2.0824599128,1.8501221466,2.3847187205\H,0,-2.5274289708,-2.3135
579942,2.4019965434\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-24
19.1432226\CCSD(T)/GTBas1=-2419.266188\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/
GTMP2LargeXP=-2418.6704336\MP2/GTMP2LargeXP=-2419.6693329\HF/GFHFB3=-2
418.7035328\HF/GFHFB4=-2418.723994\G4MP2=-2419.9806116
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### SiP4

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\0,1\P,0,-1.3884694311,1.0316246672,-0.7075354866\
Si,0,-1.4707559009,-1.2967949553,-0.7831335133\Si,0,0.9378678472,0.908
0203154,-0.7823657969\Si,0,0.8793650995,-1.4459750307,-0.8357011\Si,0,
1.0748799295,0.7591181675,1.5645559144\P,0,0.9926008286,-1.5693031647,
1.4889627527\Si,0,-1.2752406685,0.9083045863,1.6171261303\Si,0,-1.3337
381133,-1.4456908732,1.5637894632\H,0,-2.4809297123,-1.8738462108,-1.7
149957541\H,0,1.601397086,1.8633910612,-1.7144206016\H,0,1.7549246927,
-2.4013784748,-1.5722806226\H,0,2.0850524108,1.3361682713,2.4964219464
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\H,0,-2.1507904177,1.8637097241,2.3537148864\H,0,-1.9972636505,-2.4010480837,2.4958617816\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2419.135677\CCSD(T)/GTBas1=-2419.2593287\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2418.670018\MP2/GTMP2LargeXP=-2419.6684863\HF/GFHFB3=-2418.7032032\HF/GFHFB4=-2418.7237929\G4MP2=-2419.9804749

**SiP5**

\\0,1\P,0,-1.5799951812,1.1901365106,-0.8570750522\  
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**SiP6**

\\0,1\P,0,-1.6080908138,1.0490086073,-0.7315345288\  
Si,0,-1.4214692443,-1.2745380289,-0.7902911796\P,0,0.7101758686,1.329262938,-0.8271736858\Si,0,0.8977187999,-0.9728827296,-0.724171932\Si,0,0.7463407215,1.0262780596,1.4646701805\P,0,1.0245769818,-1.2673267423,1.5661435635\Si,0,-1.5864793512,0.9046526471,1.5956619346\Si,0,-1.3051481262,-1.4406684246,1.5633426879\H,0,-2.2936902133,-1.9899388118,-1.7644589611\H,0,1.9791981772,-1.6151313716,-1.5248864467\H,0,1.7178492654,1.8363578658,2.2540790814\H,0,-2.576582605,1.7460242404,2.3259769124\H,0,-1.8694994608,-2.4791982494,2.4728423736\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2470.3934965\CCSD(T)/GTBas1=-2470.5155104\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2469.9072726\MP2/GTMP2LargeXP=-2470.9363683\HF/GFHFB3=-2469.9416024\HF/GFHFB4=-2469.9621213\G4MP2=-2471.2552822

**SiP7**

\\0,1\P,0,0.99275,1.78978,-0.71559\Si,0,-0.00975,0.00026,-1.75015\Si,0,1.79728,0.02746,0.55965\P,0,1.04725,-1.75816,-0.71639\Si,0,0.01202,-0.00035,2.11663\Si,0,-0.86997,-1.56669,0.57379\Si,0,-0.91757,1.53898,0.57454\P,0,-2.05232,-0.03129,-0.69995\H,0,-0.01813,0.00052,-3.23895\H,0,3.25962,0.04989,0.83839\H,0,0.02009,-0.0007,3.6052\H,0,-1.57922,-2.8428,0.86538\H,0,-1.6656,2.79269,0.86659\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2470.4269696\CCSD(T)/GTBas1=-2470.5447807\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2469.932589\MP2/GTMP2LargeXP=-2470.9654397\HF/GFHFB3=-2469.9667057\HF/GFHFB4=-2469.987103\G4MP2=-2471.2792981

**SiP8**

\\0,1\P,0,-1.5572936931,1.1838484138,-1.3980181647\  
P,0,-1.55715511,-1.1294516209,-1.3982527684\P,0,0.7560193609,1.1839774306,-1.3983104219\P,0,0.7561385931,-1.1293252723,-1.3985491786\Si,0,0.7832382998,1.2104125722,0.9277309137\Si,0,0.7831429023,-1.1564641124,0.9274833253\Si,0,-1.5836311556,1.2105039577,0.9280323433\Si,0,-1.5837309954,-1.1563598813,0.9277868373\H,0,1.7175561331,2.1443883976,1.6220591703\H,0,1.7172233529,-2.0908186174,1.6216252811\H,0,-2.5175029179,2.1446836299,1.6226816335\H,0,-2.5179047702,-2.0903948974,1.6222310291\\

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Bas1=-2521.730691\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2521.10  
57312\MP2/GTMP2LargeXP=-2522.1595024\HF/GFHFB3=-2521.1414833\HF/GFHFB4  
=-2521.1620554\G4MP2=-2522.4929653

#### SiP9

\0,1\P,0,-1.5964205359,1.5452884127,-0.9545823102\  
P,0,-1.4237504867,-0.7546574718,-0.7096476754\P,0,0.6735328903,1.95533  
77433,-0.7096491181\Si,0,0.7915633774,-0.302365591,-0.2539278513\Si,0,  
0.1555082062,2.1470715075,1.5297086261\Si,0,0.5576365858,-0.120473087,  
2.1001225685\P,0,-2.1277487164,1.9555303862,1.2658858036\Si,0,-1.73820  
04335,-0.3020328609,1.5299515963\H,0,1.8072729791,-1.0882282495,-1.011  
5713162\H,0,0.6502118814,3.3663111745,2.2311479373\H,0,1.3426193259,-0  
.7267766345,3.2136996788\H,0,-2.7929250736,-1.0878053295,2.2322620605\  
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2521.6376761\CCSD(T)/G  
TBas1=-2521.759991\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2521.1  
300052\MP2/GTMP2LargeXP=-2522.1898059\HF/GFHFB3=-2521.1656036\HF/GFHFB  
4=-2521.1859859\G4MP2=-2522.5179702

#### SiP10

\0,1\P,0,-1.5068060295,0.7014571702,-0.6972529775\  
Si,0,-1.536177302,-1.6008319599,-0.7218643835\Si,0,0.7362007311,0.1805  
838701,-0.7219911279\P,0,0.6644408806,-2.0674820556,-1.214477055\P,0,1  
.2040411955,0.1264500429,1.5319619876\Si,0,0.6648173307,-2.0680452374,  
1.0881267404\Si,0,-1.0978735782,0.1803614844,1.5083618453\P,0,-1.59476  
56506,-2.068208402,1.5323090369\H,0,-2.5686843613,-2.2518412279,-1.571  
366031\H,0,1.6145755647,1.0281870497,-1.5714747259\H,0,1.4830920629,-3  
.1117616552,1.7610557465\H,0,-1.7621608438,1.0276309206,2.5342109441\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2521.7158849\CCSD(T)/GT  
Bas1=-2521.8277065\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2521.1  
98785\MP2/GTMP2LargeXP=-2522.2669966\HF/GFHFB3=-2521.2338434\HF/GFHFB4  
=-2521.2542195\G4MP2=-2522.582538

#### SiP11

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Si,0,-1.4844647169,-1.5067407591,-0.7097489278\P,0,0.7106186928,0.5992  
918627,-0.7352959622\P,0,0.7776412482,-1.7163678523,-0.9981647093\Si,0  
,0.7788927144,0.4015936478,1.5925824383\Si,0,0.6051593008,-1.919466178  
,1.2982853394\Si,0,-1.566242675,0.3468551534,1.554442146\P,0,-1.701740  
7416,-1.967822066,1.5278045734\H,0,-2.3779384667,-2.2580108675,-1.6367  
89481\H,0,1.74816306,1.2449520696,2.347393353\H,0,1.3479963018,-3.0350  
398625,1.9515428751\H,0,-2.563669419,1.0476277241,2.4129966279\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2521.6569846\CCSD(T)/GT  
Bas1=-2521.7765798\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2521.1494328  
\MP2/GTMP2LargeXP=-2522.2108588\HF/GFHFB3=-2521.184895\HF/GFHFB4=-2521  
.2053349\G4MP2=-2522.535727

#### SiP12

\0,1\Si,0,-1.5157669444,1.5356547823,-0.7468981319  
\P,0,-1.6781862224,-0.773891241,-0.7144034981\Si,0,0.8014352976,1.3852  
139101,-0.7467973485\P,0,0.6638606258,-0.9259462744,-0.7143025302\P,0,  
0.8443733649,1.8559395595,1.5199204365\Si,0,0.6819521332,-0.4536073426  
,1.5524132265\P,0,-1.4976743876,2.0079973346,1.5198200342\Si,0,-1.6352  
500243,-0.3031613845,1.5523161106\H,0,-2.4824635181,2.2839428975,-1.60  
05080964\H,0,1.8568420219,2.0022227227,-1.6003220194\H,0,1.6486421458,  
-1.2018974278,2.4060289708\H,0,-2.6906644923,-0.9201675364,2.405832845  
9\  
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2521.6486839\CCSD(T)

/GTBas1=-2521.7691779\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2521.1443688\MP2/GTMP2LargeXP=-2522.203838\HF/GFHFB3=-2521.1798447\HF/GFHFB4=-2521.2003423\G4MP2=-2522.529691

### SiP13

\0,1\p,0,-1.5954601028,0.8823116767,-0.7649110969\  
p,0,-1.5355376445,-1.4325518615,-0.8225985534\p,0,0.7151952195,1.1458191139,-0.6494574799\si,0,0.7531979997,-1.1577066026,-0.7539653113\si,0,0.7074878618,0.9078934461,1.6723802356\si,0,0.8148429573,-1.4580157383,1.5689858591\si,0,-1.6115830666,0.6075227977,1.5248035646\p,0,-1.5056835289,-1.6960007098,1.4907531723\h,0,1.5846006233,-1.7738128826,-1.828971289\h,0,1.5236288773,1.8813198656,2.4545096825\h,0,1.5662527974,-2.431401165,2.4135418284\h,0,-2.7166419935,1.2236220597,2.3158293879\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2521.6285866\CCSD(T)/GTBas1=-2521.7519359\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2521.1262709\MP2/GTMP2LargeXP=-2522.1839983\HF/GFHFB3=-2521.1618908\HF/GFHFB4=-2521.1823784\G4MP2=-2522.5133602

### SiP14

\0,1\si,0,-1.149099469,1.1457997739,-0.5489101943\  
si,0,-1.2320373103,-1.2009020866,-0.4746473909\si,0,1.1727391642,0.7959354255,-0.4746385825\p,0,1.0508843282,-1.5037610428,-0.615932788\p,0,1.1856474926,0.8976732921,1.8262229209\p,0,0.9620776746,-1.3967558119,1.7023314162\p,0,-1.1207234636,1.1111708508,1.7868499039\p,0,-1.3343960199,-1.1951198468,1.8261255459\h,0,-1.992519622,2.161073342,-1.2447391151\h,0,-2.0917865523,-2.1633328078,-1.2242536872\h,0,2.2767137775,1.4643189116,-1.2245080288\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2572.8670908\CCSD(T)/GTBas1=-2572.9913809\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2572.3480678\MP2/GTMP2LargeXP=-2573.4348571\HF/GFHFB3=-2572.3849868\HF/GFHFB4=-2572.4054521\G4MP2=-2573.7741924

### SiP15

\0,1\si,0,-1.466298591,1.1707882646,-0.6515501841\  
p,0,-1.6289613663,-1.1338165254,-0.731147705\si,0,0.8534242246,1.0088985828,-0.6803220137\p,0,0.7009834748,-1.2954865205,-0.8509868228\p,0,0.9101516885,1.2621470598,1.620809669\si,0,0.5448979734,-0.9893376332,1.4134126778\p,0,-1.4271299338,1.3342008338,1.6540423272\p,0,-1.7330426732,-0.9654191959,1.5814122895\h,0,-2.4406657545,1.9960295989,-1.4229875006\h,0,1.8997217807,1.7021993479,-1.4862518625\h,0,1.3282191766,-1.9041038126,2.2936691252\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2572.8908437\CCSD(T)/GTBas1=-2573.0117661\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2572.3680473\MP2/GTMP2LargeXP=-2573.4582044\HF/GFHFB3=-2572.4048029\HF/GFHFB4=-2572.425227\G4MP2=-2573.7934631

### SiP16

\0,1\si,0,-1.1194633363,1.5247254114,-0.7101261123\  
\p,0,-1.1049108411,-0.7754260577,-0.6922949704\p,0,1.1224624986,1.9887991286,-0.7979607996\si,0,1.1136854359,-0.2618085192,-0.3700895552\p,0,0.8629248276,2.1035580926,1.5118088735\p,0,1.2245462846,-0.1602744123,1.9158134465\p,0,-1.4619307386,1.9887676038,1.5068953072\si,0,-1.034281345,-0.2611924586,1.5483573607\h,0,-2.0082377358,2.1849061825,-1.7067635641\h,0,2.1108270751,-1.1106201327,-1.0801915936\h,0,-1.852122125,-1.1097348383,2.4593516075\  
Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-2572.9284062\CCSD(T)/GTBas1=-2573.0443354\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2572.3969035\MP2/GTMP2LargeXP=-2573.4937423\HF/GFHFB3=-2572.4334442\HF/GFHFB4=-2572.4537954\G4MP2=-2573.8230733



**SiP17**

\\0,1\Si,0,-1.1244049863,0.8968800992,-0.4855279717  
\P,0,-1.2582459634,-1.4071039933,-0.5331741504\Si,0,1.1992048102,0.758  
730662,-0.4854483657\P,0,1.0591102428,-1.5448788104,-0.5331101164\P,0,  
1.2077769074,0.9571362747,1.8143522914\P,0,1.06112365,-1.3492639741,1.  
7700824158\P,0,-1.109578278,1.0949145566,1.8142727252\P,0,-1.237215320  
8,-1.2126188085,1.7700144317\H,0,-2.0973830421,1.7021540433,-1.2822179  
434\H,0,2.2608119803,1.4430499505,-1.2820433166\\Version=EM64L-G09RevA  
.02\State=1-A\MP2/GTbas1=-2624.1024366\CCSD(T)/GTbas1=-2624.2280609\MP  
2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-2623.5689954\MP2/GTMP2Large  
XP=-2624.6839814\HF/GFHFB3=-2623.607211\HF/GFHFB4=-2623.6276817\G4MP2=  
-2625.0336095

**SiP18**

\\0,1\Si,0,-1.1073892032,1.1058590012,-0.4551069586  
\P,0,-1.0709632997,-1.1811178152,-0.5532426508\P,0,1.1218282985,1.6178  
795828,-0.5532755847\Si,0,1.1360710043,-0.6517142005,-0.2533362539\P,0  
,0.8962390046,1.5965774704,1.7694822228\P,0,1.175629817,-0.6826789926,  
2.0280029156\P,0,-1.399546404,1.3347669434,1.796399177\P,0,-1.10425090  
02,-0.9569531592,1.76951213\H,0,-2.0323629609,1.8304941155,-1.37330616  
68\H,0,2.1536446437,-1.4489129458,-0.9968288305\\Version=EM64L-G09RevA  
.02\State=1-A\MP2/GTbas1=-2624.1392291\CCSD(T)/GTbas1=-2624.2597204\MP  
2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-2623.5955339\MP2/GTMP2Large  
XP=-2624.7186251\HF/GFHFB3=-2623.6335429\HF/GFHFB4=-2623.653897\G4MP2=  
-2625.0622403

**SiP19**

\\0,1\Si,0,-1.4813169306,1.0904104383,-0.6464449372  
\P,0,-1.6064839606,-1.1878088931,-0.7759060343\P,0,0.7919982059,1.2897  
261692,-0.7759389538\P,0,0.7155380658,-1.0359114546,-0.8548883537\P,0,  
0.6348188533,1.4415699086,1.5421028469\Si,0,0.5096568064,-0.8366499305  
,1.4126448657\P,0,-1.687200793,1.28966462,1.6210888892\P,0,-1.76365779  
99,-1.0359727258,1.5421382879\H,0,-2.3425738896,1.9236314232,-1.536672  
8504\H,0,1.3709214423,-1.6698595553,2.3028762398\\Version=EM64L-G09Rev  
A.02\State=1-A\MP2/GTbas1=-2624.1320079\CCSD(T)/GTbas1=-2624.2534861\MP  
2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-2623.5911012\MP2/GTMP2Larg  
eXP=-2624.7112162\HF/GFHFB3=-2623.6291389\HF/GFHFB4=-2623.649487\G4MP2  
=-2625.0559073

**SiP20**

\\0,1\Si,0,-0.8639653894,0.863116134,-0.4561860156\  
P,0,-0.8984816816,-1.4169135491,-0.4956197588\P,0,1.3976052335,1.16179  
57939,-0.4954349939\P,0,1.3967781822,-1.1488316471,-0.338610142\P,0,1.  
1134381099,1.2751013808,1.799970521\P,0,1.2499153762,-1.0180731302,1.9  
555011106\P,0,-1.1995583494,1.1617804936,1.7797603459\P,0,-1.043571622  
5,-1.1488290051,1.8003580947\H,0,-1.7135598589,1.6186535292,-1.4252391  
62\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTbas1=-2675.3500256\CCSD(T)  
) /GTbas1=-2675.4754624\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-26  
74.7957269\MP2/GTMP2LargeXP=-2675.943106\HF/GFHFB3=-2674.8351968\HF/GF  
HFB4=-2674.8555765\G4MP2=-2676.3012976

**SiP2<sup>+</sup>**

\\1,2\P,0,-0.00001,-1.10061,-1.6124\Si,0,1.72  
236,-1.17953,-0.0294\P,0,0.,1.1003,-1.61257\Si,0,1.72239,1.17951,-0.02  
961\Si,0,-1.72237,1.17952,-0.02961\Si,0,0.00001,1.19599,1.62515\Si,0,-  
1.72237,-1.17951,-0.0294\Si,0,-0.00001,-1.19569,1.62537\H,0,2.80343,-2  
.15684,-0.29014\H,0,2.80345,2.15678,-0.29054\H,0,-2.80344,2.1568,-0.29

054\H,0,0.,2.0448,2.84017\H,0,-2.80345,-2.15682,-0.29013\H,0,-0.00001,  
-2.04425,2.84056\Version=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-2418.  
8593523\CCSD(T)/GTBas1=-2418.9847891\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GT  
MP2LargeXP=-2418.4102142\MP2/GTMP2LargeXP=-2419.3774259\HF/GFHFB3=-241  
8.4428945\HF/GFHFB4=-2418.4641305\G4MP2=-2419.6917288

#### SiP5<sup>+</sup>

\1,2\P,0,-1.4199925101,1.0617898744,-0.65588  
19837\P,0,-1.4097011109,-1.1665669634,-0.7537587619\P,0,0.7573393075,1  
.5352829507,-0.7538412254\Si,0,0.8798574286,-0.782969789,-0.5952549502  
\Si,0,0.600185611,1.5969946906,1.6063218232\Si,0,0.8579655226,-0.76500  
04172,1.7697298496\Si,0,-1.757994819,1.3331052761,1.6344456816\Si,0,-1  
.5036249143,-1.0261228915,1.6062917798\H,0,1.7529456804,-1.4832592452,  
-1.5647134703\H,0,1.3855415013,2.6856498001,2.2340868267\H,0,1.7606978  
821,-1.4891558634,2.6935397303\H,0,-2.865704897,2.2216362339,2.0551487  
385\H,0,-2.3959146821,-2.0287836561,2.2343859618\Version=EM64L-G09Rev  
A.02\State=2-A\MP2/GTBas1=-2470.1100581\CCSD(T)/GTBas1=-2470.238422\MP  
2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2469.6477886\MP2/GTMP2Large  
XP=-2470.6390963\HF/GFHFB3=-2469.6816\HF/GFHFB4=-2469.7026611\G4MP2=-2  
470.9648156

#### SiP6<sup>+</sup>

\1,2\P,0,-0.00043,-1.43265,-1.377\Si,0,1.709  
14,-1.15944,0.20947\P,0,-0.00047,0.75112,-1.85091\Si,0,1.60653,1.13609  
, -0.23196\Si,0,-1.60674,1.13583,-0.23109\P,0,0.0003,1.51905,1.40186\Si  
,0,-1.70912,-1.15942,0.21062\Si,0,0.00082,-0.77008,1.8094\H,0,2.8273,-  
2.13058,0.21483\H,0,2.627,2.1742,-0.49863\H,0,-2.62755,2.17405,-0.4959  
7\H,0,-2.82825,-2.1295,0.21506\H,0,0.00153,-1.21285,3.22525\Version=E  
M64L-G09RevA.02\State=2-A\MP2/GTBas1=-2470.1350186\CCSD(T)/GTBas1=-247  
0.2583852\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2469.6653176\MP  
2/GTMP2LargeXP=-2470.668673\HF/GFHFB3=-2469.6992743\HF/GFHFB4=-2469.72  
03418\G4MP2=-2470.9886757

#### SiP7<sup>+</sup>

\1,2\P,0,-0.42274,-1.13968,1.6523\Si,0,1.142  
09,-1.48494,0.00528\Si,0,-1.95893,-0.54098,0.00284\P,0,-0.42379,-1.153  
3,-1.64353\Si,0,-1.29184,1.71655,-0.00621\Si,0,0.42014,0.98518,-1.5043  
9\Si,0,0.42113,0.99751,1.49658\P,0,2.15196,0.57462,-0.00265\H,0,1.9381  
4,-2.73039,0.01069\H,0,-3.26913,-1.22832,0.00536\H,0,-2.07746,2.97184,  
-0.0124\H,0,0.7848,1.65674,-2.77382\H,0,0.78584,1.67888,2.76075\Versi  
on=EM64L-G09RevA.02\State=2-A\MP2/GTBas1=-2470.1471482\CCSD(T)/GTBas1=  
-2470.268595\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2469.6721869  
\MP2/GTMP2LargeXP=-2470.673994\HF/GFHFB3=-2469.706043\HF/GFHFB4=-2469.  
7269376\G4MP2=-2470.9921603

#### SiP8<sup>+</sup>

\1,2\P,0,0.97332,1.65683,-0.79017\P,0,-0.163  
97,0.00295,-1.7677\P,0,2.03142,-0.02844,0.43096\P,0,0.92585,-1.68244,-  
0.79097\Si,0,0.22983,-0.00394,1.89943\Si,0,-0.90778,-1.6932,0.68476\Si  
,0,-0.85854,1.71708,0.68628\Si,0,-2.09139,0.02929,-0.45718\H,0,0.48218  
, -0.00887,3.36017\H,0,-1.43379,-3.02298,1.07797\H,0,-1.34776,3.06059,1  
.08107\H,0,-3.40961,0.04845,-1.13724\Version=EM64L-G09RevA.02\State=2  
-A\MP2/GTBas1=-2521.3386723\CCSD(T)/GTBas1=-2521.4688347\MP2/GTBas2=0.  
\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2520.8606658\MP2/GTMP2LargeXP=-2521.88  
3531\HF/GFHFB3=-2520.8956902\HF/GFHFB4=-2520.9168669\G4MP2=-2522.22037  
52

**SiP9<sup>+</sup>**

\\1,2\p,0,-1.4355102709,1.4195912144,-0.72660  
14685\p,0,-1.4253472545,-0.8150502341,-0.7119696631\p,0,0.7297155007,1  
.9727300262,-0.7127646082\si,0,0.8238057584,-0.3266940681,-0.290666294  
5\si,0,0.1681769951,2.1977742299,1.5474662469\si,0,0.5183107863,-0.089  
9777768,2.044654549\p,0,-2.1493228801,1.9729301674,1.3175269523\si,0,-  
1.7838232317,-0.3265509637,1.547968921\h,0,1.8045450345,-1.0852428283,  
-1.100918853\h,0,0.6278580678,3.4458295958,2.1994629384\h,0,1.29714905  
08,-0.6929566659,3.149169584\h,0,-2.8762575565,-1.0851826968,2.2000716  
958\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-2521.3719554\CCSD(  
T)/GTbas1=-2521.496353\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-25  
20.8876268\MP2/GTMP2LargeXP=-2521.9139756\HF/GFHFB3=-2520.9225613\HF/G  
FHFB4=-2520.943534\G4MP2=-2522.243836

**SiP10<sup>+</sup>**

\\1,2\p,0,0.,1.31084,-1.61108\si,0,1.62353,0.  
97849,0.0005\si,0,-1.62351,0.97853,0.00053\p,0,0.00003,1.30884,1.61254  
\p,0,-1.80717,-1.29696,-0.00069\si,0,0.00001,-1.00155,1.41031\si,0,-0.  
00004,-0.9998,-1.41136\p,0,1.80714,-1.29699,-0.00073\h,0,2.81335,1.855  
23,0.00088\h,0,-2.8133,1.8553,0.00094\h,0,0.00002,-1.73956,2.6937\h,0,  
-0.00004,-1.73622,-2.69568\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTB  
as1=-2521.4249177\CCSD(T)/GTbas1=-2521.540397\MP2/GTbas2=0.\MP2/GTbas3  
=0.\HF/GTMP2LargeXP=-2520.9289778\MP2/GTMP2LargeXP=-2521.96592\HF/GFHF  
B3=-2520.963802\HF/GFHFB4=-2520.984664\G4MP2=-2522.2859009

**SiP11<sup>+</sup>**

\\1,2\p,0,-1.6283264929,0.7493372837,-0.72838  
88454\si,0,-1.5305786091,-1.5422685026,-0.7849996148\p,0,0.614241499,0  
.49613695,-0.6396545366\p,0,0.745363389,-1.7281905875,-1.0082699179\si  
,0,0.7920461969,0.4018787926,1.7009924799\si,0,0.6500958441,-1.9137015  
789,1.3162255436\si,0,-1.5562475447,0.3890281337,1.5763470036\p,0,-1.6  
615895322,-1.9244625968,1.4838550578\h,0,-2.4164177361,-2.286801181,-1  
.7074812299\h,0,1.7739152947,1.2639617498,2.3985375912\h,0,1.432734604  
9,-3.0250689488,1.9057783711\h,0,-2.5546369138,1.1366504858,2.37605809  
73\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-2521.387907\CCSD(T)  
/GTbas1=-2521.5156713\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=-252  
0.9029059\MP2/GTMP2LargeXP=-2521.9314291\HF/GFHFB3=-2520.9379076\HF/GF  
HFB4=-2520.9588665\G4MP2=-2522.264445

**SiP12<sup>+</sup>**

\\1,2\si,0,-1.5111900856,1.6103813499,-0.8403  
291837\p,0,-1.6316588128,-0.6999125509,-0.6528124906\si,0,0.80656866,1  
.4599194348,-0.8402173778\p,0,0.6272869101,-0.8465689085,-0.6527274814  
\p,0,0.7978461584,1.7819591856,1.4583395599\si,0,0.6773769626,-0.52834  
49099,1.6458293884\p,0,-1.4611002987,1.9286191045,1.4582384107\si,0,-1  
.6403801883,-0.3778581225,1.6457518252\h,0,-2.5138328863,2.3314045534,  
-1.6570594542\h,0,1.8940924203,2.0452223778,-1.6568736082\h,0,1.680012  
9325,-1.249353279,2.4625812242\h,0,-2.7279217722,-0.9631682353,2.46237  
91874\\Version=EM64L-G09RevA.02\State=2-A\MP2/GTbas1=-2521.4008345\CCS  
D(T)/GTbas1=-2521.5162814\MP2/GTbas2=0.\MP2/GTbas3=0.\HF/GTMP2LargeXP=  
-2520.9064655\MP2/GTMP2LargeXP=-2521.9506207\HF/GFHFB3=-2520.9415971\H  
F/GFHFB4=-2520.9626741\G4MP2=-2522.2708275

**SiP14<sup>+</sup>**

\\1,2\si,0,-2.05236,0.0001,-0.47534\si,0,-0.8  
136,1.63014,0.69616\si,0,-0.81376,-1.63007,0.69613\p,0,0.18611,-0.0000  
2,2.0019\p,0,0.95336,-1.65542,-0.80379\p,0,1.90517,-0.00009,0.51197\p,

0,-0.1677,0.00002,-1.86586\ P,0,0.95351,1.65534,-0.80378\ H,0,-3.42942,0.00017,-1.0277\ H,0,-1.25558,2.91405,1.29189\ H,0,-1.25586,-2.91395,1.29185\ \Version=EM64L-G09RevA.02\ State=2-A\ MP2/GTBas1=-2572.599789\ CCSD(T)/GTBas1=-2572.7302777\ MP2/GTBas2=0.\ MP2/GTBas3=0.\ HF/GTMP2LargeXP=-2572.0986339\ MP2/GTMP2LargeXP=-2573.1610328\ HF/GFHFB3=-2572.134976\ HF/GFHFB4=-2572.1560679\ G4MP2=-2573.5065471

**SiP15<sup>+</sup>**

\ \1,2\ Si,0,-1.4653996742,1.2516813444,-0.7353239193\ P,0,-1.5760073605,-1.062838114,-0.6489936362\ Si,0,0.854315378,1.0866466818,-0.7608506375\ P,0,0.6721535914,-1.2356030007,-0.783139487\ P,0,0.870946253,1.1951676012,1.5660491647\ Si,0,0.5345881136,-1.0754713376,1.5034064295\ P,0,-1.3872085566,1.2457547336,1.5821193929\ P,0,-1.7518342694,-1.0353555926,1.6553775452\ H,0,-2.4929760186,2.0351149201,-1.4590157462\ H,0,1.9298250321,1.7482332796,-1.5364195314\ H,0,1.3528975112,-1.9672305158,2.3568904253\ \Version=EM64L-G09RevA.02\ State=2-A\ MP2/GTBas1=-2572.6386118\ CCSD(T)/GTBas1=-2572.7544805\ MP2/GTBas2=0.\ MP2/GTBas3=0.\ HF/GTMP2LargeXP=-2572.1239639\ MP2/GTMP2LargeXP=-2573.2005594\ HF/GFHFB3=-2572.1602451\ HF/GFHFB4=-2572.1813157\ G4MP2=-2573.5303336

**SiP16<sup>+</sup>**

\ \1,2\ Si,0,-1.144385412,1.5730383951,-0.737146313\ P,0,-1.0735662722,-0.7295700538,-0.6579036054\ P,0,1.1243077872,1.9853694356,-0.8311638097\ Si,0,1.170942802,-0.2794990279,-0.3862571497\ P,0,0.7656693083,1.9613942607,1.402189371\ P,0,1.2275310049,-0.1917670419,1.9198894407\ P,0,-1.4939602653,1.9863941159,1.5066260985\ Si,0,-1.0568241074,-0.2778867777,1.6025133098\ H,0,-2.0125231573,2.2734618353,-1.7100950354\ H,0,2.1993238648,-1.0951889193,-1.0701482343\ H,0,-1.8530155531,-1.0940462219,2.5462959275\ \Version=EM64L-G09RevA.02\ State=2-A\ MP2/GTBas1=-2572.6545857\ CCSD(T)/GTBas1=-2572.7773039\ MP2/GTBas2=0.\ MP2/GTBas3=0.\ HF/GTMP2LargeXP=-2572.1463918\ MP2/GTMP2LargeXP=-2573.2097669\ HF/GFHFB3=-2572.1824093\ HF/GFHFB4=-2572.2033074\ G4MP2=-2573.5458137

**SiP17<sup>+</sup>**

\ \1,2\ Si,0,-1.1194014407,0.9723455685,-0.5662426211\ P,0,-1.2167876701,-1.3457436831,-0.4440062059\ Si,0,1.2031912129,0.8341892646,-0.5661664948\ P,0,1.0253001326,-1.4791084042,-0.4439703296\ P,0,1.1645852717,0.8664045961,1.7566314223\ P,0,1.0624742352,-1.4305383907,1.8566482895\ P,0,-1.0775049146,0.9997225696,1.7565708907\ P,0,-1.2482197973,-1.2931726948,1.8565480107\ H,0,-2.1402460045,1.739715238,-1.3194696263\ H,0,2.3078089748,1.475185936,-1.3193433356\ \Version=EM64L-G09RevA.02\ State=2-A\ MP2/GTBas1=-2623.8470774\ CCSD(T)/GTBas1=-2623.9663747\ MP2/GTBas2=0.\ MP2/GTBas3=0.\ HF/GTMP2LargeXP=-2623.3210105\ MP2/GTMP2LargeXP=-2624.4273652\ HF/GFHFB3=-2623.3586015\ HF/GFHFB4=-2623.3798473\ G4MP2=-2624.7703478

**SiP18<sup>+</sup>**

\ \1,2\ Si,0,-1.2030923253,1.1808315054,-0.4466268124\ P,0,-1.0197501533,-1.1137287714,-0.5357027231\ P,0,1.0686591778,1.5520221143,-0.535732501\ Si,0,1.2298784334,-0.7252022681,-0.2278142411\ P,0,0.8342250157,1.5103157889,1.707571351\ P,0,1.2356807996,-0.7297172101,2.0639529793\ P,0,-1.4629845929,1.3844608415,1.8212440394\ P,0,-1.0353346906,-0.8760954028,1.7075974552\ H,0,-2.106659895,1.8887234989,-1.3830320347\ H,0,2.2282782306,-1.5074100966,-0.9931575127\ \Version=EM64L-G09RevA.02\ State=2-A\ MP2/GTBas1=-2623.8836311\ CCSD(T)/GTBas1=-2623.9989795\ MP2/GTBas2=0.\ MP2/GTBas3=0.\ HF/GTMP2LargeXP=-2623.3448229\ MP2/GTMP2LargeXP=-2624.4562476\ HF/GFHFB3=-2623.3822137\ HF/GFHFB4=-2623.4032125\ G4MP2=-2624.7944052

**SiP19<sup>+</sup>**

```
\\1,2\Si,0,-1.5662316414,1.0863442602,-0.7343  
297687\P,0,-1.6787834711,-1.1986810309,-0.8505711157\P,0,0.7207683827,  
1.2532202773,-0.7023797008\P,0,0.6391142679,-0.9988209327,-0.786298765  
9\P,0,0.7071223269,1.4524422822,1.616767519\Si,0,0.5945735157,-0.83258  
26437,1.5005320567\P,0,-1.6107781088,1.2525782334,1.552500743\P,0,-1.6  
924266299,-0.9994631793,1.4685755747\H,0,-2.3917504183,1.9718574294,-1  
.5879186272\H,0,1.4200917762,-1.7180946959,2.3541220849\\Version=EM64L  
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73543\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-2623.3368535\MP2/GT  
MP2LargeXP=-2624.4470655\HF/GFHFB3=-2623.3743108\HF/GFHFB4=-2623.39539  
34\G4MP2=-2624.7857551
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**END OF SUPPORTING INFORMATION**