

**Electronic Supplementary Information belonging to the manuscript:**

**Aromaticity-enhanced reactivity of Geminal Frustrated Lewis  
Pairs**

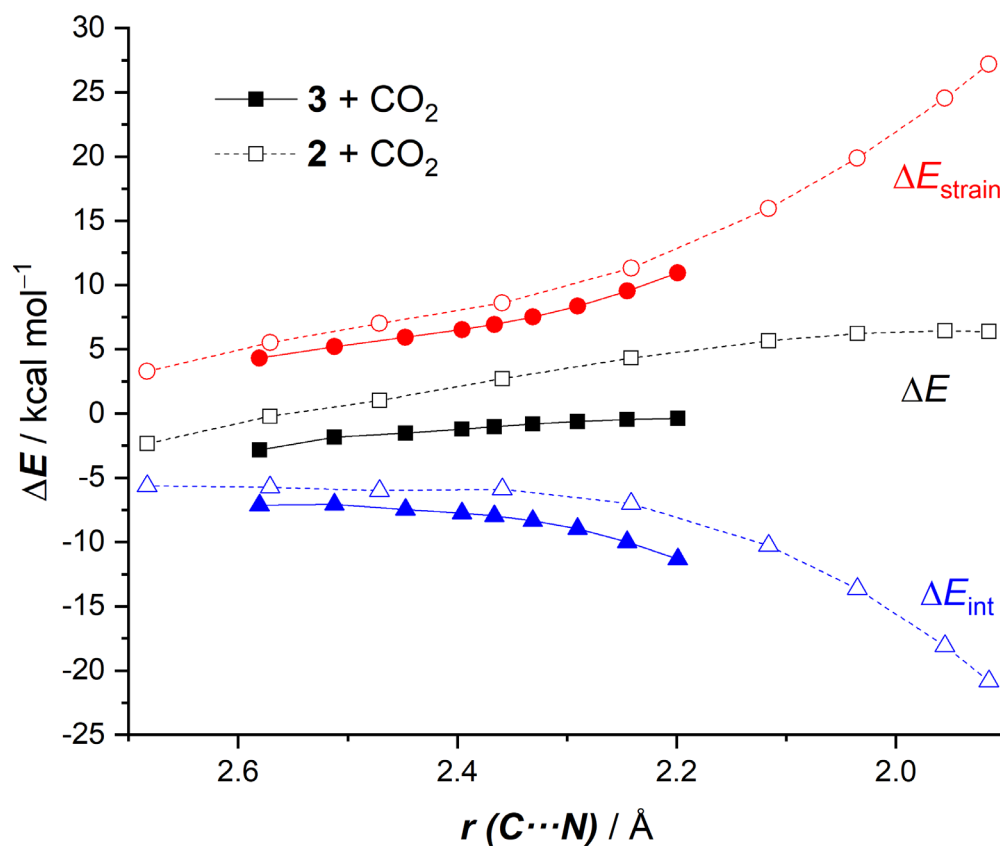
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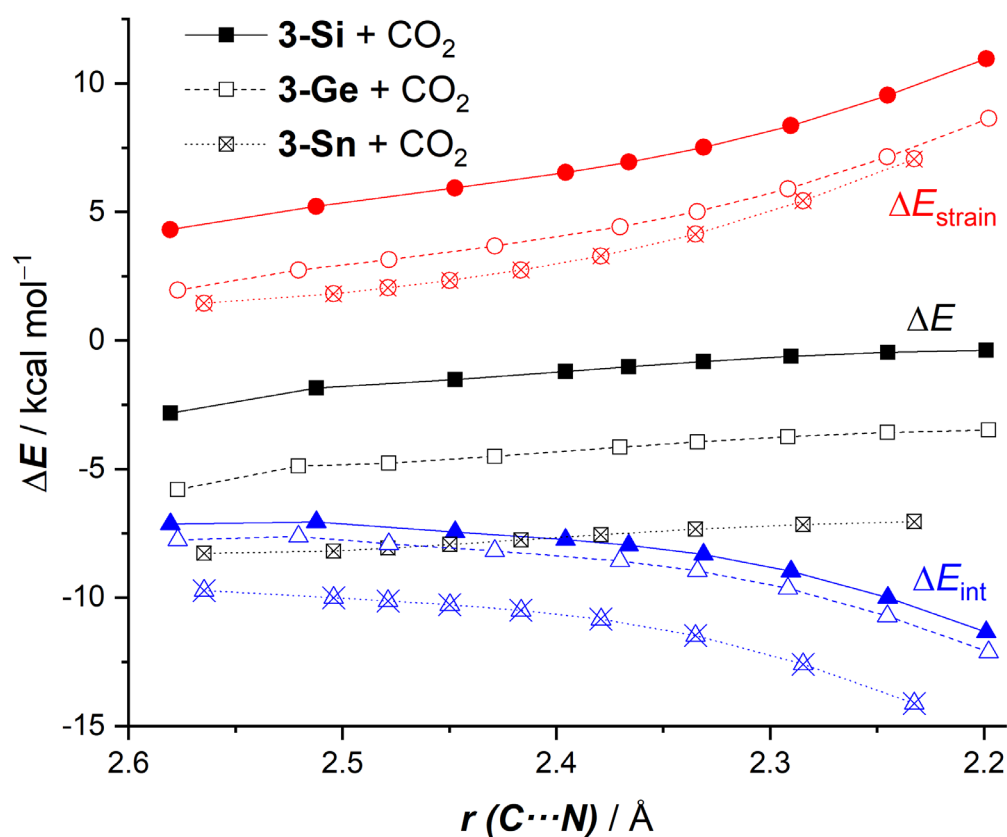
[israel@quim.ucm.es](mailto:israel@quim.ucm.es)

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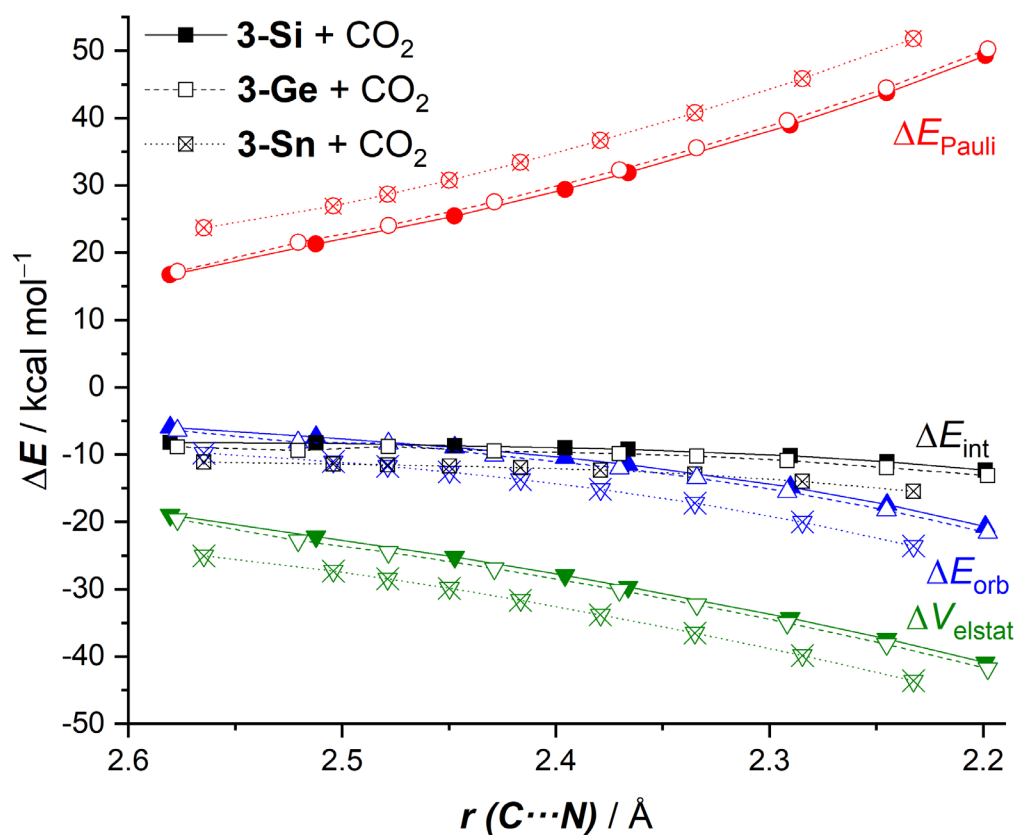
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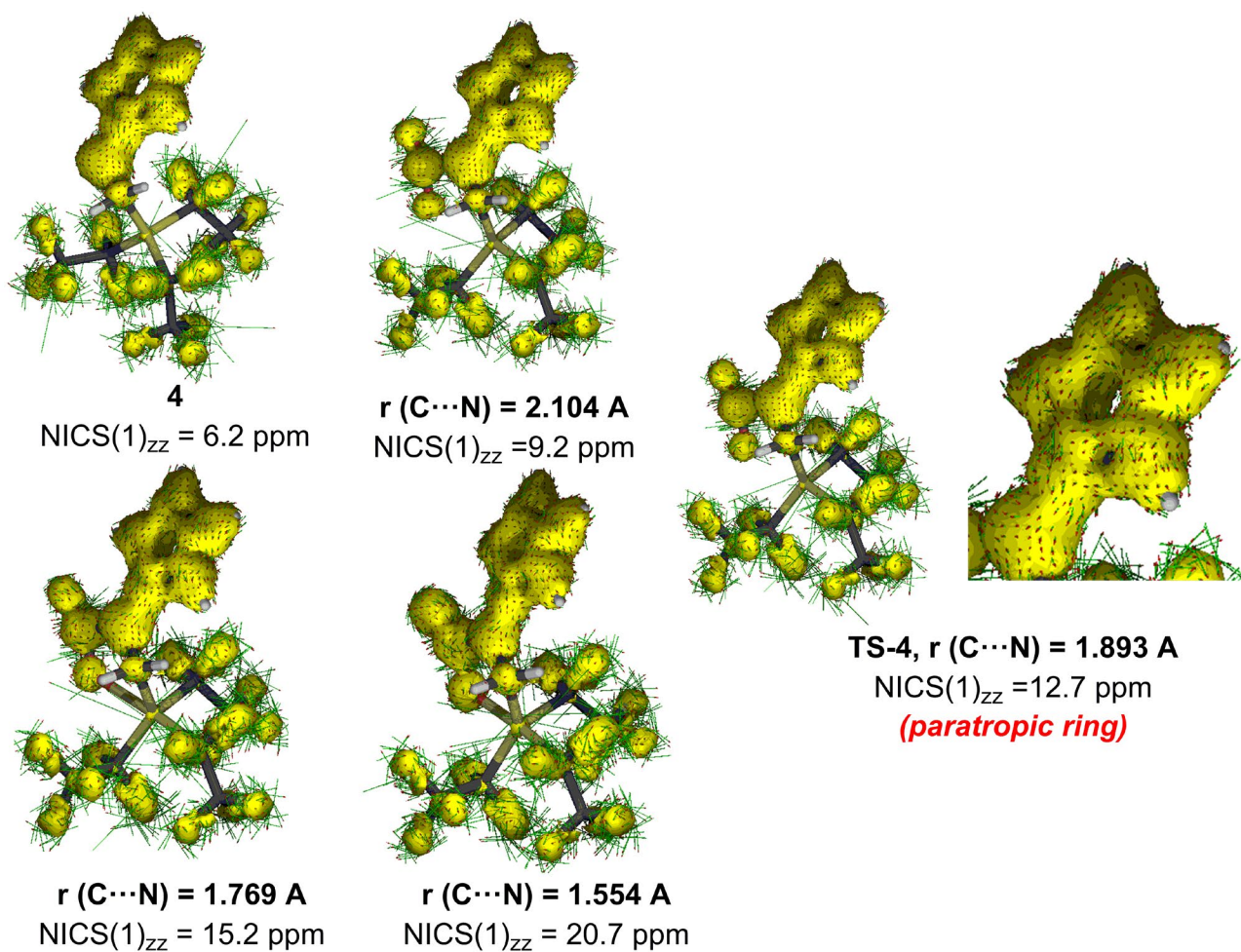
**Figure S1.** Activation strain diagrams for the CO<sub>2</sub> activation reactions mediated by FLP **3** (solid lines) and FLP **2** (dashed lines) along the entire reaction coordinate projected onto the forming C...N bond length. All data were computed at the PCM(toluene)-M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory.



**Figure S2.** Activation strain diagrams for the CO<sub>2</sub> activation reactions mediated by FLP **3-Si** (solid lines), FLP **3-Ge** (dashed lines), and FLP **3-Sn** (dotted lines) along the entire reaction coordinate projected onto the forming C $\cdots$ N bond length. All data were computed at the PCM(toluene)-M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory.



**Figure S3.** Comparative energy decomposition analyses for the CO<sub>2</sub> activation reactions mediated by FLP **3-Si** (solid lines), FLP **3-Ge** (dashed lines), and FLP **3-Sn** (dotted lines) along the entire reaction coordinate projected onto the forming C...N bond length. All data were computed at the ZORA-M06-2X/TZ2P//M06-2X/def2-SVP level of theory.



**Figure S4.** Computed ACID plots for the key points of the CO<sub>2</sub> activation reaction mediated by FLP 4 (isosurface value of 0.04)

## Computational Details

Geometry optimizations of the molecules were performed without symmetry constraints using the Gaussian09 suite of programs<sup>1</sup> employing the meta-hybrid M06-2X exchange-correlation functional<sup>2</sup> combined with the double- $\zeta$  quality def2-SVP basis set.<sup>3</sup> Reactants and products were characterized by frequency calculations and have positive definite Hessian matrices. Transition structures (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.<sup>4</sup> In addition, the vibrational calculation provides the thermal Gibbs energy corrections by using the gas ideal-rigid-rotor-harmonic-oscillator approximation. Solvent effects were taken into account by means of the Polarizable Continuum Model (PCM)<sup>5</sup> using the gas-phase optimized geometries at the same DFT level in conjunction with the triple- $\zeta$  quality def2-TZVPP basis set.<sup>3</sup> This level is denoted PCM(solvent)/M06-2X/def2-TZVPP//M06-2X/def2-SVP. Moreover, more accurate energies were computed at the Domain Based Local Pair-Natural Coupled-Cluster (DLPNO-CCSD(T))<sup>6</sup> as implemented in Orca 5.0.1<sup>7</sup> using the def2-TZVP basis sets<sup>3</sup> and the CPCM solvation model on the M06-2X/def2-SVP geometries. This level is denoted CPCM(solvent)DLPNO-CCSD(T)/def2-TZVP//M06-2X-def2-SVP.

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<sup>1</sup> Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

<sup>2</sup> Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

<sup>3</sup> Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

<sup>4</sup> Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.

<sup>5</sup> (a) Miertuš, S.; Scrocco, E.; Tomasi, J. *Chem. Phys.* **1981**, *55*, 117; (b) Pascual-Ahuir, J. L.; Silla, E.; Tuñón, I. *J. Comp. Chem.* **1994**, *15*, 1127; (c) Barone, V.; Cossi, M. *J. Phys. Chem. A*, **1998**, *102*, 1995.

<sup>6</sup> Riplinger, C.; Sandhoefer, B.; Hansen, A.; Neese, F. *J. Chem. Phys.* **2013**, *139*, 134101.

<sup>7</sup> Neese, F. *WIREs Comput. Mol. Sci.* **2018**, *8*, e1327.

The aromaticity of the considered species has been assessed by the computation of the NICS<sup>8</sup> values using the gauge invariant atomic orbital (GIAO) method,<sup>9</sup> at the B3LYP<sup>10</sup> level using the def2-SVP basis set, with the optimized M06-2X/def2-SVP geometries. This scheme is denoted as GIAO-B3LYP/def2-SVP//M06-2X/def2-SVP. In addition, the HOMA method<sup>11</sup> was also used as a structural criterion for aromaticity.

#### *Activation Strain Model (ASM) of Reactivity and Energy Decomposition Analysis (EDA)*

Within the ASM method,<sup>12</sup> the potential energy surface  $\Delta E(\zeta)$  is decomposed along the reaction coordinate,  $\zeta$ , into two contributions, namely the strain  $\Delta E_{\text{strain}}(\zeta)$  associated with the deformation (or distortion) required by the individual reactants during the process and the interaction  $\Delta E_{\text{int}}(\zeta)$  between these increasingly deformed reactants:

$$\Delta E(\zeta) = \Delta E_{\text{strain}}(\zeta) + \Delta E_{\text{int}}(\zeta)$$

Within the Energy Decomposition Analysis (EDA) method,<sup>13</sup> the interaction energy can be further decomposed into the following chemically meaningful terms:

$$\Delta E_{\text{int}}(\zeta) = \Delta V_{\text{elstat}}(\zeta) + \Delta E_{\text{Pauli}}(\zeta) + \Delta E_{\text{orb}}(\zeta) + \Delta E_{\text{disp}}(\zeta)$$

The term  $\Delta V_{\text{elstat}}$  corresponds to the classical electrostatic interaction between the unperturbed charge distributions of the deformed reactants and is usually attractive. The Pauli repulsion  $\Delta E_{\text{Pauli}}$  comprises the destabilizing interactions between occupied orbitals and is responsible for any steric repulsion. The orbital interaction  $\Delta E_{\text{orb}}$  accounts for bond pair formation, charge transfer (interaction between occupied orbitals on one moiety with unoccupied orbitals on the other, including HOMO-

<sup>8</sup> Chen, Z.; Wannere, C. S.; Corminboeuf, C.; Puchta, R.; Schleyer, P. v. R. *Chem. Rev.* **2005**, *105*, 3842.

<sup>9</sup> Wolinski, K.; Hilton, J. F.; Pulay, P. *J. Am. Chem. Soc.* **1990**, *112*, 8251.

<sup>10</sup> (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648; (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B: Condens. Matter Mater. Phys.* **1988**, *37*, 785; (c) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200.

<sup>11</sup> Kruszewski, J.; Krygowski, T. M. Definition of aromaticity basing on the Harmonic Oscillator Model. *Tetrahedron Lett.* **1972**, *13*, 3839.

<sup>12</sup> For reviews on the ASM method, see: (a) van Zeist, W.-J.; Bickelhaupt, F. M. *Org. Biomol. Chem.* **2010**, *8*, 3118-3127. (b) Fernández, I.; Bickelhaupt, F. M. *Chem. Soc. Rev.* **2014**, *43*, 4953-4967. (c) Wolters, L. P.; Bickelhaupt, F. M. *WIREs Comput. Mol. Sci.* **2015**, *5*, 324-343. (d) Bickelhaupt, F. M.; Houk, K. N. *Angew. Chem. Int. Ed.* **2017**, *56*, 10070-10086. See also, (e) Fernández, I. in *Discovering the Future of Molecular Sciences* (Ed.: B. Pignataro), Wiley-VCH, Weinheim, 2014, pp. 165-187.

<sup>13</sup> For reviews on the EDA method, see: (a) von Hopffgarten, M.; Frenking, G. *WIREs Comput. Mol. Sci.* **2012**, *2*, 43-62. (b) Zhao, L.; von Hopffgarten, M.; Andrada, D. M.; Frenking, G. *WIREs Comput. Mol. Sci.* **2018**, *8*, e1345.

LUMO interactions), and polarization (empty-occupied orbital mixing on one fragment due to the presence of another fragment). Finally, the  $\Delta E_{\text{disp}}$  term accounts for the interactions coming from dispersion forces.

The program package ADF<sup>14</sup> was used for EDA calculations using the optimized M06-2X/def2-SVP geometries at the same DFT level in conjunction with a triple- $\zeta$ -quality basis set using uncontracted Slater-type orbitals (STOs) augmented by two sets of polarization functions with a frozen-core approximation for the core electrons.<sup>15</sup> Auxiliary sets of s, p, d, f, and g STOs were used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle.<sup>16</sup> Scalar relativistic effects were incorporated by applying the zeroth-order regular approximation (ZORA).<sup>17</sup> This level of theory is denoted ZORA-M06-2X/TZ2P//M06-2X/def2-SVP.

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<sup>14</sup> (a) te Velde, G.; Bickelhaupt, F. M.; Baerends, E. J.; Fonseca Guerra, C.; van Gisbergen, S. J. A.; Snijders, J. G.; Ziegler, T. *J. Comput. Chem.* **2001**, *22*, 931-967. (b) ADF2019, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>.

<sup>15</sup> Snijders, J. G.; Vernooijs, P.; Baerends, E. J. *At. Data Nucl. Data Tables*, **1981**, *26*, 483-509.

<sup>16</sup> Krijn, J.; Baerends, E. J. Internal Report, in Dutch, Vrije Universiteit Amsterdam, The Netherlands, 1984.

<sup>17</sup> (a) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1993**, *99*, 4597. (b) van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1994**, *101*, 9783. (c) van Lenthe, E.; Ehlers, A.; Baerends, E. J. *J. Chem. Phys.* **1999**, *110*, 8943.



Cartesian coordinates (in Å) and free energy (in a.u.) of all the stationary points discussed in the text. Free energy plain values have been performed at the PCM(toluene)-M06-2X/def2-TZVPP//M06-2X/def2-SVP level whereas values within parenthesis have been calculated at the CPCM(toluene)-DLPNO-CCSD(T)/def2-TZVPP//M06-2X/def2-SVP level.

**CO<sub>2</sub>:** E= -188.5980863 (-188.3538733)  
C 0.000000000 0.000000000 0.000000000  
O 0.000000000 0.000000000 1.156136000  
O 0.000000000 0.000000000 -1.156136000

**CS<sub>2</sub>:** E= -834.4970336 (-833.5166977)  
C -0.000001000 0.000110000 0.000210000  
S -0.790328000 1.190763000 -0.610055000  
S 0.790328000 -1.190804000 0.609977000

**PhNCO:** E= -399.7579615 (-399.0790651)  
C -0.804474000 -1.278881000 -0.000004000  
C 0.086645000 -0.200924000 -0.000008000  
C -2.176171000 -1.041594000 0.000014000  
H -2.866305000 -1.886371000 0.000021000  
C -0.402378000 1.111799000 -0.000014000  
C -2.667720000 0.263358000 0.000015000  
H 0.299679000 1.946656000 -0.000027000  
H -3.742987000 0.444732000 0.000030000  
C -1.775964000 1.335935000 -0.000001000  
H -2.151251000 2.360344000 -0.000002000  
H -0.404090000 -2.292617000 -0.000011000  
N 1.451364000 -0.457612000 -0.000041000  
C 2.579265000 -0.059940000 0.000008000  
O 3.708774000 0.231503000 0.000028000

**HC≡CH:** E= -77.3461880 (-77.2102867)  
C 0.000000000 0.000000000 0.602879000  
C 0.000000000 0.000000000 -0.602879000  
H 0.000000000 0.000000000 -1.677248000  
H 0.000000000 0.000000000 1.677248000

**SiH<sub>4</sub>:** E= -291.8740738 (-291.4554405)  
Si 0.000000000 0.000000000 0.000000000  
H 0.857178000 0.857178000 0.857178000  
H -0.857178000 -0.857178000 0.857178000  
H 0.857178000 -0.857178000 -0.857178000  
H -0.857178000 0.857178000 -0.857178000

**1:** E= -2712.3575533 (-2708.7280471)  
P -2.436886000 0.003036000 0.192247000  
Si 0.750906000 0.030976000 -0.053336000  
F 1.864997000 1.129840000 -2.212634000  
F 3.256870000 1.030099000 -0.519117000  
F 2.612023000 3.520147000 -1.286594000  
F 1.859553000 3.064992000 0.678879000  
F 0.512474000 3.118682000 -1.000863000

|   |              |              |              |
|---|--------------|--------------|--------------|
| F | 2.033013000  | 0.881050000  | 2.165434000  |
| F | -0.081049000 | 1.442568000  | 2.071123000  |
| F | 1.500576000  | -1.545932000 | 2.866030000  |
| F | -0.604271000 | -1.362318000 | 2.462127000  |
| F | 0.292314000  | -0.210032000 | 4.047603000  |
| F | 0.932903000  | -2.641748000 | 0.331719000  |
| F | 2.843341000  | -1.589534000 | 0.488322000  |
| F | 2.982537000  | -1.316033000 | -2.137087000 |
| F | 2.518300000  | -3.354237000 | -1.621963000 |
| F | 0.976623000  | -2.065341000 | -2.407714000 |
| C | 1.983535000  | 1.293620000  | -0.867358000 |
| C | 1.747597000  | 2.788165000  | -0.608961000 |
| C | 0.797018000  | 0.437647000  | 1.843324000  |
| C | 0.484517000  | -0.696892000 | 2.834256000  |
| C | 1.692138000  | -1.659782000 | -0.211107000 |
| C | 2.061017000  | -2.116255000 | -1.628340000 |
| C | -0.898409000 | 0.219471000  | -0.880130000 |
| H | -0.926833000 | -0.388869000 | -1.797629000 |
| H | -0.882775000 | 1.267086000  | -1.216615000 |
| C | -3.438187000 | 1.506707000  | -0.398502000 |
| C | -4.886645000 | 1.330470000  | 0.070149000  |
| H | -5.419822000 | 0.578063000  | -0.528594000 |
| H | -5.424840000 | 2.285443000  | -0.041054000 |
| H | -4.937411000 | 1.035653000  | 1.129912000  |
| C | -3.423734000 | 1.825839000  | -1.895600000 |
| H | -2.409752000 | 2.011933000  | -2.278460000 |
| H | -4.001618000 | 2.748340000  | -2.070267000 |
| H | -3.877531000 | 1.032413000  | -2.500588000 |
| C | -2.818455000 | 2.687971000  | 0.366453000  |
| H | -2.868195000 | 2.531048000  | 1.453523000  |
| H | -3.366015000 | 3.612480000  | 0.121466000  |
| H | -1.762546000 | 2.849769000  | 0.099176000  |
| C | -3.159342000 | -1.593887000 | -0.531758000 |
| C | -3.674759000 | -1.521879000 | -1.968009000 |
| H | -4.577245000 | -0.898984000 | -2.046384000 |
| H | -3.942298000 | -2.534665000 | -2.312297000 |
| C | -4.286149000 | -2.046654000 | 0.409006000  |
| H | -3.917694000 | -2.147446000 | 1.440500000  |
| H | -4.662591000 | -3.029237000 | 0.081321000  |
| H | -5.135428000 | -1.350747000 | 0.415771000  |
| C | -2.038110000 | -2.638741000 | -0.445156000 |
| H | -1.238973000 | -2.461304000 | -1.179249000 |
| H | -2.456620000 | -3.635707000 | -0.657845000 |
| H | -1.586585000 | -2.672427000 | 0.557750000  |
| H | -2.918683000 | -1.126665000 | -2.664425000 |

**2:** E= -2227.9999605 (-2225.0603158)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 2.556512000  | 1.048914000  | 0.792062000  |
| C  | 3.636240000  | 0.386049000  | 0.921181000  |
| C  | 1.395749000  | 0.758902000  | 1.596904000  |
| H  | 0.970113000  | 1.694885000  | 1.997489000  |
| H  | 1.522673000  | 0.058060000  | 2.442471000  |
| Si | 0.141350000  | 0.089275000  | 0.383145000  |
| C  | -1.485469000 | -0.308812000 | 1.365536000  |
| C  | -2.843174000 | -0.257462000 | 0.654541000  |
| C  | 0.860928000  | -1.559935000 | -0.345124000 |
| C  | -0.043084000 | -2.413465000 | -1.241299000 |
| C  | -0.172793000 | 1.307945000  | -1.090952000 |
| C  | -0.302225000 | 2.771474000  | -0.639241000 |
| F  | 1.967749000  | -1.273753000 | -1.064886000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| F | 1.239592000  | -2.346099000 | 0.695835000  |
| F | 0.650479000  | -3.379967000 | -1.817318000 |
| F | -0.574761000 | -1.641600000 | -2.182618000 |
| F | -1.015040000 | -2.950929000 | -0.521888000 |
| F | -1.347785000 | -1.554866000 | 1.877301000  |
| F | -1.556926000 | 0.557151000  | 2.404617000  |
| F | -3.798363000 | -0.701446000 | 1.454054000  |
| F | -3.122165000 | 0.988307000  | 0.303759000  |
| F | -2.809244000 | -1.014506000 | -0.435293000 |
| F | 0.874493000  | 3.263161000  | -0.298893000 |
| F | -1.097570000 | 2.806005000  | 0.437103000  |
| F | -0.832588000 | 3.523265000  | -1.584446000 |
| F | 0.822227000  | 1.228237000  | -1.992322000 |
| F | -1.328960000 | 0.992008000  | -1.716898000 |
| H | 5.673458000  | 0.958841000  | 0.534561000  |
| H | 5.001129000  | -0.217365000 | -0.608982000 |
| H | 4.479843000  | 1.497054000  | -0.699931000 |
| C | 3.867748000  | -0.710813000 | 1.936616000  |
| H | 3.224341000  | -1.575731000 | 1.715858000  |
| H | 4.911370000  | -1.046215000 | 1.919145000  |
| H | 3.630937000  | -0.368295000 | 2.954724000  |
| C | 4.764644000  | 0.684752000  | -0.022623000 |

**3-Si:** E= -2493.4531714 (-2490.0518980)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.298935000 | 0.923039000  | -1.262467000 |
| N  | -3.885327000 | -1.835870000 | -1.378259000 |
| N  | -4.272061000 | 1.230140000  | 0.682073000  |
| C  | -2.430446000 | 0.377308000  | -0.973046000 |
| C  | -3.417319000 | -0.636015000 | -0.962118000 |
| C  | -3.606505000 | 0.490649000  | -0.213190000 |
| C  | -0.321169000 | 0.165635000  | -2.023092000 |
| H  | 0.101220000  | 0.744208000  | -2.859262000 |
| C  | -5.082139000 | -2.348881000 | -0.749235000 |
| H  | -5.836019000 | -1.552737000 | -0.683696000 |
| H  | -5.497449000 | -3.156878000 | -1.366521000 |
| H  | -4.894251000 | -2.747386000 | 0.265897000  |
| C  | -2.952107000 | -2.804237000 | -1.917273000 |
| H  | -2.434399000 | -3.377177000 | -1.128245000 |
| H  | -3.492055000 | -3.504404000 | -2.569656000 |
| H  | -2.197873000 | -2.286389000 | -2.522130000 |
| C  | -5.569385000 | 0.830932000  | 1.173856000  |
| H  | -6.393461000 | 1.170021000  | 0.520639000  |
| H  | -5.615109000 | -0.262329000 | 1.265653000  |
| H  | -5.723509000 | 1.260272000  | 2.173705000  |
| C  | -3.784788000 | 2.563472000  | 0.981672000  |
| H  | -2.763790000 | 2.663735000  | 0.592786000  |
| H  | -4.420224000 | 3.340754000  | 0.524136000  |
| H  | -3.766566000 | 2.722670000  | 2.070406000  |
| H  | -0.645462000 | -0.819891000 | -2.402755000 |
| Si | 0.844778000  | 0.048671000  | -0.590213000 |
| C  | 2.423832000  | -0.986124000 | -1.066347000 |
| C  | 3.669770000  | -0.992548000 | -0.136927000 |
| C  | -0.125484000 | -0.829139000 | 0.856300000  |
| C  | 0.655291000  | -1.579390000 | 1.944522000  |
| C  | 1.547556000  | 1.730724000  | 0.061401000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.829328000  | 3.044393000  | -0.281383000 |
| F | -0.925136000 | 0.037964000  | 1.511819000  |
| F | -0.924523000 | -1.766582000 | 0.266973000  |
| F | -0.177490000 | -2.292081000 | 2.690178000  |
| F | 1.299369000  | -0.728742000 | 2.722046000  |
| F | 1.533020000  | -2.408489000 | 1.384307000  |
| F | 2.019864000  | -2.268198000 | -1.242811000 |
| F | 2.818438000  | -0.526111000 | -2.279551000 |
| F | 4.099526000  | -2.224027000 | 0.080942000  |
| F | 4.654693000  | -0.282715000 | -0.654882000 |
| F | 3.345250000  | -0.451048000 | 1.040546000  |
| F | -0.311461000 | 3.151539000  | 0.379906000  |
| F | 0.605836000  | 3.120512000  | -1.585847000 |
| F | 1.602170000  | 4.068141000  | 0.067674000  |
| F | 1.664141000  | 1.695352000  | 1.406170000  |
| F | 2.799382000  | 1.845851000  | -0.462830000 |

**3-Ge:** E= -4280.9727964 (-4276.6036428)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.457469000  | 0.621319000  | -1.386870000 |
| N  | 4.365477000  | -1.729012000 | -0.779290000 |
| N  | 4.472675000  | 1.905939000  | -0.009931000 |
| C  | 2.661057000  | 0.326165000  | -1.054218000 |
| C  | 3.790327000  | -0.503884000 | -0.822288000 |
| C  | 3.861594000  | 0.821012000  | -0.511740000 |
| C  | 0.551398000  | -0.433307000 | -1.769676000 |
| H  | 0.946735000  | -1.464337000 | -1.717867000 |
| C  | 5.744001000  | -1.818380000 | -0.355605000 |
| H  | 5.901057000  | -1.185164000 | 0.528261000  |
| H  | 5.970993000  | -2.855857000 | -0.074356000 |
| H  | 6.455471000  | -1.508444000 | -1.144900000 |
| C  | 3.860857000  | -2.774736000 | -1.642037000 |
| H  | 4.322889000  | -2.756611000 | -2.646184000 |
| H  | 4.055028000  | -3.755513000 | -1.185269000 |
| H  | 2.776208000  | -2.659495000 | -1.756343000 |
| C  | 5.795751000  | 1.807239000  | 0.558006000  |
| H  | 5.782495000  | 1.446206000  | 1.603390000  |
| H  | 6.410105000  | 1.125826000  | -0.045962000 |
| H  | 6.272427000  | 2.797468000  | 0.542221000  |
| C  | 3.638841000  | 3.032234000  | 0.371605000  |
| H  | 2.663987000  | 2.937206000  | -0.124469000 |
| H  | 3.471914000  | 3.057471000  | 1.462537000  |
| H  | 4.111925000  | 3.977496000  | 0.066221000  |
| H  | 0.136902000  | -0.279517000 | -2.780300000 |
| Ge | -0.880930000 | -0.158462000 | -0.480593000 |
| C  | -2.508939000 | -1.255978000 | -0.941725000 |
| C  | -3.612265000 | -1.406351000 | 0.142855000  |
| C  | -1.274161000 | 1.816950000  | -0.491197000 |
| C  | -2.659164000 | 2.255642000  | -0.002394000 |
| C  | -0.425489000 | -0.700584000 | 1.405241000  |
| C  | 1.060142000  | -0.847041000 | 1.744996000  |
| F  | -0.371690000 | 2.484024000  | 0.255580000  |
| F  | -1.169327000 | 2.236884000  | -1.771012000 |
| F  | -2.871192000 | 3.533030000  | -0.276117000 |
| F  | -2.767311000 | 2.074096000  | 1.303454000  |
| F  | -3.595684000 | 1.529943000  | -0.614887000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| F | -3.068635000 | -0.726069000 | -2.050930000 |
| F | -2.071158000 | -2.495171000 | -1.267130000 |
| F | -4.811193000 | -1.156203000 | -0.351486000 |
| F | -3.605544000 | -2.620403000 | 0.661871000  |
| F | -3.380014000 | -0.534627000 | 1.130038000  |
| F | 1.663121000  | 0.333144000  | 1.720137000  |
| F | 1.645601000  | -1.650022000 | 0.856118000  |
| F | 1.217224000  | -1.374071000 | 2.949541000  |
| F | -0.953012000 | 0.146881000  | 2.308057000  |
| F | -0.979120000 | -1.926717000 | 1.601623000  |

**3-Sn:** E= -2418.1827288 (-2414.6387587)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.501214000  | 0.921336000  | -1.538874000 |
| N  | 4.481255000  | -1.316475000 | -0.881389000 |
| N  | 4.126244000  | 2.074166000  | 0.580666000  |
| C  | 2.659428000  | 0.639222000  | -1.050193000 |
| C  | 3.808023000  | -0.150869000 | -0.788684000 |
| C  | 3.701632000  | 1.086596000  | -0.222443000 |
| C  | 0.727272000  | -0.108806000 | -2.182594000 |
| H  | 1.195299000  | -1.104296000 | -2.273750000 |
| C  | 5.735099000  | -1.458888000 | -0.179074000 |
| H  | 5.657153000  | -0.998311000 | 0.815271000  |
| H  | 5.953517000  | -2.526919000 | -0.041214000 |
| H  | 6.582958000  | -0.997921000 | -0.719869000 |
| C  | 4.200772000  | -2.235181000 | -1.961645000 |
| H  | 4.918739000  | -2.130561000 | -2.794776000 |
| H  | 4.240229000  | -3.271637000 | -1.594636000 |
| H  | 3.193010000  | -2.044351000 | -2.348676000 |
| C  | 5.338710000  | 1.916267000  | 1.348499000  |
| H  | 5.178099000  | 1.336723000  | 2.276895000  |
| H  | 6.101356000  | 1.410811000  | 0.740887000  |
| H  | 5.724977000  | 2.907419000  | 1.624352000  |
| C  | 3.139391000  | 3.033770000  | 1.046591000  |
| H  | 2.285556000  | 3.033570000  | 0.357196000  |
| H  | 2.769407000  | 2.773921000  | 2.053444000  |
| H  | 3.580458000  | 4.040855000  | 1.080069000  |
| H  | 0.327390000  | 0.202767000  | -3.157514000 |
| Sn | -0.790319000 | -0.028651000 | -0.658647000 |
| C  | -2.631201000 | -1.300880000 | -0.779886000 |
| C  | -3.402369000 | -1.592871000 | 0.504244000  |
| C  | -1.286593000 | 2.127126000  | -0.445894000 |
| C  | -2.621586000 | 2.435124000  | 0.227641000  |
| C  | 0.243526000  | -0.570205000 | 1.240338000  |
| C  | 0.881246000  | -1.956539000 | 1.182971000  |
| F  | -0.339864000 | 2.758721000  | 0.281370000  |
| F  | -1.318956000 | 2.686536000  | -1.674129000 |
| F  | -2.851603000 | 3.738336000  | 0.282784000  |
| F  | -2.611323000 | 1.952402000  | 1.465830000  |
| F  | -3.609664000 | 1.857173000  | -0.447927000 |
| F  | -3.500865000 | -0.735685000 | -1.648889000 |
| F  | -2.261052000 | -2.499803000 | -1.295657000 |
| F  | -4.510314000 | -2.276517000 | 0.256645000  |
| F  | -2.645613000 | -2.297056000 | 1.336293000  |
| F  | -3.731843000 | -0.451351000 | 1.098847000  |
| F  | 1.806809000  | -1.985294000 | 0.219901000  |

|   |              |              |             |
|---|--------------|--------------|-------------|
| F | -0.041851000 | -2.864078000 | 0.883194000 |
| F | 1.456459000  | -2.290736000 | 2.325667000 |
| F | 1.237274000  | 0.300075000  | 1.543390000 |
| F | -0.623517000 | -0.574492000 | 2.278527000 |

**4:** E= -2302.9627002 (-2299.8811555)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.210109000 | 1.391659000  | -0.698920000 |
| C  | -3.332088000 | 0.788193000  | -0.727124000 |
| C  | -1.104891000 | 0.932880000  | -1.492080000 |
| H  | -0.578345000 | 1.795878000  | -1.933347000 |
| H  | -1.342784000 | 0.223928000  | -2.306481000 |
| Si | 0.116226000  | 0.127228000  | -0.320037000 |
| C  | 1.573155000  | -0.526790000 | -1.422679000 |
| C  | 2.982197000  | -0.652714000 | -0.829172000 |
| C  | -0.793182000 | -1.367504000 | 0.512039000  |
| C  | 0.051209000  | -2.312412000 | 1.372662000  |
| C  | 0.724814000  | 1.326770000  | 1.074494000  |
| C  | 0.995236000  | 2.748017000  | 0.560539000  |
| F  | -1.780156000 | -0.890831000 | 1.299066000  |
| F  | -1.359659000 | -2.108789000 | -0.469267000 |
| F  | -0.713348000 | -3.157824000 | 2.038589000  |
| F  | 0.756457000  | -1.588686000 | 2.236883000  |
| F  | 0.885290000  | -2.997314000 | 0.605341000  |
| F  | 1.210185000  | -1.750813000 | -1.870949000 |
| F  | 1.673500000  | 0.292534000  | -2.495975000 |
| F  | 3.783181000  | -1.271678000 | -1.678979000 |
| F  | 3.470228000  | 0.551723000  | -0.576167000 |
| F  | 2.935539000  | -1.345111000 | 0.301933000  |
| F  | -0.141950000 | 3.352791000  | 0.263082000  |
| F  | 1.724871000  | 2.659413000  | -0.556416000 |
| F  | 1.654986000  | 3.466251000  | 1.447296000  |
| F  | -0.189096000 | 1.405600000  | 2.058969000  |
| F  | 1.880149000  | 0.873438000  | 1.607385000  |
| C  | -4.478245000 | 1.206035000  | 0.123855000  |
| H  | -4.429368000 | 2.047682000  | 0.810143000  |
| C  | -5.499420000 | 0.370306000  | -0.126050000 |
| H  | -6.488029000 | 0.394243000  | 0.329341000  |
| C  | -5.071671000 | -0.624685000 | -1.145611000 |
| H  | -5.710040000 | -1.421561000 | -1.525845000 |
| C  | -3.798000000 | -0.390948000 | -1.512357000 |
| H  | -3.214079000 | -0.962198000 | -2.229086000 |

## CO<sub>2</sub> activation

**TS-1 (CO<sub>2</sub>):** E= -2900.9454157 (-2897.0442215) (i = -154 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| P  | 2.439236000  | -0.166248000 | 0.161773000  |
| Si | -0.819004000 | -0.060303000 | -0.307251000 |
| F  | -2.638550000 | 1.851126000  | -1.001753000 |
| F  | -1.267574000 | 1.182379000  | -2.578802000 |
| F  | -0.914800000 | 3.654533000  | -2.195242000 |
| F  | 0.745859000  | 2.613635000  | -1.303906000 |
| F  | -0.788537000 | 3.510417000  | -0.061967000 |
| F  | -3.139992000 | -0.266628000 | 0.850407000  |
| F  | -1.627399000 | -1.424765000 | 1.926249000  |
| F  | -2.005436000 | 2.034297000  | 1.954480000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| F | -0.851796000 | 0.727422000  | 3.248080000  |
| F | -2.986380000 | 0.589443000  | 3.208516000  |
| F | -3.041526000 | -0.840717000 | -1.804059000 |
| F | -1.104310000 | -1.499237000 | -2.571953000 |
| F | -0.927962000 | -3.191794000 | -0.342442000 |
| F | -3.012173000 | -2.769048000 | 0.023711000  |
| F | -2.400864000 | -3.568005000 | -1.871551000 |
| O | 0.484525000  | 1.570841000  | 1.190426000  |
| O | 2.548084000  | 2.492170000  | 1.633191000  |
| C | -1.354711000 | 1.549498000  | -1.268881000 |
| C | -0.564612000 | 2.867637000  | -1.189346000 |
| C | -1.870713000 | -0.232585000 | 1.331645000  |
| C | -1.914585000 | 0.815255000  | 2.460930000  |
| C | -1.838071000 | -1.319063000 | -1.437608000 |
| C | -2.067073000 | -2.741626000 | -0.894764000 |
| C | 0.913325000  | -0.643752000 | -0.747674000 |
| H | 0.852284000  | -1.735545000 | -0.871603000 |
| H | 1.000217000  | -0.241580000 | -1.772741000 |
| C | 3.755231000  | -0.113055000 | -1.183709000 |
| C | 3.504269000  | 1.207987000  | -1.927806000 |
| H | 2.523050000  | 1.227007000  | -2.424690000 |
| H | 4.271899000  | 1.334029000  | -2.707447000 |
| H | 3.556451000  | 2.069968000  | -1.246618000 |
| C | 3.697953000  | -1.272984000 | -2.181348000 |
| H | 3.877760000  | -2.246416000 | -1.708429000 |
| H | 4.476479000  | -1.123877000 | -2.946969000 |
| H | 2.731862000  | -1.316794000 | -2.704815000 |
| C | 5.133847000  | -0.044492000 | -0.517525000 |
| H | 5.172737000  | 0.743101000  | 0.251059000  |
| H | 5.890476000  | 0.192390000  | -1.281947000 |
| H | 5.417662000  | -1.001630000 | -0.057332000 |
| C | 2.701563000  | -1.566277000 | 1.392213000  |
| C | 3.159101000  | -2.887260000 | 0.773687000  |
| H | 2.473786000  | -3.234344000 | -0.014942000 |
| H | 3.179924000  | -3.662695000 | 1.556373000  |
| H | 4.171196000  | -2.813869000 | 0.352458000  |
| C | 3.715850000  | -1.082151000 | 2.438272000  |
| H | 4.711653000  | -0.912291000 | 2.009029000  |
| H | 3.816107000  | -1.846016000 | 3.225338000  |
| H | 3.385154000  | -0.145375000 | 2.910724000  |
| C | 1.347199000  | -1.773128000 | 2.084353000  |
| H | 0.920237000  | -0.829756000 | 2.459934000  |
| H | 1.483550000  | -2.439582000 | 2.950304000  |
| H | 0.613341000  | -2.251795000 | 1.420881000  |
| C | 1.638725000  | 1.842894000  | 1.295809000  |

**TS-2 (CO<sub>2</sub>)**: E= -2416.5893926 (-2413.3786092) (i = -182 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.567994000 | 0.658718000  | -1.025678000 |
| C  | -3.393518000 | -0.223442000 | -1.448103000 |
| C  | -1.207634000 | 0.746413000  | -1.508617000 |
| H  | -0.971082000 | 1.792377000  | -1.761224000 |
| H  | -1.019795000 | 0.133529000  | -2.397290000 |
| Si | -0.016719000 | 0.213534000  | -0.128257000 |
| C  | 1.194993000  | -0.848154000 | -1.272147000 |
| C  | 2.649446000  | -1.216551000 | -0.929382000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.934954000 | -1.115226000 | 0.981291000  |
| C | -0.032737000 | -1.998017000 | 1.860661000  |
| C | 1.141036000  | 1.431468000  | 0.859588000  |
| C | 1.498647000  | 2.672086000  | 0.028353000  |
| F | -1.848291000 | -0.562292000 | 1.798940000  |
| F | -1.608849000 | -1.950598000 | 0.143740000  |
| F | -0.741293000 | -2.621673000 | 2.784875000  |
| F | 0.875268000  | -1.229875000 | 2.455685000  |
| F | 0.585527000  | -2.900047000 | 1.116923000  |
| F | 0.540711000  | -2.016346000 | -1.516639000 |
| F | 1.275226000  | -0.195712000 | -2.465278000 |
| F | 3.078558000  | -2.149674000 | -1.768975000 |
| F | 3.427258000  | -0.153173000 | -1.053821000 |
| F | 2.747541000  | -1.687968000 | 0.304845000  |
| F | 0.459491000  | 3.481024000  | -0.095506000 |
| F | 1.843808000  | 2.254166000  | -1.196566000 |
| F | 2.507846000  | 3.336989000  | 0.552416000  |
| F | 0.672093000  | 1.821659000  | 2.048224000  |
| F | 2.310425000  | 0.784097000  | 1.086780000  |
| C | -2.717682000 | 1.814072000  | 0.494334000  |
| H | -5.510677000 | -0.370655000 | -1.631075000 |
| H | -4.794616000 | -1.347799000 | -0.341828000 |
| H | -4.972339000 | 0.424995000  | -0.112544000 |
| C | -3.042318000 | -1.197952000 | -2.542791000 |
| H | -2.144024000 | -1.771011000 | -2.269877000 |
| H | -3.867452000 | -1.897511000 | -2.715662000 |
| H | -2.832547000 | -0.664298000 | -3.481859000 |
| O | -1.568672000 | 1.860797000  | 0.829989000  |
| O | -3.834468000 | 2.138734000  | 0.644716000  |
| C | -4.751975000 | -0.363294000 | -0.835139000 |

**TS-3-Si (CO<sub>2</sub>)** : E= -2682.0559890 (-2678.3860539) (i = -163 cm<sup>-1</sup>)

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 1.699192000 | -1.026415000 | -0.978020000 |
| N | 3.383412000 | 2.308197000  | -0.889947000 |
| N | 5.202474000 | -0.760273000 | 0.041848000  |
| C | 2.722972000 | -0.272120000 | -0.762793000 |
| C | 3.401858000 | 0.967555000  | -0.734194000 |
| C | 4.074894000 | -0.167641000 | -0.379721000 |
| C | 0.492996000 | -0.438844000 | -1.507009000 |
| H | 0.058529000 | -1.089710000 | -2.285504000 |
| C | 4.622819000 | 3.011854000  | -1.140892000 |
| H | 4.861175000 | 3.063355000  | -2.219109000 |
| H | 4.552089000 | 4.037263000  | -0.751501000 |
| H | 5.448379000 | 2.505192000  | -0.628185000 |
| C | 2.166274000 | 2.929524000  | -1.368766000 |
| H | 2.180413000 | 3.996989000  | -1.109685000 |
| H | 2.045954000 | 2.838278000  | -2.464478000 |
| H | 1.302192000 | 2.478874000  | -0.869696000 |
| C | 6.377425000 | 0.038112000  | 0.307405000  |
| H | 6.950216000 | 0.272009000  | -0.608941000 |
| H | 6.088765000 | 0.976289000  | 0.800135000  |
| H | 7.036914000 | -0.512899000 | 0.991862000  |
| C | 5.383628000 | -2.188587000 | -0.139128000 |
| H | 4.405446000 | -2.667947000 | -0.248203000 |
| H | 6.000444000 | -2.405867000 | -1.028690000 |



|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 5.883152000  | -2.613349000 | 0.743837000  |
| H  | 0.652601000  | 0.545653000  | -1.981922000 |
| Si | -0.853808000 | -0.176739000 | -0.199019000 |
| C  | -1.599378000 | 1.582624000  | -0.663174000 |
| C  | -3.041171000 | 2.026768000  | -0.368860000 |
| C  | 0.050545000  | 0.024242000  | 1.510488000  |
| C  | -0.781708000 | 0.493641000  | 2.707743000  |
| C  | -2.357297000 | -1.402106000 | 0.016031000  |
| C  | -2.860325000 | -1.952058000 | -1.329902000 |
| F  | 0.614549000  | -1.146612000 | 1.875241000  |
| F  | 1.047950000  | 0.931043000  | 1.344855000  |
| F  | -0.070100000 | 0.446774000  | 3.821839000  |
| F  | -1.842727000 | -0.293282000 | 2.839640000  |
| F  | -1.191635000 | 1.738839000  | 2.515312000  |
| F  | -0.801061000 | 2.515064000  | -0.075162000 |
| F  | -1.448798000 | 1.726276000  | -2.006149000 |
| F  | -3.181804000 | 3.299316000  | -0.719528000 |
| F  | -3.900653000 | 1.305886000  | -1.071480000 |
| F  | -3.318901000 | 1.915717000  | 0.919861000  |
| F  | -2.080974000 | -2.915896000 | -1.781769000 |
| F  | -2.832168000 | -0.945454000 | -2.216125000 |
| F  | -4.097897000 | -2.400462000 | -1.239437000 |
| F  | -2.132024000 | -2.421448000 | 0.852713000  |
| F  | -3.386457000 | -0.684529000 | 0.534894000  |
| C  | 1.313939000  | -2.983847000 | -0.053111000 |
| O  | 0.159629000  | -2.963888000 | -0.247534000 |
| O  | 2.376741000  | -3.318130000 | 0.286550000  |

**TS-3-Ge (CO<sub>2</sub>)** : E= -4469.5782182 (-4464.9408656) (i = -168 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.759552000  | 1.060996000  | 1.057594000  |
| N  | 3.411465000  | -2.284712000 | 0.910578000  |
| N  | 5.239268000  | 0.784905000  | -0.022200000 |
| C  | 2.773707000  | 0.300016000  | 0.814971000  |
| C  | 3.441477000  | -0.944457000 | 0.764500000  |
| C  | 4.116791000  | 0.189670000  | 0.408415000  |
| C  | 0.561062000  | 0.478844000  | 1.599682000  |
| H  | 0.109083000  | 1.153461000  | 2.343885000  |
| C  | 4.646647000  | -3.009028000 | 1.119806000  |
| H  | 4.904055000  | -3.091020000 | 2.191580000  |
| H  | 4.556716000  | -4.023191000 | 0.705540000  |
| H  | 5.468306000  | -2.498275000 | 0.604825000  |
| C  | 2.194287000  | -2.898590000 | 1.399064000  |
| H  | 2.196018000  | -3.964150000 | 1.132213000  |
| H  | 2.086074000  | -2.813218000 | 2.496244000  |
| H  | 1.328457000  | -2.438721000 | 0.911347000  |
| C  | 6.412564000  | -0.010637000 | -0.303230000 |
| H  | 6.990611000  | -0.254151000 | 0.607280000  |
| H  | 6.120829000  | -0.943656000 | -0.803886000 |
| H  | 7.067924000  | 0.547418000  | -0.985850000 |
| C  | 5.420078000  | 2.211223000  | 0.176210000  |
| H  | 4.441315000  | 2.688104000  | 0.293461000  |
| H  | 6.038219000  | 2.418151000  | 1.067314000  |
| H  | 5.917259000  | 2.647182000  | -0.702478000 |
| H  | 0.718188000  | -0.493973000 | 2.096090000  |
| Ge | -0.803955000 | 0.181046000  | 0.203970000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.517934000 | -1.688116000 | 0.621610000  |
| C | -2.964447000 | -2.110685000 | 0.342311000  |
| C | 0.190048000  | -0.034034000 | -1.539763000 |
| C | -0.649887000 | -0.475165000 | -2.741529000 |
| C | -2.400920000 | 1.399471000  | -0.044265000 |
| C | -2.896809000 | 1.963129000  | 1.295709000  |
| F | 0.804150000  | 1.112591000  | -1.894470000 |
| F | 1.151428000  | -0.973054000 | -1.352119000 |
| F | 0.054864000  | -0.431241000 | -3.860168000 |
| F | -1.698062000 | 0.333606000  | -2.859591000 |
| F | -1.086166000 | -1.712765000 | -2.558389000 |
| F | -0.733103000 | -2.588403000 | -0.025273000 |
| F | -1.326675000 | -1.884133000 | 1.953091000  |
| F | -3.125738000 | -3.386362000 | 0.672915000  |
| F | -3.803353000 | -1.383958000 | 1.065421000  |
| F | -3.253164000 | -1.970992000 | -0.941897000 |
| F | -2.103079000 | 2.925834000  | 1.729779000  |
| F | -2.875561000 | 0.971307000  | 2.196486000  |
| F | -4.130050000 | 2.424803000  | 1.205307000  |
| F | -2.191204000 | 2.412933000  | -0.891474000 |
| F | -3.415973000 | 0.658045000  | -0.548152000 |
| C | 1.333965000  | 2.958242000  | 0.032959000  |
| O | 0.170861000  | 2.891625000  | 0.162897000  |
| O | 2.395754000  | 3.332258000  | -0.263934000 |

**TS-3-Sn (CO<sub>2</sub>):** E= -2606.7931652 (-2602.9792591) (i = -189 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.745918000  | -1.239108000 | -1.492287000 |
| N  | 3.222106000  | 2.188947000  | -1.151767000 |
| N  | 5.119257000  | -0.810389000 | -0.170211000 |
| C  | 2.707657000  | -0.428363000 | -1.181126000 |
| C  | 3.283677000  | 0.852786000  | -1.020865000 |
| C  | 4.003865000  | -0.258822000 | -0.671211000 |
| C  | 0.521337000  | -0.676051000 | -1.985578000 |
| H  | -0.034713000 | -1.415212000 | -2.579366000 |
| C  | 4.315886000  | 2.991158000  | -0.649978000 |
| H  | 4.271125000  | 3.987208000  | -1.110542000 |
| H  | 4.275817000  | 3.113431000  | 0.448059000  |
| H  | 5.275075000  | 2.532026000  | -0.924481000 |
| C  | 1.945262000  | 2.849442000  | -1.338973000 |
| H  | 1.526125000  | 3.218927000  | -0.390102000 |
| H  | 2.062155000  | 3.693623000  | -2.033992000 |
| H  | 1.227125000  | 2.149215000  | -1.781068000 |
| C  | 6.220627000  | 0.035946000  | 0.228010000  |
| H  | 6.846866000  | 0.347530000  | -0.628736000 |
| H  | 5.841363000  | 0.931208000  | 0.738079000  |
| H  | 6.855805000  | -0.513711000 | 0.935883000  |
| C  | 5.397785000  | -2.213126000 | -0.417187000 |
| H  | 4.462986000  | -2.731716000 | -0.654385000 |
| H  | 6.108546000  | -2.339356000 | -1.252329000 |
| H  | 5.830926000  | -2.670751000 | 0.484113000  |
| H  | 0.649043000  | 0.227421000  | -2.605568000 |
| Sn | -0.736399000 | -0.170097000 | -0.279281000 |
| C  | -1.473565000 | 1.946783000  | -0.559116000 |
| C  | -2.961145000 | 2.232113000  | -0.373805000 |
| C  | 0.641631000  | 0.189987000  | 1.444888000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.088447000 | 0.403608000  | 2.767859000  |
| C | -2.507969000 | -1.396848000 | 0.294480000  |
| C | -3.078458000 | -2.133939000 | -0.919717000 |
| F | 1.548769000  | -0.793009000 | 1.642491000  |
| F | 1.344583000  | 1.327048000  | 1.186330000  |
| F | 0.734812000  | 0.763941000  | 3.739455000  |
| F | -0.702258000 | -0.720076000 | 3.116181000  |
| F | -1.009214000 | 1.353092000  | 2.612035000  |
| F | -0.806831000 | 2.815764000  | 0.237600000  |
| F | -1.183051000 | 2.287472000  | -1.849074000 |
| F | -3.261188000 | 3.470286000  | -0.744905000 |
| F | -3.667920000 | 1.388373000  | -1.121359000 |
| F | -3.303290000 | 2.078406000  | 0.895761000  |
| F | -2.232752000 | -3.068907000 | -1.331128000 |
| F | -3.240404000 | -1.260238000 | -1.919326000 |
| F | -4.244085000 | -2.695112000 | -0.654371000 |
| F | -2.238640000 | -2.310620000 | 1.239801000  |
| F | -3.491528000 | -0.597525000 | 0.766028000  |
| C | 1.363467000  | -2.894228000 | -0.043489000 |
| O | 0.216275000  | -2.669006000 | 0.088844000  |
| O | 2.413479000  | -3.375227000 | 0.065349000  |

**TS-4 (CO<sub>2</sub>):** E= -2491.5485079 (-2488.1962672) (i = -189 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.335777000 | 0.989712000  | -0.733518000 |
| C  | -3.388425000 | 0.296412000  | -0.940435000 |
| C  | -1.072301000 | 0.740255000  | -1.372645000 |
| H  | -0.714807000 | 1.666077000  | -1.853373000 |
| H  | -1.129180000 | -0.047192000 | -2.133333000 |
| Si | 0.231085000  | 0.235954000  | -0.075069000 |
| C  | 1.152720000  | -1.047461000 | -1.268026000 |
| C  | 2.586410000  | -1.577846000 | -1.086328000 |
| C  | -0.685694000 | -0.883952000 | 1.239437000  |
| C  | 0.201155000  | -1.849969000 | 2.039454000  |
| C  | 1.657073000  | 1.356943000  | 0.643670000  |
| C  | 2.039319000  | 2.501947000  | -0.306072000 |
| F  | -1.374042000 | -0.161219000 | 2.142206000  |
| F  | -1.587590000 | -1.633494000 | 0.554063000  |
| F  | -0.454478000 | -2.350922000 | 3.070626000  |
| F  | 1.263915000  | -1.184733000 | 2.484283000  |
| F  | 0.606285000  | -2.844281000 | 1.267031000  |
| F  | 0.339474000  | -2.134505000 | -1.333930000 |
| F  | 1.147097000  | -0.487913000 | -2.511654000 |
| F  | 2.776847000  | -2.615102000 | -1.891044000 |
| F  | 3.461421000  | -0.638053000 | -1.406710000 |
| F  | 2.801686000  | -1.970880000 | 0.160132000  |
| F  | 1.111458000  | 3.443536000  | -0.328577000 |
| F  | 2.136191000  | 1.988801000  | -1.539915000 |
| F  | 3.195513000  | 3.040482000  | 0.023927000  |
| F  | 1.409507000  | 1.860014000  | 1.857121000  |
| F  | 2.762184000  | 0.580712000  | 0.753223000  |
| C  | -2.101953000 | 2.218589000  | 0.687240000  |
| O  | -0.924285000 | 2.090395000  | 0.880565000  |
| O  | -3.125636000 | 2.723295000  | 0.951409000  |
| C  | -4.684970000 | 0.492578000  | -0.229267000 |
| H  | -4.858129000 | 1.259311000  | 0.518663000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -5.532243000 | -0.431822000 | -0.706075000 |
| H | -6.568614000 | -0.571745000 | -0.403458000 |
| C | -4.839341000 | -1.263737000 | -1.732881000 |
| H | -5.304631000 | -2.092726000 | -2.264594000 |
| C | -3.574092000 | -0.840495000 | -1.884624000 |
| H | -2.815180000 | -1.255227000 | -2.541855000 |

**Adduct-1 (CO<sub>2</sub>):** E= -2900.9750628 (-2897.0748580)

|    |              |              |              |
|----|--------------|--------------|--------------|
| P  | 2.339923000  | -0.359712000 | -0.091206000 |
| Si | -0.723356000 | 0.094383000  | -0.218966000 |
| F  | -2.649737000 | 2.012684000  | -0.492010000 |
| F  | -1.349597000 | 1.774863000  | -2.242191000 |
| F  | -1.074900000 | 4.115378000  | -1.239045000 |
| F  | 0.684988000  | 2.948988000  | -0.822224000 |
| F  | -0.728145000 | 3.407432000  | 0.754287000  |
| F  | -3.096661000 | -0.403898000 | 0.928629000  |
| F  | -1.575478000 | -1.843235000 | 1.559110000  |
| F  | -1.827425000 | 1.499653000  | 2.501321000  |
| F  | -0.552460000 | -0.078937000 | 3.265396000  |
| F  | -2.683358000 | -0.230209000 | 3.449848000  |
| F  | -3.070664000 | -0.304394000 | -1.798597000 |
| F  | -1.192004000 | -0.837515000 | -2.779270000 |
| F  | -1.030535000 | -3.025084000 | -1.031292000 |
| F  | -3.080505000 | -2.616328000 | -0.488069000 |
| F  | -2.561893000 | -2.942818000 | -2.541825000 |
| O  | 0.395034000  | 0.978394000  | 1.033878000  |
| O  | 2.423167000  | 1.553460000  | 1.824384000  |
| C  | -1.374193000 | 1.815559000  | -0.882262000 |
| C  | -0.614627000 | 3.100626000  | -0.520306000 |
| C  | -1.802619000 | -0.523857000 | 1.298946000  |
| C  | -1.705735000 | 0.192588000  | 2.656893000  |
| C  | -1.872344000 | -0.889475000 | -1.586990000 |
| C  | -2.160843000 | -2.389762000 | -1.405559000 |
| C  | 0.877427000  | -0.593767000 | -1.091340000 |
| H  | 0.741445000  | -1.632593000 | -1.414747000 |
| H  | 0.944375000  | 0.017600000  | -2.006157000 |
| C  | 3.751302000  | 0.363761000  | -1.056286000 |
| C  | 3.320454000  | 1.777377000  | -1.473543000 |
| H  | 2.405715000  | 1.774950000  | -2.082477000 |
| H  | 4.125950000  | 2.211414000  | -2.084827000 |
| H  | 3.158621000  | 2.427788000  | -0.603186000 |
| C  | 4.013534000  | -0.481804000 | -2.309028000 |
| H  | 4.325900000  | -1.506851000 | -2.071078000 |
| H  | 4.825598000  | -0.007134000 | -2.880649000 |
| H  | 3.129233000  | -0.526740000 | -2.961181000 |
| C  | 4.999750000  | 0.450234000  | -0.171817000 |
| H  | 4.779763000  | 0.951250000  | 0.782100000  |
| H  | 5.759843000  | 1.041075000  | -0.705124000 |
| H  | 5.429743000  | -0.541646000 | 0.025087000  |
| C  | 2.685376000  | -1.882088000 | 0.921071000  |
| C  | 3.318381000  | -2.971936000 | 0.050042000  |
| H  | 2.725025000  | -3.184387000 | -0.852222000 |
| H  | 3.368240000  | -3.900015000 | 0.639597000  |
| H  | 4.343911000  | -2.714172000 | -0.249795000 |
| C  | 3.587112000  | -1.545583000 | 2.118202000  |

|   |             |              |             |
|---|-------------|--------------|-------------|
| H | 4.607355000 | -1.276621000 | 1.821216000 |
| H | 3.649014000 | -2.443612000 | 2.751323000 |
| H | 3.174378000 | -0.728481000 | 2.725444000 |
| C | 1.323000000 | -2.351678000 | 1.451660000 |
| H | 0.836869000 | -1.587451000 | 2.074882000 |
| H | 1.490695000 | -3.231155000 | 2.091496000 |
| H | 0.628154000 | -2.653061000 | 0.656102000 |
| C | 1.675372000 | 0.936487000  | 1.116165000 |

**Adduct-2 (CO<sub>2</sub>):** E= -2416.6073881 (-2413.3951974)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.557419000 | 0.774481000  | -1.035525000 |
| C  | -3.691205000 | 0.173209000  | -1.203460000 |
| C  | -1.293240000 | 0.409356000  | -1.662680000 |
| H  | -0.972105000 | 1.201559000  | -2.355057000 |
| H  | -1.360501000 | -0.545721000 | -2.188254000 |
| Si | -0.081817000 | 0.289992000  | -0.144252000 |
| C  | 1.127095000  | -0.828468000 | -1.318369000 |
| C  | 2.608679000  | -1.181332000 | -1.123809000 |
| C  | -1.061181000 | -1.049253000 | 0.904636000  |
| C  | -0.281657000 | -1.938445000 | 1.873379000  |
| C  | 1.274905000  | 1.135865000  | 0.981906000  |
| C  | 1.919179000  | 2.349117000  | 0.266646000  |
| F  | -2.034914000 | -0.444102000 | 1.636550000  |
| F  | -1.711180000 | -1.888004000 | 0.044529000  |
| F  | -1.099136000 | -2.766253000 | 2.508744000  |
| F  | 0.342033000  | -1.184138000 | 2.765748000  |
| F  | 0.612215000  | -2.651532000 | 1.205873000  |
| F  | 0.491356000  | -2.017425000 | -1.527312000 |
| F  | 1.116671000  | -0.180230000 | -2.528316000 |
| F  | 3.033761000  | -1.876021000 | -2.175860000 |
| F  | 3.335533000  | -0.070299000 | -1.049771000 |
| F  | 2.812071000  | -1.915525000 | -0.044896000 |
| F  | 1.385215000  | 3.484879000  | 0.671664000  |
| F  | 1.666172000  | 2.228618000  | -1.054276000 |
| F  | 3.226150000  | 2.399930000  | 0.427784000  |
| F  | 0.784103000  | 1.550502000  | 2.162490000  |
| F  | 2.250330000  | 0.241196000  | 1.257034000  |
| C  | -2.335578000 | 1.836594000  | 0.032782000  |
| H  | -4.576001000 | 0.549415000  | 0.719849000  |
| H  | -5.319847000 | 1.417842000  | -0.617514000 |
| H  | -5.612217000 | -0.343289000 | -0.451993000 |
| C  | -3.819369000 | -0.871213000 | -2.262884000 |
| H  | -4.873904000 | -1.057157000 | -2.491215000 |
| H  | -3.277506000 | -0.596867000 | -3.176036000 |
| H  | -3.377077000 | -1.804204000 | -1.872610000 |
| O  | -1.130166000 | 1.762172000  | 0.432325000  |
| O  | -3.235999000 | 2.556842000  | 0.325434000  |
| C  | -4.872227000 | 0.454685000  | -0.331628000 |

**Adduct-3-Si (CO<sub>2</sub>):** E= -2682.0963888 (-2678.4243228)

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -1.672047000 | 1.017634000  | -0.781340000 |
| N | -3.759035000 | -1.937824000 | -1.227433000 |
| N | -5.269329000 | 1.136431000  | 0.139509000  |
| C | -2.879144000 | 0.464799000  | -0.706507000 |
| C | -3.659470000 | -0.664325000 | -0.870206000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -4.217265000 | 0.502053000  | -0.352294000 |
| C  | -0.539753000 | 0.330530000  | -1.396095000 |
| H  | -0.255353000 | 0.822633000  | -2.338848000 |
| C  | -5.049287000 | -2.575249000 | -1.410356000 |
| H  | -5.088642000 | -3.064715000 | -2.394947000 |
| H  | -5.230006000 | -3.335588000 | -0.634134000 |
| H  | -5.845720000 | -1.823450000 | -1.372905000 |
| C  | -2.564232000 | -2.733192000 | -1.486416000 |
| H  | -2.775382000 | -3.776344000 | -1.215848000 |
| H  | -2.274206000 | -2.697239000 | -2.548534000 |
| H  | -1.732683000 | -2.385734000 | -0.861221000 |
| C  | -6.522930000 | 0.436497000  | 0.343157000  |
| H  | -7.227236000 | 0.612238000  | -0.487006000 |
| H  | -6.342079000 | -0.640105000 | 0.447141000  |
| H  | -6.986627000 | 0.795113000  | 1.272527000  |
| C  | -5.256247000 | 2.576378000  | 0.364712000  |
| H  | -4.228051000 | 2.946503000  | 0.285581000  |
| H  | -5.905455000 | 3.080956000  | -0.368040000 |
| H  | -5.632461000 | 2.786190000  | 1.376092000  |
| H  | -0.789985000 | -0.711302000 | -1.614117000 |
| Si | 0.825427000  | 0.448119000  | -0.054852000 |
| C  | 1.682180000  | -1.202052000 | -0.902997000 |
| C  | 3.072937000  | -1.823765000 | -0.693591000 |
| C  | -0.004335000 | -0.427240000 | 1.509876000  |
| C  | 0.870669000  | -1.259920000 | 2.456468000  |
| C  | 2.465499000  | 1.476243000  | 0.248798000  |
| C  | 2.922361000  | 2.269485000  | -0.978854000 |
| F  | -0.623651000 | 0.483816000  | 2.291005000  |
| F  | -0.995268000 | -1.262399000 | 1.056003000  |
| F  | 0.240089000  | -1.486273000 | 3.602675000  |
| F  | 1.990353000  | -0.592242000 | 2.713774000  |
| F  | 1.174782000  | -2.429296000 | 1.918558000  |
| F  | 0.794309000  | -2.228081000 | -0.681394000 |
| F  | 1.629197000  | -0.973368000 | -2.255284000 |
| F  | 3.114068000  | -3.033203000 | -1.253558000 |
| F  | 4.004607000  | -1.081691000 | -1.274554000 |
| F  | 3.369028000  | -1.963865000 | 0.591024000  |
| F  | 2.036458000  | 3.206283000  | -1.290731000 |
| F  | 3.023348000  | 1.438070000  | -2.017657000 |
| F  | 4.096302000  | 2.845149000  | -0.778897000 |
| F  | 2.343383000  | 2.347352000  | 1.267212000  |
| F  | 3.487383000  | 0.643549000  | 0.562335000  |
| C  | -1.309131000 | 2.109661000  | 0.105643000  |
| O  | -0.046464000 | 2.077461000  | 0.335968000  |
| O  | -2.149761000 | 2.860022000  | 0.522081000  |

**Adduct-3-Ge (CO<sub>2</sub>):** E= -4469.6032211 (-4464.9620931)

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -1.725851000 | 1.072107000  | -0.798972000 |
| N | -3.748969000 | -1.930472000 | -1.287442000 |
| N | -5.324940000 | 1.076863000  | 0.132919000  |
| C | -2.914110000 | 0.484907000  | -0.727964000 |
| C | -3.670715000 | -0.659964000 | -0.907017000 |
| C | -4.253528000 | 0.482563000  | -0.370145000 |
| C | -0.594253000 | 0.415818000  | -1.438229000 |
| H | -0.281123000 | 0.965885000  | -2.337924000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -5.029245000 | -2.583375000 | -1.482028000 |
| H  | -5.055532000 | -3.068739000 | -2.469233000 |
| H  | -5.207323000 | -3.350217000 | -0.711148000 |
| H  | -5.835557000 | -1.841962000 | -1.447335000 |
| C  | -2.545096000 | -2.703439000 | -1.562871000 |
| H  | -2.732915000 | -3.751589000 | -1.293294000 |
| H  | -2.267368000 | -2.660267000 | -2.628399000 |
| H  | -1.711816000 | -2.345179000 | -0.946724000 |
| C  | -6.549787000 | 0.328330000  | 0.334959000  |
| H  | -7.260746000 | 0.475442000  | -0.495608000 |
| H  | -6.327562000 | -0.740594000 | 0.439719000  |
| H  | -7.028931000 | 0.668712000  | 1.263456000  |
| C  | -5.369789000 | 2.515373000  | 0.361599000  |
| H  | -4.359698000 | 2.928437000  | 0.264297000  |
| H  | -6.055173000 | 2.990720000  | -0.357963000 |
| H  | -5.735825000 | 2.707921000  | 1.380286000  |
| H  | -0.850301000 | -0.607919000 | -1.729901000 |
| Ge | 0.817610000  | 0.394432000  | -0.049767000 |
| C  | 1.654819000  | -1.309896000 | -0.932939000 |
| C  | 3.034914000  | -1.916929000 | -0.665306000 |
| C  | -0.115431000 | -0.453698000 | 1.550346000  |
| C  | 0.727237000  | -1.320003000 | 2.493074000  |
| C  | 2.476482000  | 1.496375000  | 0.278618000  |
| C  | 2.929789000  | 2.260938000  | -0.966454000 |
| F  | -0.713322000 | 0.475249000  | 2.316933000  |
| F  | -1.114385000 | -1.254096000 | 1.061170000  |
| F  | 0.079740000  | -1.559027000 | 3.625599000  |
| F  | 1.857391000  | -0.679767000 | 2.776127000  |
| F  | 1.018345000  | -2.480491000 | 1.927432000  |
| F  | 0.747363000  | -2.315455000 | -0.719917000 |
| F  | 1.622956000  | -1.070657000 | -2.278740000 |
| F  | 3.120093000  | -3.131471000 | -1.205558000 |
| F  | 3.980538000  | -1.162167000 | -1.204518000 |
| F  | 3.263970000  | -2.031010000 | 0.636850000  |
| F  | 2.031728000  | 3.173646000  | -1.306035000 |
| F  | 3.045371000  | 1.398932000  | -1.979577000 |
| F  | 4.095654000  | 2.855759000  | -0.778173000 |
| F  | 2.325067000  | 2.378087000  | 1.276243000  |
| F  | 3.493100000  | 0.666935000  | 0.616116000  |
| C  | -1.403635000 | 2.189405000  | 0.114658000  |
| O  | -0.165150000 | 2.207484000  | 0.371994000  |
| O  | -2.310318000 | 2.884939000  | 0.500431000  |

**Adduct-3-Sn (CO<sub>2</sub>):** E= -2606.8208961 (-2603.0039388)

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 1.765842000 | -1.140719000 | -0.978966000 |
| N | 3.843809000 | 1.838221000  | -1.419421000 |
| N | 5.325094000 | -1.138813000 | 0.129948000  |
| C | 2.956363000 | -0.565009000 | -0.866467000 |
| C | 3.729117000 | 0.573138000  | -1.025194000 |
| C | 4.276961000 | -0.560903000 | -0.440028000 |
| C | 0.666585000 | -0.462897000 | -1.660805000 |
| H | 0.358736000 | -1.025646000 | -2.553152000 |
| C | 5.143963000 | 2.463971000  | -1.566124000 |
| H | 5.230218000 | 2.920193000  | -2.563913000 |
| H | 5.297281000 | 3.249196000  | -0.808555000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 5.933861000  | 1.710667000  | -1.469017000 |
| C  | 2.673585000  | 2.623005000  | -1.785636000 |
| H  | 2.873335000  | 3.677348000  | -1.551740000 |
| H  | 2.446358000  | 2.540384000  | -2.860998000 |
| H  | 1.803613000  | 2.313115000  | -1.194872000 |
| C  | 6.524341000  | -0.369060000 | 0.395572000  |
| H  | 7.278145000  | -0.495893000 | -0.400187000 |
| H  | 6.277882000  | 0.694771000  | 0.498882000  |
| H  | 6.963809000  | -0.709592000 | 1.343429000  |
| C  | 5.380918000  | -2.572859000 | 0.380882000  |
| H  | 4.390906000  | -3.008655000 | 0.209431000  |
| H  | 6.128487000  | -3.041150000 | -0.278927000 |
| H  | 5.672187000  | -2.746803000 | 1.426846000  |
| H  | 0.966569000  | 0.545000000  | -1.967384000 |
| Sn | -0.847290000 | -0.369886000 | -0.106296000 |
| C  | -1.686925000 | 1.585942000  | -0.896724000 |
| C  | -3.030831000 | 2.154305000  | -0.460616000 |
| C  | 0.475011000  | 0.458421000  | 1.494429000  |
| C  | -0.189468000 | 1.239637000  | 2.622372000  |
| C  | -2.676510000 | -1.520003000 | 0.370160000  |
| C  | -3.282093000 | -2.155991000 | -0.879244000 |
| F  | 1.227200000  | -0.504860000 | 2.065324000  |
| F  | 1.349867000  | 1.314144000  | 0.875783000  |
| F  | 0.678509000  | 1.578054000  | 3.566283000  |
| F  | -1.140692000 | 0.487727000  | 3.170470000  |
| F  | -0.744832000 | 2.343821000  | 2.143690000  |
| F  | -0.747250000 | 2.545938000  | -0.639251000 |
| F  | -1.735824000 | 1.463348000  | -2.254293000 |
| F  | -3.213123000 | 3.389794000  | -0.918559000 |
| F  | -4.013426000 | 1.390425000  | -0.919203000 |
| F  | -3.103671000 | 2.190820000  | 0.866558000  |
| F  | -2.459247000 | -3.075795000 | -1.367756000 |
| F  | -3.441427000 | -1.211412000 | -1.810547000 |
| F  | -4.454542000 | -2.714894000 | -0.635610000 |
| F  | -2.465313000 | -2.490121000 | 1.271197000  |
| F  | -3.609100000 | -0.676903000 | 0.874610000  |
| C  | 1.443988000  | -2.303245000 | -0.102968000 |
| O  | 0.216011000  | -2.340463000 | 0.188228000  |
| O  | 2.362202000  | -3.014651000 | 0.222784000  |

**Adduct-4 (CO<sub>2</sub>):** E= -2491.5619987 (-2488.2088183)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.340610000 | 0.992820000  | -0.629630000 |
| C  | -3.503954000 | 0.469146000  | -0.807971000 |
| C  | -1.137215000 | 0.654944000  | -1.360800000 |
| H  | -0.813536000 | 1.521200000  | -1.959879000 |
| H  | -1.284017000 | -0.216971000 | -2.001945000 |
| Si | 0.183375000  | 0.318082000  | 0.023780000  |
| C  | 1.143959000  | -0.856435000 | -1.312008000 |
| C  | 2.567158000  | -1.436343000 | -1.239636000 |
| C  | -0.683042000 | -1.038448000 | 1.149270000  |
| C  | 0.206622000  | -2.095612000 | 1.817333000  |
| C  | 1.717894000  | 1.278852000  | 0.769660000  |
| C  | 2.148563000  | 2.485441000  | -0.071934000 |
| F  | -1.386029000 | -0.452010000 | 2.144088000  |
| F  | -1.592901000 | -1.699902000 | 0.379059000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| F | -0.444236000 | -2.710782000 | 2.792698000  |
| F | 1.276999000  | -1.494982000 | 2.329906000  |
| F | 0.596695000  | -3.000012000 | 0.936458000  |
| F | 0.319524000  | -1.924801000 | -1.519297000 |
| F | 1.131924000  | -0.147985000 | -2.486657000 |
| F | 2.719251000  | -2.354541000 | -2.190656000 |
| F | 3.467394000  | -0.486916000 | -1.445683000 |
| F | 2.801596000  | -2.014229000 | -0.070612000 |
| F | 1.174298000  | 3.386686000  | -0.129202000 |
| F | 2.395318000  | 2.074150000  | -1.316075000 |
| F | 3.233151000  | 3.057851000  | 0.415114000  |
| F | 1.482256000  | 1.714181000  | 2.019438000  |
| F | 2.787103000  | 0.453180000  | 0.831424000  |
| C | -2.020394000 | 1.913644000  | 0.580985000  |
| O | -0.810619000 | 1.727647000  | 0.885184000  |
| O | -2.884794000 | 2.609375000  | 1.002776000  |
| C | -4.701590000 | 0.654745000  | 0.057739000  |
| H | -4.731650000 | 1.283467000  | 0.940458000  |
| C | -5.672974000 | -0.095798000 | -0.482826000 |
| H | -6.686003000 | -0.203068000 | -0.098739000 |
| C | -5.158909000 | -0.784851000 | -1.708253000 |
| H | -5.752367000 | -1.450996000 | -2.332811000 |
| C | -3.872578000 | -0.456892000 | -1.905370000 |
| H | -3.214437000 | -0.786046000 | -2.703437000 |

## CS<sub>2</sub> activation

**TS-2 (CS<sub>2</sub>):** E= -3062.4507005 (-3058.5267846) (I = -310 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.416740000 | -0.272511000 | -0.951857000 |
| C  | -2.757085000 | -1.437134000 | -1.352327000 |
| C  | -1.198734000 | 0.375030000  | -1.373466000 |
| H  | -1.366196000 | 1.460784000  | -1.437637000 |
| H  | -0.842975000 | 0.026205000  | -2.352310000 |
| Si | 0.203645000  | 0.086541000  | -0.119415000 |
| C  | 1.611720000  | -0.598392000 | -1.317344000 |
| C  | 3.117165000  | -0.447906000 | -1.039328000 |
| C  | -0.232475000 | -1.417895000 | 1.059100000  |
| C  | 0.924989000  | -1.949766000 | 1.921251000  |
| C  | 0.965402000  | 1.616640000  | 0.827549000  |
| C  | 0.954852000  | 2.879091000  | -0.053143000 |
| F  | -1.236086000 | -1.127089000 | 1.897654000  |
| F  | -0.645849000 | -2.451006000 | 0.276406000  |
| F  | 0.474357000  | -2.741693000 | 2.876486000  |
| F  | 1.555081000  | -0.917387000 | 2.475637000  |
| F  | 1.781155000  | -2.625360000 | 1.173062000  |
| F  | 1.372137000  | -1.928654000 | -1.465105000 |
| F  | 1.422239000  | -0.030737000 | -2.536958000 |
| F  | 3.798497000  | -1.173368000 | -1.913783000 |
| F  | 3.474724000  | 0.819458000  | -1.174972000 |
| F  | 3.422171000  | -0.860639000 | 0.180692000  |
| F  | -0.252588000 | 3.416603000  | -0.088980000 |
| F  | 1.281060000  | 2.510602000  | -1.299988000 |
| F  | 1.820063000  | 3.777291000  | 0.366732000  |
| F  | 0.382317000  | 1.901919000  | 1.998838000  |
| F  | 2.264322000  | 1.338040000  | 1.081922000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.467940000 | 0.937761000  | 0.175675000  |
| H | -4.732622000 | -2.248943000 | -1.495310000 |
| H | -3.597406000 | -3.161805000 | -0.480689000 |
| H | -4.320363000 | -1.639400000 | 0.135104000  |
| C | -1.991455000 | -2.174178000 | -2.423050000 |
| H | -0.944974000 | -2.331705000 | -2.122481000 |
| H | -2.446944000 | -3.150942000 | -2.620826000 |
| H | -1.992131000 | -1.590851000 | -3.356326000 |
| S | -2.416838000 | 1.526749000  | 1.245901000  |
| S | -4.951631000 | 0.994966000  | -0.409457000 |
| C | -3.929297000 | -2.147684000 | -0.749352000 |

**TS-3-Si (CS<sub>2</sub>):** E= -3327.9219249 (-3323.5399108) (I = -270 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.537762000 | 0.893479000  | -0.951270000 |
| N  | -2.955318000 | -2.443544000 | -1.815979000 |
| N  | -4.642181000 | -0.186374000 | 0.584079000  |
| C  | -2.461506000 | -0.002906000 | -0.882886000 |
| C  | -3.026847000 | -1.261240000 | -1.175725000 |
| C  | -3.671355000 | -0.422603000 | -0.305659000 |
| C  | -0.260817000 | 0.578589000  | -1.529215000 |
| H  | 0.148541000  | 1.461918000  | -2.047148000 |
| C  | -3.626254000 | -3.596702000 | -1.249680000 |
| H  | -3.924032000 | -4.284164000 | -2.053867000 |
| H  | -2.979413000 | -4.143622000 | -0.540727000 |
| H  | -4.529609000 | -3.273434000 | -0.718906000 |
| C  | -1.801945000 | -2.702342000 | -2.657107000 |
| H  | -2.036822000 | -3.526076000 | -3.344653000 |
| H  | -1.577507000 | -1.810933000 | -3.257765000 |
| H  | -0.907160000 | -2.974137000 | -2.071197000 |
| C  | -5.751244000 | -1.103194000 | 0.717901000  |
| H  | -5.986447000 | -1.547692000 | -0.257881000 |
| H  | -5.543560000 | -1.909680000 | 1.444826000  |
| H  | -6.638309000 | -0.552001000 | 1.061615000  |
| C  | -4.385445000 | 0.715341000  | 1.694253000  |
| H  | -3.460126000 | 1.270412000  | 1.504053000  |
| H  | -5.210696000 | 1.433633000  | 1.809017000  |
| H  | -4.272631000 | 0.144912000  | 2.632318000  |
| H  | -0.285488000 | -0.250501000 | -2.258134000 |
| Si | 0.940596000  | 0.104539000  | -0.148607000 |
| C  | 1.518634000  | -1.725413000 | -0.534005000 |
| C  | 2.902690000  | -2.240568000 | -0.118262000 |
| C  | -0.018429000 | 0.067669000  | 1.549558000  |
| C  | 0.768324000  | -0.402787000 | 2.779949000  |
| C  | 2.501612000  | 1.248103000  | 0.072875000  |
| C  | 3.056099000  | 1.727886000  | -1.279286000 |
| F  | -0.467911000 | 1.305828000  | 1.827646000  |
| F  | -1.091587000 | -0.758646000 | 1.455096000  |
| F  | 0.097220000  | -0.152375000 | 3.891571000  |
| F  | 1.935919000  | 0.227701000  | 2.829801000  |
| F  | 0.989161000  | -1.707538000 | 2.700191000  |
| F  | 0.598125000  | -2.558602000 | 0.017601000  |
| F  | 1.454359000  | -1.904810000 | -1.880182000 |
| F  | 3.000801000  | -3.535075000 | -0.385814000 |
| F  | 3.838275000  | -1.595798000 | -0.799151000 |
| F  | 3.100989000  | -2.060185000 | 1.178099000  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| F | 2.298446000  | 2.688500000 | -1.783006000 |
| F | 3.031680000  | 0.691509000 | -2.127597000 |
| F | 4.295880000  | 2.162557000 | -1.174936000 |
| F | 2.220429000  | 2.325663000 | 0.826122000  |
| F | 3.503951000  | 0.571472000 | 0.677297000  |
| C | -1.939908000 | 2.963869000 | -0.620546000 |
| S | -0.482049000 | 3.582883000 | -0.479419000 |
| S | -3.523672000 | 3.060172000 | -0.682236000 |

**TS-3-Ge (CS<sub>2</sub>)**: E= -5115.4441870 (-5110.0943551) (I = -269 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.600641000 | 0.912949000  | -1.053386000 |
| N  | -3.141315000 | -2.377192000 | -1.858837000 |
| N  | -4.720929000 | -0.049487000 | 0.549155000  |
| C  | -2.558197000 | 0.056771000  | -0.959647000 |
| C  | -3.170077000 | -1.186906000 | -1.230561000 |
| C  | -3.770244000 | -0.320932000 | -0.357510000 |
| C  | -0.344890000 | 0.545980000  | -1.635387000 |
| H  | 0.086967000  | 1.385911000  | -2.201175000 |
| C  | -3.873024000 | -3.491138000 | -1.288998000 |
| H  | -4.144345000 | -4.198562000 | -2.084666000 |
| H  | -3.283303000 | -4.028822000 | -0.525105000 |
| H  | -4.796265000 | -3.124895000 | -0.824710000 |
| C  | -1.984113000 | -2.694675000 | -2.674806000 |
| H  | -2.233858000 | -3.531717000 | -3.340315000 |
| H  | -1.725807000 | -1.828944000 | -3.298891000 |
| H  | -1.105508000 | -2.974636000 | -2.067894000 |
| C  | -5.817283000 | -0.974641000 | 0.729485000  |
| H  | -6.154045000 | -1.349649000 | -0.246071000 |
| H  | -5.544957000 | -1.830698000 | 1.374706000  |
| H  | -6.659093000 | -0.446698000 | 1.198420000  |
| C  | -4.375343000 | 0.788346000  | 1.686090000  |
| H  | -3.500083000 | 1.397074000  | 1.434965000  |
| H  | -5.212478000 | 1.456959000  | 1.933229000  |
| H  | -4.136049000 | 0.169115000  | 2.568454000  |
| H  | -0.388709000 | -0.333000000 | -2.300350000 |
| Ge | 0.888819000  | 0.110745000  | -0.161364000 |
| C  | 1.438695000  | -1.819281000 | -0.495148000 |
| C  | 2.796914000  | -2.348172000 | -0.023243000 |
| C  | -0.172239000 | 0.087222000  | 1.564074000  |
| C  | 0.595715000  | -0.396509000 | 2.800080000  |
| C  | 2.559146000  | 1.224554000  | 0.080167000  |
| C  | 3.144787000  | 1.653992000  | -1.272046000 |
| F  | -0.638572000 | 1.315459000  | 1.847751000  |
| F  | -1.238100000 | -0.741023000 | 1.424099000  |
| F  | -0.071325000 | -0.133502000 | 3.911620000  |
| F  | 1.775317000  | 0.214285000  | 2.850893000  |
| F  | 0.795435000  | -1.704249000 | 2.721512000  |
| F  | 0.484009000  | -2.616310000 | 0.046823000  |
| F  | 1.404409000  | -2.022366000 | -1.838579000 |
| F  | 2.882364000  | -3.653279000 | -0.241674000 |
| F  | 3.766306000  | -1.742571000 | -0.693231000 |
| F  | 2.957484000  | -2.124906000 | 1.272752000  |
| F  | 2.393664000  | 2.595679000  | -1.822866000 |
| F  | 3.143534000  | 0.593795000  | -2.088305000 |
| F  | 4.380772000  | 2.097983000  | -1.153179000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| F | 2.334111000  | 2.326783000 | 0.812537000  |
| F | 3.511401000  | 0.500501000 | 0.706182000  |
| C | -1.844912000 | 3.003294000 | -0.606399000 |
| S | -0.339539000 | 3.497764000 | -0.463207000 |
| S | -3.415546000 | 3.212668000 | -0.638006000 |

**TS-3-Sn (CS<sub>2</sub>)** : E= -3252.6547553 (-3248.1293174) (i = -284 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.804248000 | 1.057386000  | -1.562519000 |
| N  | -2.791386000 | -2.535623000 | -1.530205000 |
| N  | -4.823474000 | 0.015008000  | 0.206732000  |
| C  | -2.633495000 | 0.109290000  | -1.262100000 |
| C  | -3.021962000 | -1.249418000 | -1.215058000 |
| C  | -3.791417000 | -0.305697000 | -0.586899000 |
| C  | -0.489136000 | 0.704866000  | -1.981054000 |
| H  | 0.013596000  | 1.549878000  | -2.473415000 |
| C  | -3.401620000 | -3.571223000 | -0.719966000 |
| H  | -4.442501000 | -3.305128000 | -0.499572000 |
| H  | -3.402124000 | -4.515143000 | -1.280889000 |
| H  | -2.861014000 | -3.719432000 | 0.231101000  |
| C  | -1.544356000 | -2.869039000 | -2.193090000 |
| H  | -0.699573000 | -2.924382000 | -1.486949000 |
| H  | -1.650192000 | -3.844525000 | -2.686615000 |
| H  | -1.327355000 | -2.121861000 | -2.967024000 |
| C  | -5.598965000 | -1.048867000 | 0.809007000  |
| H  | -5.874568000 | -1.788174000 | 0.045086000  |
| H  | -5.052716000 | -1.558467000 | 1.623369000  |
| H  | -6.525118000 | -0.627319000 | 1.220302000  |
| C  | -4.787365000 | 1.298806000  | 0.887925000  |
| H  | -4.367313000 | 2.053169000  | 0.212688000  |
| H  | -5.811412000 | 1.598303000  | 1.148278000  |
| H  | -4.177090000 | 1.261247000  | 1.806441000  |
| H  | -0.434985000 | -0.167611000 | -2.654719000 |
| Sn | 0.705876000  | 0.126140000  | -0.235451000 |
| C  | 1.808522000  | -1.750345000 | -0.873143000 |
| C  | 3.314593000  | -1.872591000 | -0.653598000 |
| C  | -0.614038000 | -0.840499000 | 1.305729000  |
| C  | 0.128808000  | -1.117075000 | 2.609942000  |
| C  | 2.290146000  | 1.406375000  | 0.698745000  |
| C  | 2.872106000  | 2.388995000  | -0.323986000 |
| F  | -1.727521000 | -0.142770000 | 1.624041000  |
| F  | -1.034048000 | -2.042649000 | 0.821013000  |
| F  | -0.606842000 | -1.808939000 | 3.465845000  |
| F  | 0.468308000  | 0.038018000  | 3.170302000  |
| F  | 1.240928000  | -1.799191000 | 2.349374000  |
| F  | 1.260005000  | -2.859429000 | -0.313704000 |
| F  | 1.610227000  | -1.850836000 | -2.219696000 |
| F  | 3.798412000  | -2.941185000 | -1.275605000 |
| F  | 3.928748000  | -0.796841000 | -1.136966000 |
| F  | 3.581845000  | -1.984818000 | 0.637837000  |
| F  | 2.002332000  | 3.357738000  | -0.573634000 |
| F  | 3.099438000  | 1.739571000  | -1.471496000 |
| F  | 4.006231000  | 2.922834000  | 0.089553000  |
| F  | 1.854503000  | 2.126223000  | 1.750004000  |
| F  | 3.304416000  | 0.628112000  | 1.131883000  |
| C  | -1.876605000 | 2.994817000  | -0.454345000 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| S | -0.842905000 | 2.717718000 | 0.729476000  |
| S | -2.892208000 | 3.851165000 | -1.291414000 |

**Adduct-2 (CS<sub>2</sub>):** E= -3062.4721343 (-3058.5473311)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.562220000 | 0.162001000  | -0.991614000 |
| C  | -3.353298000 | -0.862029000 | -1.092640000 |
| C  | -1.228260000 | 0.211043000  | -1.579938000 |
| H  | -1.110124000 | 1.138475000  | -2.157446000 |
| H  | -1.061663000 | -0.651692000 | -2.228321000 |
| Si | 0.040608000  | 0.172332000  | -0.095896000 |
| C  | 1.363497000  | -0.683639000 | -1.384356000 |
| C  | 2.893221000  | -0.803051000 | -1.275670000 |
| C  | -0.626022000 | -1.361265000 | 0.949814000  |
| C  | 0.340488000  | -2.023599000 | 1.933745000  |
| C  | 1.346112000  | 1.191042000  | 0.970471000  |
| C  | 1.829813000  | 2.479031000  | 0.255328000  |
| F  | -1.737060000 | -1.049921000 | 1.656129000  |
| F  | -1.009658000 | -2.338412000 | 0.076793000  |
| F  | -0.243611000 | -3.047448000 | 2.539678000  |
| F  | 0.719646000  | -1.143963000 | 2.848328000  |
| F  | 1.406062000  | -2.465235000 | 1.284169000  |
| F  | 0.924515000  | -1.947845000 | -1.645719000 |
| F  | 1.193436000  | 0.019115000  | -2.551103000 |
| F  | 3.363377000  | -1.348484000 | -2.393965000 |
| F  | 3.440924000  | 0.401988000  | -1.150157000 |
| F  | 3.269453000  | -1.565302000 | -0.265250000 |
| F  | 1.173262000  | 3.534288000  | 0.702461000  |
| F  | 1.564461000  | 2.359972000  | -1.056487000 |
| F  | 3.123370000  | 2.680427000  | 0.402479000  |
| F  | 0.852482000  | 1.549314000  | 2.171455000  |
| F  | 2.413533000  | 0.399505000  | 1.207801000  |
| C  | -2.859315000 | 1.354925000  | -0.161762000 |
| H  | -4.465738000 | -0.477042000 | 0.723555000  |
| H  | -5.448011000 | -0.748201000 | -0.739316000 |
| H  | -4.608963000 | -2.125729000 | 0.017526000  |
| C  | -3.078128000 | -1.927134000 | -2.107380000 |
| H  | -3.955342000 | -2.575180000 | -2.208528000 |
| H  | -2.835435000 | -1.484147000 | -3.082434000 |
| H  | -2.223505000 | -2.542382000 | -1.786519000 |
| S  | -1.559213000 | 1.792856000  | 0.840445000  |
| S  | -4.288875000 | 2.109487000  | -0.372583000 |
| C  | -4.535194000 | -1.052027000 | -0.204276000 |

**Adduct-3-Si (CS<sub>2</sub>):** E= -3327.9654198 (-3323.5809147)

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 1.801789000 | -0.846759000 | -0.485187000 |
| N | 3.418478000 | 2.411027000  | -0.752899000 |
| N | 5.550673000 | -0.539942000 | -0.441546000 |
| C | 2.951096000 | -0.149176000 | -0.518542000 |
| C | 3.529823000 | 1.100806000  | -0.624868000 |
| C | 4.328934000 | -0.041623000 | -0.496287000 |
| C | 0.629147000 | -0.253612000 | -1.129352000 |
| H | 0.433873000 | -0.757148000 | -2.090287000 |
| C | 4.561151000 | 3.241757000  | -1.087590000 |
| H | 4.300849000 | 3.900221000  | -1.929229000 |
| H | 4.858212000 | 3.868835000  | -0.232247000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 5.406819000  | 2.614837000  | -1.391905000 |
| C  | 2.130535000  | 3.080115000  | -0.604078000 |
| H  | 2.280775000  | 4.014838000  | -0.046011000 |
| H  | 1.688079000  | 3.318273000  | -1.583758000 |
| H  | 1.437973000  | 2.449839000  | -0.037570000 |
| C  | 6.689750000  | 0.330659000  | -0.211843000 |
| H  | 7.263555000  | 0.495081000  | -1.138688000 |
| H  | 6.353381000  | 1.294129000  | 0.188304000  |
| H  | 7.354676000  | -0.132508000 | 0.531087000  |
| C  | 5.843267000  | -1.951712000 | -0.649616000 |
| H  | 4.941315000  | -2.472952000 | -0.981723000 |
| H  | 6.637113000  | -2.036756000 | -1.407485000 |
| H  | 6.181168000  | -2.418373000 | 0.287103000  |
| H  | 0.844651000  | 0.798810000  | -1.343214000 |
| Si | -0.931837000 | -0.419291000 | -0.018396000 |
| C  | -1.631493000 | 1.261833000  | -0.956299000 |
| C  | -3.040685000 | 1.869390000  | -0.955905000 |
| C  | -0.409278000 | 0.312833000  | 1.741872000  |
| C  | -1.379432000 | 1.225855000  | 2.508591000  |
| C  | -2.648004000 | -1.388824000 | 0.052226000  |
| C  | -3.011002000 | -2.074432000 | -1.282550000 |
| F  | -0.096375000 | -0.667831000 | 2.605789000  |
| F  | 0.736407000  | 1.044008000  | 1.544688000  |
| F  | -0.967565000 | 1.394341000  | 3.758862000  |
| F  | -2.581879000 | 0.665781000  | 2.531804000  |
| F  | -1.465917000 | 2.420710000  | 1.944084000  |
| F  | -0.804385000 | 2.284178000  | -0.556655000 |
| F  | -1.357028000 | 1.085500000  | -2.287132000 |
| F  | -3.019678000 | 3.048679000  | -1.576555000 |
| F  | -3.883623000 | 1.084528000  | -1.615003000 |
| F  | -3.491578000 | 2.067832000  | 0.273208000  |
| F  | -2.493202000 | -3.289525000 | -1.346236000 |
| F  | -2.496987000 | -1.352363000 | -2.287647000 |
| F  | -4.317533000 | -2.157641000 | -1.458785000 |
| F  | -2.653197000 | -2.335384000 | 1.011934000  |
| F  | -3.648788000 | -0.530538000 | 0.345442000  |
| C  | 1.683742000  | -2.049882000 | 0.243400000  |
| S  | 0.067331000  | -2.602875000 | 0.408317000  |
| S  | 3.006004000  | -2.783483000 | 0.905773000  |

**Adduct-3-Ge (CS<sub>2</sub>):** E= -5115.4807301 (-5110.1260919)

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 1.863484000 | -0.860408000 | -0.510006000 |
| N | 3.455147000 | 2.410463000  | -0.838427000 |
| N | 5.608713000 | -0.511833000 | -0.454012000 |
| C | 3.004518000 | -0.148534000 | -0.549578000 |
| C | 3.574170000 | 1.103327000  | -0.681440000 |
| C | 4.381724000 | -0.028761000 | -0.525177000 |
| C | 0.698432000 | -0.294424000 | -1.190485000 |
| H | 0.490959000 | -0.850925000 | -2.117590000 |
| C | 4.592963000 | 3.240063000  | -1.191383000 |
| H | 4.328607000 | 3.880534000  | -2.045618000 |
| H | 4.888981000 | 3.885370000  | -0.349271000 |
| H | 5.441285000 | 2.611395000  | -1.484598000 |
| C | 2.162349000 | 3.072074000  | -0.705405000 |
| H | 2.306956000 | 4.030303000  | -0.187188000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 1.706764000  | 3.266482000  | -1.688930000 |
| H  | 1.483013000  | 2.458940000  | -0.105245000 |
| C  | 6.735110000  | 0.376580000  | -0.230839000 |
| H  | 7.314722000  | 0.531849000  | -1.155695000 |
| H  | 6.384176000  | 1.342663000  | 0.150007000  |
| H  | 7.399588000  | -0.065552000 | 0.525275000  |
| C  | 5.921876000  | -1.922877000 | -0.635352000 |
| H  | 5.028259000  | -2.463242000 | -0.958973000 |
| H  | 6.719083000  | -2.010059000 | -1.389629000 |
| H  | 6.263794000  | -2.367074000 | 0.310744000  |
| H  | 0.914522000  | 0.747099000  | -1.454246000 |
| Ge | -0.905550000 | -0.386197000 | -0.012846000 |
| C  | -1.606989000 | 1.371591000  | -0.942937000 |
| C  | -3.020748000 | 1.953749000  | -0.888545000 |
| C  | -0.289701000 | 0.347805000  | 1.788519000  |
| C  | -1.265659000 | 1.231338000  | 2.577513000  |
| C  | -2.660215000 | -1.420415000 | 0.023431000  |
| C  | -3.012805000 | -2.049124000 | -1.335706000 |
| F  | 0.077730000  | -0.636631000 | 2.621131000  |
| F  | 0.827910000  | 1.101702000  | 1.542750000  |
| F  | -0.856872000 | 1.391128000  | 3.828623000  |
| F  | -2.460399000 | 0.650334000  | 2.592678000  |
| F  | -1.375048000 | 2.428641000  | 2.021873000  |
| F  | -0.774623000 | 2.376921000  | -0.521543000 |
| F  | -1.340486000 | 1.218548000  | -2.274768000 |
| F  | -3.044376000 | 3.159418000  | -1.454319000 |
| F  | -3.864620000 | 1.176336000  | -1.554297000 |
| F  | -3.438350000 | 2.081364000  | 0.363111000  |
| F  | -2.398393000 | -3.210623000 | -1.485509000 |
| F  | -2.594801000 | -1.232667000 | -2.311370000 |
| F  | -4.314448000 | -2.230142000 | -1.473341000 |
| F  | -2.648175000 | -2.402911000 | 0.940855000  |
| F  | -3.660036000 | -0.573772000 | 0.350220000  |
| C  | 1.766100000  | -2.056586000 | 0.250286000  |
| S  | 0.179742000  | -2.678137000 | 0.407540000  |
| S  | 3.114860000  | -2.711907000 | 0.950391000  |

**Adduct-3-Sn (CS<sub>2</sub>):** E= -3252.7024794 (-3248.1745247)

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 1.983230000 | -0.964286000 | -0.605355000 |
| N | 3.543730000 | 2.315575000  | -0.872868000 |
| N | 5.728477000 | -0.608298000 | -0.575665000 |
| C | 3.127169000 | -0.250943000 | -0.648420000 |
| C | 3.684333000 | 1.007320000  | -0.756403000 |
| C | 4.502440000 | -0.123439000 | -0.629232000 |
| C | 0.834196000 | -0.402095000 | -1.321793000 |
| H | 0.622124000 | -1.002688000 | -2.219088000 |
| C | 4.663399000 | 3.177269000  | -1.206499000 |
| H | 4.385420000 | 3.832820000  | -2.044757000 |
| H | 4.946488000 | 3.807247000  | -0.348652000 |
| H | 5.523782000 | 2.572643000  | -1.515003000 |
| C | 2.240363000 | 2.948286000  | -0.700311000 |
| H | 2.373889000 | 3.888271000  | -0.146964000 |
| H | 1.765921000 | 3.168864000  | -1.668470000 |
| H | 1.582230000 | 2.300692000  | -0.112332000 |
| C | 6.861971000 | 0.271301000  | -0.353739000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 7.442678000  | 0.418134000  | -1.279003000 |
| H  | 6.518112000  | 1.241500000  | 0.022815000  |
| H  | 7.522236000  | -0.173392000 | 0.404607000  |
| C  | 6.028665000  | -2.021032000 | -0.765664000 |
| H  | 5.123055000  | -2.555359000 | -1.065445000 |
| H  | 6.805828000  | -2.114632000 | -1.539779000 |
| H  | 6.391232000  | -2.466573000 | 0.172032000  |
| H  | 1.071762000  | 0.621034000  | -1.637405000 |
| Sn | -0.904618000 | -0.413275000 | 0.002634000  |
| C  | -1.646618000 | 1.406847000  | -1.169449000 |
| C  | -2.988931000 | 2.099536000  | -0.980279000 |
| C  | -0.130124000 | 0.464463000  | 1.905421000  |
| C  | -0.850294000 | 1.675377000  | 2.490008000  |
| C  | -2.848837000 | -1.476162000 | 0.224174000  |
| C  | -3.352889000 | -2.123070000 | -1.063580000 |
| F  | -0.076559000 | -0.460464000 | 2.878695000  |
| F  | 1.159264000  | 0.863084000  | 1.653159000  |
| F  | -0.331985000 | 2.034514000  | 3.656780000  |
| F  | -2.133106000 | 1.383924000  | 2.667111000  |
| F  | -0.754664000 | 2.707132000  | 1.656415000  |
| F  | -0.691705000 | 2.382319000  | -1.011139000 |
| F  | -1.578378000 | 1.040726000  | -2.482944000 |
| F  | -3.070838000 | 3.207850000  | -1.713793000 |
| F  | -3.978709000 | 1.294103000  | -1.339600000 |
| F  | -3.152048000 | 2.436995000  | 0.295342000  |
| F  | -2.569158000 | -3.144766000 | -1.389044000 |
| F  | -3.301013000 | -1.234570000 | -2.056504000 |
| F  | -4.597375000 | -2.556994000 | -0.948180000 |
| F  | -2.763040000 | -2.444830000 | 1.157672000  |
| F  | -3.785985000 | -0.587986000 | 0.628017000  |
| C  | 1.888076000  | -2.107833000 | 0.229500000  |
| S  | 0.307148000  | -2.728981000 | 0.508795000  |
| S  | 3.250244000  | -2.748522000 | 0.918247000  |

#### PhNCO activation

**TS-2 (PhNCO):** E= -2627.7222453 (-2624.1017774) (i = -142 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.128366000 | -1.193023000 | -1.661356000 |
| C  | -1.155907000 | -2.462193000 | -1.815955000 |
| C  | 0.077446000  | -0.434237000 | -1.915836000 |
| H  | -0.191652000 | 0.524880000  | -2.383579000 |
| H  | 0.789535000  | -0.943498000 | -2.577587000 |
| Si | 0.962001000  | -0.005846000 | -0.295725000 |
| C  | 2.790648000  | -0.606980000 | -0.687150000 |
| C  | 4.037993000  | -0.006575000 | -0.019628000 |
| C  | 0.306823000  | -1.161279000 | 1.136894000  |
| C  | 1.117542000  | -1.145736000 | 2.441863000  |
| C  | 1.048479000  | 1.853985000  | 0.281683000  |
| C  | 1.116130000  | 2.811209000  | -0.919067000 |
| F  | -0.960413000 | -0.857769000 | 1.468183000  |
| F  | 0.316991000  | -2.443323000 | 0.686050000  |
| F  | 0.448947000  | -1.735235000 | 3.416487000  |
| F  | 1.361281000  | 0.115351000  | 2.785511000  |
| F  | 2.267630000  | -1.776467000 | 2.268638000  |
| F  | 2.817078000  | -1.943509000 | -0.441394000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| F | 2.989451000  | -0.449567000 | -2.021521000 |
| F | 5.098737000  | -0.741488000 | -0.321316000 |
| F | 4.237481000  | 1.224176000  | -0.464224000 |
| F | 3.904157000  | 0.019456000  | 1.297740000  |
| F | -0.063743000 | 2.937032000  | -1.500118000 |
| F | 1.962392000  | 2.277331000  | -1.812781000 |
| F | 1.559953000  | 4.001807000  | -0.571362000 |
| F | 0.055375000  | 2.233559000  | 1.091906000  |
| F | 2.209086000  | 2.023860000  | 0.960394000  |
| C | -2.421972000 | 0.102557000  | -0.736869000 |
| H | -2.632665000 | -3.917533000 | -2.312677000 |
| H | -2.155806000 | -3.878513000 | -0.607249000 |
| H | -3.229288000 | -2.587892000 | -1.248969000 |
| C | 0.033162000  | -3.253507000 | -2.304152000 |
| H | 0.926052000  | -3.037996000 | -1.699312000 |
| H | -0.173150000 | -4.328404000 | -2.251149000 |
| H | 0.262473000  | -2.997432000 | -3.350256000 |
| O | -1.630313000 | 0.935655000  | -0.434882000 |
| N | -3.538333000 | -0.415461000 | -0.823994000 |
| C | -2.386685000 | -3.244375000 | -1.478467000 |
| C | -4.689079000 | 0.131988000  | -0.217839000 |
| C | -5.904619000 | -0.531706000 | -0.417434000 |
| C | -4.657372000 | 1.291798000  | 0.569549000  |
| C | -7.072798000 | -0.044623000 | 0.161696000  |
| C | -5.831101000 | 1.771439000  | 1.144966000  |
| C | -7.042113000 | 1.108562000  | 0.945500000  |
| H | -5.911980000 | -1.430542000 | -1.035158000 |
| H | -3.710466000 | 1.810620000  | 0.728975000  |
| H | -8.015098000 | -0.570286000 | -0.001137000 |
| H | -5.797730000 | 2.673931000  | 1.757607000  |
| H | -7.957948000 | 1.489763000  | 1.398886000  |

**TS-3-Si (PhNCO):** E= -2893.1854104 (-2889.1062882) (i = -197 cm<sup>-1</sup>)

|   |              |             |              |
|---|--------------|-------------|--------------|
| N | 1.016700000  | 0.509718000 | -1.628454000 |
| N | 1.312158000  | 4.050024000 | -0.400349000 |
| N | 4.286298000  | 1.935078000 | -0.979990000 |
| C | 1.678259000  | 1.541524000 | -1.236857000 |
| C | 1.840478000  | 2.865460000 | -0.757434000 |
| C | 2.944921000  | 2.091107000 | -0.975926000 |
| C | -0.412561000 | 0.573062000 | -1.778138000 |
| H | -0.728956000 | 0.009151000 | -2.673516000 |
| C | 2.194757000  | 5.097621000 | 0.061743000  |
| H | 1.689042000  | 6.067554000 | -0.040198000 |
| H | 2.486808000  | 4.968413000 | 1.120353000  |
| H | 3.102340000  | 5.119737000 | -0.556340000 |
| C | -0.087297000 | 4.141064000 | -0.035644000 |
| H | -0.245774000 | 4.022446000 | 1.049839000  |
| H | -0.487254000 | 5.115586000 | -0.350613000 |
| H | -0.652366000 | 3.352076000 | -0.542476000 |
| C | 5.111641000  | 3.046382000 | -0.565046000 |
| H | 5.208335000  | 3.821347000 | -1.349972000 |
| H | 4.691149000  | 3.505805000 | 0.339478000  |
| H | 6.118158000  | 2.676815000 | -0.324497000 |
| C | 4.854699000  | 1.021978000 | -1.958159000 |
| H | 4.138815000  | 0.211684000 | -2.138861000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 5.077604000  | 1.539025000  | -2.909005000 |
| H  | 5.785487000  | 0.588097000  | -1.564629000 |
| H  | -0.793458000 | 1.601115000  | -1.924716000 |
| Si | -1.419520000 | -0.120501000 | -0.330478000 |
| C  | -2.955679000 | 1.095957000  | -0.298997000 |
| C  | -4.328989000 | 0.755073000  | 0.300907000  |
| C  | -0.414851000 | 0.166311000  | 1.310176000  |
| C  | -1.176636000 | 0.057869000  | 2.636415000  |
| C  | -2.129676000 | -1.937656000 | -0.312172000 |
| C  | -2.563469000 | -2.405743000 | -1.709003000 |
| F  | 0.605863000  | -0.712402000 | 1.382446000  |
| F  | 0.114620000  | 1.417262000  | 1.265268000  |
| F  | -0.341272000 | 0.059969000  | 3.661709000  |
| F  | -1.872549000 | -1.073671000 | 2.648965000  |
| F  | -2.010893000 | 1.079191000  | 2.766197000  |
| F  | -2.529003000 | 2.219506000  | 0.342992000  |
| F  | -3.203447000 | 1.449610000  | -1.586294000 |
| F  | -5.079659000 | 1.849683000  | 0.326919000  |
| F  | -4.941784000 | -0.151884000 | -0.442448000 |
| F  | -4.206324000 | 0.302360000  | 1.539737000  |
| F  | -1.524088000 | -2.692254000 | -2.469967000 |
| F  | -3.232250000 | -1.394536000 | -2.281585000 |
| F  | -3.358051000 | -3.457357000 | -1.644376000 |
| F  | -1.317678000 | -2.851589000 | 0.231143000  |
| F  | -3.262238000 | -1.919298000 | 0.438082000  |
| C  | 1.761511000  | -1.468133000 | -0.947027000 |
| O  | 0.749886000  | -2.029900000 | -1.147743000 |
| N  | 2.893836000  | -1.146855000 | -0.614050000 |
| C  | 3.844075000  | -1.910372000 | 0.079077000  |
| C  | 3.760551000  | -3.306194000 | 0.172180000  |
| C  | 4.911182000  | -1.239342000 | 0.687572000  |
| C  | 4.737850000  | -4.015777000 | 0.864432000  |
| C  | 5.883022000  | -1.958100000 | 1.378729000  |
| C  | 5.803623000  | -3.347817000 | 1.468211000  |
| H  | 2.925184000  | -3.826684000 | -0.300740000 |
| H  | 4.940613000  | -0.150470000 | 0.616598000  |
| H  | 4.664579000  | -5.102469000 | 0.932122000  |
| H  | 6.708321000  | -1.427639000 | 1.856975000  |
| H  | 6.566948000  | -3.908085000 | 2.009407000  |

**TS-3-Ge (PhNCO) :** E= -4680.7078037 (-4675.6607897) (i = 202 cm<sup>-1</sup>)

|   |              |             |              |
|---|--------------|-------------|--------------|
| N | 1.132652000  | 0.604852000 | -1.655795000 |
| N | 1.555820000  | 3.990164000 | -0.088325000 |
| N | 4.456058000  | 1.854952000 | -0.986479000 |
| C | 1.835658000  | 1.574140000 | -1.179188000 |
| C | 2.051839000  | 2.847965000 | -0.598777000 |
| C | 3.125182000  | 2.058408000 | -0.906352000 |
| C | -0.290277000 | 0.746175000 | -1.777515000 |
| H | -0.646793000 | 0.285876000 | -2.713553000 |
| C | 2.399929000  | 5.161889000 | -0.003066000 |
| H | 2.353819000  | 5.777037000 | -0.920202000 |
| H | 2.086338000  | 5.783205000 | 0.847693000  |
| H | 3.440732000  | 4.858183000 | 0.158713000  |
| C | 0.122952000  | 4.202786000 | -0.103860000 |
| H | -0.144074000 | 4.919322000 | 0.685136000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | -0.232869000 | 4.601315000  | -1.071498000 |
| H  | -0.392569000 | 3.261833000  | 0.113783000  |
| C  | 5.355533000  | 2.897834000  | -0.546544000 |
| H  | 5.445047000  | 3.720433000  | -1.281072000 |
| H  | 5.010335000  | 3.308031000  | 0.412073000  |
| H  | 6.354590000  | 2.467522000  | -0.391165000 |
| C  | 4.936426000  | 0.962768000  | -2.029108000 |
| H  | 4.174898000  | 0.195208000  | -2.211705000 |
| H  | 5.142747000  | 1.511440000  | -2.965580000 |
| H  | 5.861798000  | 0.469026000  | -1.698144000 |
| H  | -0.635042000 | 1.795922000  | -1.794152000 |
| Ge | -1.326823000 | -0.095740000 | -0.318900000 |
| C  | -2.859982000 | 1.240965000  | -0.139703000 |
| C  | -4.239584000 | 0.868399000  | 0.415459000  |
| C  | -0.278081000 | 0.099094000  | 1.399029000  |
| C  | -1.068178000 | -0.101216000 | 2.698167000  |
| C  | -2.170752000 | -1.932533000 | -0.433537000 |
| C  | -2.567510000 | -2.283913000 | -1.872563000 |
| F  | 0.756069000  | -0.763910000 | 1.443709000  |
| F  | 0.233819000  | 1.356609000  | 1.424876000  |
| F  | -0.258856000 | -0.199096000 | 3.739571000  |
| F  | -1.782490000 | -1.219259000 | 2.601404000  |
| F  | -1.892808000 | 0.916155000  | 2.894203000  |
| F  | -2.401438000 | 2.268752000  | 0.624173000  |
| F  | -3.083858000 | 1.744146000  | -1.381155000 |
| F  | -4.969787000 | 1.963499000  | 0.585843000  |
| F  | -4.870947000 | 0.074516000  | -0.435199000 |
| F  | -4.124672000 | 0.256536000  | 1.585794000  |
| F  | -1.502453000 | -2.531649000 | -2.614071000 |
| F  | -3.200614000 | -1.226295000 | -2.395664000 |
| F  | -3.377259000 | -3.326058000 | -1.913877000 |
| F  | -1.413591000 | -2.918064000 | 0.062118000  |
| F  | -3.320602000 | -1.912419000 | 0.281844000  |
| C  | 1.766951000  | -1.416698000 | -0.949693000 |
| O  | 0.703420000  | -1.900001000 | -1.089125000 |
| N  | 2.932270000  | -1.180055000 | -0.672353000 |
| C  | 3.830723000  | -1.978542000 | 0.052713000  |
| C  | 3.632034000  | -3.354305000 | 0.227973000  |
| C  | 4.958173000  | -1.364600000 | 0.609006000  |
| C  | 4.558367000  | -4.102267000 | 0.949066000  |
| C  | 5.878475000  | -2.121466000 | 1.329443000  |
| C  | 5.685533000  | -3.492203000 | 1.500247000  |
| H  | 2.748245000  | -3.828818000 | -0.203227000 |
| H  | 5.075195000  | -0.287391000 | 0.478084000  |
| H  | 4.395939000  | -5.173091000 | 1.082062000  |
| H  | 6.752098000  | -1.635304000 | 1.766890000  |
| H  | 6.407839000  | -4.082682000 | 2.065027000  |

**TS-3-Sn (PhNCO) :** E= -2817.9214659 (-2813.6986646) (i = -228 cm-1)

|   |             |             |              |
|---|-------------|-------------|--------------|
| N | 1.196456000 | 0.433690000 | -1.961680000 |
| N | 1.186212000 | 3.942592000 | -0.635588000 |
| N | 4.306704000 | 1.980645000 | -0.880504000 |
| C | 1.778762000 | 1.480465000 | -1.475034000 |
| C | 1.807627000 | 2.795329000 | -0.945788000 |
| C | 2.970376000 | 2.078028000 | -1.043819000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -0.221634000 | 0.473579000  | -2.175658000 |
| H  | -0.514087000 | -0.227520000 | -2.970335000 |
| C  | 1.947697000  | 5.012503000  | -0.028830000 |
| H  | 1.422441000  | 5.964074000  | -0.187542000 |
| H  | 2.080622000  | 4.865768000  | 1.058386000  |
| H  | 2.935354000  | 5.085646000  | -0.503189000 |
| C  | -0.257230000 | 3.996251000  | -0.502054000 |
| H  | -0.577600000 | 3.913889000  | 0.547818000  |
| H  | -0.633100000 | 4.940678000  | -0.922106000 |
| H  | -0.714589000 | 3.171477000  | -1.061034000 |
| C  | 5.023178000  | 3.113015000  | -0.337826000 |
| H  | 5.184163000  | 3.911858000  | -1.087002000 |
| H  | 4.471578000  | 3.529790000  | 0.515384000  |
| H  | 6.005600000  | 2.776901000  | 0.021682000  |
| C  | 5.034753000  | 1.112190000  | -1.791404000 |
| H  | 4.390494000  | 0.267822000  | -2.067000000 |
| H  | 5.339714000  | 1.653804000  | -2.704830000 |
| H  | 5.933875000  | 0.722610000  | -1.292931000 |
| H  | -0.618574000 | 1.467791000  | -2.442241000 |
| Sn | -1.231846000 | -0.163221000 | -0.356388000 |
| C  | -2.867784000 | 1.377600000  | -0.092328000 |
| C  | -4.276704000 | 0.934838000  | 0.288933000  |
| C  | 0.034489000  | 0.410199000  | 1.394259000  |
| C  | -0.598726000 | 0.061775000  | 2.738612000  |
| C  | -2.191036000 | -2.147696000 | -0.052165000 |
| C  | -2.621698000 | -2.769909000 | -1.381000000 |
| F  | 1.270686000  | -0.132010000 | 1.386364000  |
| F  | 0.198375000  | 1.762288000  | 1.366976000  |
| F  | 0.129161000  | 0.495993000  | 3.755651000  |
| F  | -0.727654000 | -1.256729000 | 2.832997000  |
| F  | -1.809117000 | 0.606820000  | 2.813683000  |
| F  | -2.504523000 | 2.331021000  | 0.801756000  |
| F  | -2.980583000 | 2.001546000  | -1.303425000 |
| F  | -5.126362000 | 1.954780000  | 0.250027000  |
| F  | -4.698537000 | 0.006173000  | -0.564728000 |
| F  | -4.283033000 | 0.429564000  | 1.513352000  |
| F  | -1.554240000 | -3.073086000 | -2.108582000 |
| F  | -3.344446000 | -1.878503000 | -2.065490000 |
| F  | -3.347932000 | -3.859704000 | -1.208367000 |
| F  | -1.386952000 | -3.025690000 | 0.568830000  |
| F  | -3.305121000 | -2.007241000 | 0.701732000  |
| C  | 1.824371000  | -1.404847000 | -0.882387000 |
| O  | 0.726134000  | -1.839228000 | -0.765202000 |
| N  | 3.019376000  | -1.221894000 | -0.797617000 |
| C  | 4.038572000  | -1.879207000 | -0.092595000 |
| C  | 4.245419000  | -3.256691000 | -0.221906000 |
| C  | 4.876241000  | -1.119934000 | 0.731664000  |
| C  | 5.284492000  | -3.866610000 | 0.476899000  |
| C  | 5.908063000  | -1.741879000 | 1.430061000  |
| C  | 6.118917000  | -3.115057000 | 1.303904000  |
| H  | 3.590305000  | -3.839106000 | -0.871377000 |
| H  | 4.686905000  | -0.048203000 | 0.815213000  |
| H  | 5.440792000  | -4.941554000 | 0.374012000  |
| H  | 6.551832000  | -1.147336000 | 2.080484000  |
| H  | 6.929874000  | -3.599405000 | 1.849111000  |

**Adduct-2 (PhNCO):** E= -2627.7569655 (-2624.1363629)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.182395000 | -1.771840000 | -1.324878000 |
| C  | -1.505733000 | -3.025893000 | -1.259999000 |
| C  | 0.113653000  | -1.259510000 | -1.767040000 |
| H  | -0.008768000 | -0.671559000 | -2.688235000 |
| H  | 0.835647000  | -2.063456000 | -1.919717000 |
| Si | 0.632869000  | -0.101951000 | -0.280160000 |
| C  | 2.519663000  | -0.200285000 | -0.999582000 |
| C  | 3.716571000  | 0.703715000  | -0.674859000 |
| C  | 0.612492000  | -1.450415000 | 1.145375000  |
| C  | 1.490971000  | -1.239169000 | 2.377683000  |
| C  | 0.706466000  | 1.679651000  | 0.537778000  |
| C  | 0.488591000  | 2.779844000  | -0.529972000 |
| F  | -0.660084000 | -1.603512000 | 1.603953000  |
| F  | 0.965976000  | -2.660240000 | 0.619535000  |
| F  | 1.338627000  | -2.236943000 | 3.238141000  |
| F  | 1.154875000  | -0.104707000 | 2.975294000  |
| F  | 2.764202000  | -1.177196000 | 2.018535000  |
| F  | 2.956960000  | -1.476208000 | -0.796447000 |
| F  | 2.379261000  | -0.062501000 | -2.357196000 |
| F  | 4.750141000  | 0.355788000  | -1.437402000 |
| F  | 3.418106000  | 1.971160000  | -0.947504000 |
| F  | 4.090416000  | 0.599128000  | 0.587801000  |
| F  | -0.772131000 | 3.176820000  | -0.559553000 |
| F  | 0.773305000  | 2.247339000  | -1.735731000 |
| F  | 1.266477000  | 3.828545000  | -0.351503000 |
| F  | -0.227836000 | 1.846018000  | 1.499831000  |
| F  | 1.903889000  | 1.887534000  | 1.126738000  |
| C  | -1.979377000 | -0.673228000 | -0.736553000 |
| H  | -3.602907000 | -3.376911000 | -1.135644000 |
| H  | -2.574858000 | -4.572718000 | -0.282526000 |
| H  | -2.866559000 | -2.927106000 | 0.398905000  |
| C  | -0.621054000 | -4.042989000 | -1.903703000 |
| H  | 0.220794000  | -4.246270000 | -1.219558000 |
| H  | -1.170991000 | -4.977185000 | -2.059737000 |
| H  | -0.208798000 | -3.686890000 | -2.855357000 |
| O  | -1.187775000 | 0.241083000  | -0.276142000 |
| N  | -3.234798000 | -0.761545000 | -0.798552000 |
| C  | -2.704612000 | -3.509575000 | -0.515162000 |
| C  | -4.120585000 | 0.199364000  | -0.275203000 |
| C  | -5.480995000 | -0.038779000 | -0.523824000 |
| C  | -3.749050000 | 1.335913000  | 0.466041000  |
| C  | -6.456359000 | 0.830732000  | -0.049454000 |
| C  | -4.735341000 | 2.199019000  | 0.938835000  |
| C  | -6.085050000 | 1.956146000  | 0.686597000  |
| H  | -5.748043000 | -0.924057000 | -1.102530000 |
| H  | -2.701184000 | 1.542808000  | 0.672213000  |
| H  | -7.509242000 | 0.629989000  | -0.253444000 |
| H  | -4.439052000 | 3.076909000  | 1.515238000  |
| H  | -6.844812000 | 2.642294000  | 1.063616000  |

**Adduct-3-Si (PhNCO):** E= -2893.2425057 (-2889.1632589)

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | -1.424043000 | -0.576120000 | -0.955799000 |
| N | -2.404539000 | -4.034693000 | -0.452470000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -5.026978000 | -1.443163000 | -0.535311000 |
| C  | -2.413507000 | -1.443854000 | -0.775631000 |
| C  | -2.769358000 | -2.766797000 | -0.586276000 |
| C  | -3.748209000 | -1.775647000 | -0.612626000 |
| C  | -0.077277000 | -1.012458000 | -1.315258000 |
| H  | 0.102084000  | -0.869986000 | -2.391937000 |
| C  | -3.369723000 | -5.115123000 | -0.529571000 |
| H  | -3.016597000 | -5.878842000 | -1.238304000 |
| H  | -3.514617000 | -5.590603000 | 0.453585000  |
| H  | -4.330580000 | -4.732727000 | -0.892585000 |
| C  | -1.005778000 | -4.390064000 | -0.240800000 |
| H  | -0.964222000 | -5.266944000 | 0.419595000  |
| H  | -0.501630000 | -4.637741000 | -1.188145000 |
| H  | -0.475404000 | -3.567969000 | 0.255513000  |
| C  | -6.026599000 | -2.446754000 | -0.225647000 |
| H  | -6.495754000 | -2.850010000 | -1.139052000 |
| H  | -5.572565000 | -3.266530000 | 0.344310000  |
| H  | -6.811196000 | -1.992902000 | 0.395223000  |
| C  | -5.492257000 | -0.130856000 | -0.964029000 |
| H  | -4.628014000 | 0.541140000  | -1.043888000 |
| H  | -6.017031000 | -0.208092000 | -1.929787000 |
| H  | -6.189187000 | 0.269784000  | -0.214005000 |
| H  | 0.060018000  | -2.072001000 | -1.081066000 |
| Si | 1.077383000  | 0.069462000  | -0.222187000 |
| C  | 2.530342000  | -1.320529000 | -0.566996000 |
| C  | 4.041412000  | -1.250365000 | -0.312094000 |
| C  | 0.554219000  | -0.439811000 | 1.606912000  |
| C  | 1.629870000  | -0.522753000 | 2.697741000  |
| C  | 2.185636000  | 1.687399000  | -0.314127000 |
| C  | 2.357057000  | 2.216360000  | -1.745765000 |
| F  | -0.379308000 | 0.416971000  | 2.076276000  |
| F  | -0.051787000 | -1.669092000 | 1.558577000  |
| F  | 1.076745000  | -0.556320000 | 3.903626000  |
| F  | 2.411189000  | 0.549555000  | 2.620430000  |
| F  | 2.371587000  | -1.608880000 | 2.554749000  |
| F  | 2.107621000  | -2.458789000 | 0.073624000  |
| F  | 2.443508000  | -1.610593000 | -1.905548000 |
| F  | 4.589047000  | -2.450634000 | -0.506401000 |
| F  | 4.614170000  | -0.407424000 | -1.161996000 |
| F  | 4.317324000  | -0.876104000 | 0.928420000  |
| F  | 1.268490000  | 2.853827000  | -2.156060000 |
| F  | 2.555644000  | 1.174896000  | -2.563647000 |
| F  | 3.389645000  | 3.034590000  | -1.853298000 |
| F  | 1.680652000  | 2.691517000  | 0.431636000  |
| F  | 3.431167000  | 1.443245000  | 0.152696000  |
| C  | -1.510628000 | 0.798389000  | -0.551183000 |
| O  | -0.325325000 | 1.291340000  | -0.386270000 |
| N  | -2.657180000 | 1.319286000  | -0.380240000 |
| C  | -2.818790000 | 2.645892000  | 0.057030000  |
| C  | -1.891171000 | 3.679249000  | -0.165313000 |
| C  | -4.018381000 | 2.952254000  | 0.717868000  |
| C  | -2.174518000 | 4.973211000  | 0.264865000  |
| C  | -4.289038000 | 4.246005000  | 1.152127000  |
| C  | -3.367337000 | 5.267171000  | 0.924424000  |
| H  | -0.948249000 | 3.466109000  | -0.665068000 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| H | -4.731292000 | 2.145636000 | 0.895364000 |
| H | -1.443282000 | 5.763184000 | 0.084683000 |
| H | -5.225528000 | 4.457763000 | 1.671174000 |
| H | -3.575553000 | 6.283970000 | 1.260236000 |

**Adduct-3-Ge (PhNCO):** E= -4680.7498363 (-4675.7008226)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.402388000  | 0.523033000  | -1.164546000 |
| N  | 2.034360000  | 4.058477000  | -0.526279000 |
| N  | 4.886784000  | 1.734370000  | -0.654769000 |
| C  | 2.289294000  | 1.487922000  | -0.939220000 |
| C  | 2.511492000  | 2.831720000  | -0.695054000 |
| C  | 3.582035000  | 1.941449000  | -0.740482000 |
| C  | 0.023873000  | 0.856081000  | -1.505824000 |
| H  | -0.199220000 | 0.580220000  | -2.547590000 |
| C  | 2.903673000  | 5.219072000  | -0.555479000 |
| H  | 2.496250000  | 5.971712000  | -1.246976000 |
| H  | 2.993960000  | 5.675048000  | 0.443438000  |
| H  | 3.898943000  | 4.931715000  | -0.913356000 |
| C  | 0.610444000  | 4.290878000  | -0.319240000 |
| H  | 0.488501000  | 5.103903000  | 0.409907000  |
| H  | 0.106788000  | 4.580403000  | -1.255320000 |
| H  | 0.132735000  | 3.395967000  | 0.096250000  |
| C  | 5.774734000  | 2.812007000  | -0.265696000 |
| H  | 6.230628000  | 3.302693000  | -1.142517000 |
| H  | 5.227500000  | 3.555858000  | 0.326000000  |
| H  | 6.581082000  | 2.404959000  | 0.360044000  |
| C  | 5.491244000  | 0.506933000  | -1.155012000 |
| H  | 4.704550000  | -0.249342000 | -1.273233000 |
| H  | 6.004167000  | 0.697130000  | -2.111688000 |
| H  | 6.228734000  | 0.142504000  | -0.425829000 |
| H  | -0.148015000 | 1.930885000  | -1.390357000 |
| Ge | -1.087905000 | -0.168265000 | -0.224531000 |
| C  | -2.599857000 | 1.273754000  | -0.387319000 |
| C  | -4.053953000 | 1.146628000  | 0.073712000  |
| C  | -0.327991000 | 0.309586000  | 1.604055000  |
| C  | -1.301613000 | 0.390881000  | 2.785478000  |
| C  | -2.165498000 | -1.865850000 | -0.420397000 |
| C  | -2.460191000 | -2.200109000 | -1.884392000 |
| F  | 0.640604000  | -0.546606000 | 1.970142000  |
| F  | 0.262550000  | 1.540432000  | 1.483485000  |
| F  | -0.650808000 | 0.412514000  | 3.940106000  |
| F  | -2.094782000 | -0.676552000 | 2.765475000  |
| F  | -2.045576000 | 1.483014000  | 2.707223000  |
| F  | -2.097821000 | 2.396910000  | 0.217797000  |
| F  | -2.669891000 | 1.580304000  | -1.717199000 |
| F  | -4.654772000 | 2.334666000  | 0.055568000  |
| F  | -4.719812000 | 0.338448000  | -0.738439000 |
| F  | -4.125392000 | 0.670039000  | 1.310657000  |
| F  | -1.338122000 | -2.499254000 | -2.526632000 |
| F  | -2.997435000 | -1.127395000 | -2.469837000 |
| F  | -3.301927000 | -3.212800000 | -1.998777000 |
| F  | -1.569317000 | -2.933290000 | 0.133704000  |
| F  | -3.363724000 | -1.704700000 | 0.189198000  |
| C  | 1.627229000  | -0.837753000 | -0.701430000 |
| O  | 0.524706000  | -1.453002000 | -0.517062000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 2.841855000 | -1.179943000 | -0.498229000 |
| C | 3.170753000 | -2.435646000 | 0.034473000  |
| C | 2.389848000 | -3.598188000 | -0.099435000 |
| C | 4.393726000 | -2.530671000 | 0.719261000  |
| C | 2.835761000 | -4.804832000 | 0.435345000  |
| C | 4.828028000 | -3.737762000 | 1.256760000  |
| C | 4.050982000 | -4.886618000 | 1.114660000  |
| H | 1.431697000 | -3.547098000 | -0.613015000 |
| H | 4.989352000 | -1.623968000 | 0.834948000  |
| H | 2.216144000 | -5.696395000 | 0.321948000  |
| H | 5.778212000 | -3.781070000 | 1.792516000  |
| H | 4.387555000 | -5.836631000 | 1.532259000  |

**Adduct-3-Sn (PhNCO):** E= -2817.9666670 (-2813.7432043)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.505837000  | 0.432584000  | -1.290485000 |
| N  | 2.198356000  | 3.968907000  | -0.708744000 |
| N  | 5.011382000  | 1.594743000  | -0.812093000 |
| C  | 2.409907000  | 1.389503000  | -1.091797000 |
| C  | 2.654959000  | 2.732506000  | -0.866718000 |
| C  | 3.710149000  | 1.822608000  | -0.899782000 |
| C  | 0.148785000  | 0.795841000  | -1.690638000 |
| H  | -0.052551000 | 0.474331000  | -2.722987000 |
| C  | 3.085624000  | 5.115255000  | -0.753412000 |
| H  | 2.684393000  | 5.869982000  | -1.446310000 |
| H  | 3.192113000  | 5.576394000  | 0.241619000  |
| H  | 4.072918000  | 4.809162000  | -1.117893000 |
| C  | 0.781211000  | 4.225108000  | -0.486073000 |
| H  | 0.680187000  | 5.045110000  | 0.238570000  |
| H  | 0.269173000  | 4.515200000  | -1.417387000 |
| H  | 0.296485000  | 3.340834000  | -0.056788000 |
| C  | 5.915906000  | 2.661090000  | -0.430308000 |
| H  | 6.380419000  | 3.137604000  | -1.310550000 |
| H  | 5.379815000  | 3.418364000  | 0.154530000  |
| H  | 6.715231000  | 2.246527000  | 0.199556000  |
| C  | 5.599756000  | 0.359112000  | -1.312039000 |
| H  | 4.802928000  | -0.384411000 | -1.435714000 |
| H  | 6.121562000  | 0.545972000  | -2.264692000 |
| H  | 6.325739000  | -0.021684000 | -0.579819000 |
| H  | 0.016726000  | 1.882364000  | -1.635939000 |
| Sn | -1.116082000 | -0.200812000 | -0.233924000 |
| C  | -2.689397000 | 1.422422000  | -0.413950000 |
| C  | -4.073630000 | 1.296778000  | 0.207106000  |
| C  | -0.123780000 | 0.389907000  | 1.674277000  |
| C  | -1.010183000 | 0.726619000  | 2.870675000  |
| C  | -2.332610000 | -2.043835000 | -0.339073000 |
| C  | -2.743100000 | -2.350808000 | -1.777189000 |
| F  | 0.747240000  | -0.550059000 | 2.080059000  |
| F  | 0.607804000  | 1.518697000  | 1.393740000  |
| F  | -0.294767000 | 0.900965000  | 3.973496000  |
| F  | -1.867070000 | -0.270436000 | 3.074120000  |
| F  | -1.696008000 | 1.837204000  | 2.636573000  |
| F  | -2.120479000 | 2.557876000  | 0.099479000  |
| F  | -2.867302000 | 1.663366000  | -1.743133000 |
| F  | -4.727972000 | 2.454232000  | 0.200067000  |
| F  | -4.790655000 | 0.407598000  | -0.466425000 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| F | -3.966156000 | 0.888599000  | 1.470272000  |
| F | -1.666543000 | -2.633460000 | -2.503610000 |
| F | -3.318661000 | -1.266367000 | -2.302931000 |
| F | -3.590170000 | -3.361865000 | -1.854762000 |
| F | -1.698893000 | -3.121502000 | 0.150058000  |
| F | -3.472033000 | -1.867915000 | 0.371091000  |
| C | 1.731019000  | -0.908240000 | -0.749345000 |
| O | 0.649456000  | -1.551439000 | -0.555586000 |
| N | 2.953091000  | -1.196943000 | -0.498228000 |
| C | 3.314918000  | -2.412801000 | 0.095883000  |
| C | 2.610171000  | -3.620805000 | -0.054249000 |
| C | 4.496191000  | -2.421789000 | 0.856703000  |
| C | 3.088025000  | -4.788156000 | 0.536450000  |
| C | 4.962765000  | -3.590208000 | 1.450276000  |
| C | 4.261812000  | -4.785022000 | 1.289786000  |
| H | 1.685882000  | -3.633816000 | -0.628857000 |
| H | 5.028731000  | -1.477932000 | 0.986125000  |
| H | 2.528815000  | -5.716802000 | 0.407263000  |
| H | 5.878472000  | -3.568071000 | 2.044312000  |
| H | 4.624743000  | -5.704931000 | 1.750382000  |

#### Acetylene activation

**TS-2 (HC≡CH):** E= -2305.2827656 (-2302.1996411) (i = -767 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 2.209819000  | -1.541753000 | -1.262331000 |
| C  | 3.360734000  | -1.021735000 | -1.444471000 |
| C  | 0.952515000  | -1.056356000 | -1.763225000 |
| H  | 0.407877000  | -1.880650000 | -2.251519000 |
| H  | 1.041217000  | -0.209905000 | -2.450944000 |
| Si | -0.047706000 | -0.594864000 | -0.177061000 |
| C  | -1.771644000 | -1.523226000 | 0.138988000  |
| C  | -3.122601000 | -0.833194000 | -0.112810000 |
| C  | -0.551528000 | 1.174960000  | -0.979290000 |
| C  | -1.418086000 | 2.239950000  | -0.251263000 |
| C  | 1.053033000  | 0.024858000  | 1.367078000  |
| C  | 1.829026000  | 1.358283000  | 1.308609000  |
| F  | 0.641893000  | 1.778508000  | -1.274811000 |
| F  | -1.127622000 | 0.933381000  | -2.185039000 |
| F  | -0.922697000 | 3.458458000  | -0.403502000 |
| F  | -1.464740000 | 1.970817000  | 1.053350000  |
| F  | -2.654559000 | 2.235359000  | -0.722598000 |
| F  | -1.782229000 | -2.587887000 | -0.701469000 |
| F  | -1.866879000 | -1.969040000 | 1.407465000  |
| F  | -4.099916000 | -1.713224000 | 0.051859000  |
| F  | -3.304391000 | 0.157424000  | 0.747545000  |
| F  | -3.191159000 | -0.359935000 | -1.348448000 |
| F  | 1.054011000  | 2.414859000  | 1.158877000  |
| F  | 2.701197000  | 1.309194000  | 0.293408000  |
| F  | 2.518807000  | 1.514598000  | 2.428013000  |
| F  | 0.236349000  | 0.095057000  | 2.440341000  |
| F  | 2.051652000  | -0.843628000 | 1.656882000  |
| C  | 3.587018000  | 0.104594000  | -2.412694000 |
| H  | 4.643715000  | 0.393247000  | -2.439374000 |
| H  | 3.270901000  | -0.189423000 | -3.424148000 |
| H  | 2.987129000  | 0.976479000  | -2.110944000 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 4.510407000 | -1.516581000 | -0.627324000 |
| H | 4.213505000 | -2.355052000 | 0.012905000  |
| H | 5.345739000 | -1.812065000 | -1.278277000 |
| H | 4.862434000 | -0.685776000 | 0.004600000  |
| C | 0.765760000 | -2.718234000 | 0.509915000  |
| C | 0.393628000 | -3.576410000 | 1.296717000  |
| H | 0.030935000 | -4.319512000 | 1.985415000  |
| H | 1.758644000 | -2.283887000 | -0.330788000 |

**TS-3-Si (HC≡CH):** E= -2570.7484026 (-2567.2058530) (i = -829 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.361970000  | -1.375986000 | -1.708823000 |
| N  | 3.577734000  | 1.624412000  | -1.562557000 |
| N  | 4.546220000  | -1.653414000 | -0.075537000 |
| C  | 2.486877000  | -0.781606000 | -1.419504000 |
| C  | 3.339014000  | 0.325527000  | -1.327397000 |
| C  | 3.725831000  | -0.877897000 | -0.787284000 |
| C  | 0.174137000  | -0.568941000 | -1.874543000 |
| H  | -0.490937000 | -0.987474000 | -2.646774000 |
| C  | 4.520771000  | 2.338356000  | -0.725807000 |
| H  | 5.011968000  | 3.129593000  | -1.309444000 |
| H  | 4.020634000  | 2.796595000  | 0.144997000  |
| H  | 5.289998000  | 1.646521000  | -0.362527000 |
| C  | 2.556099000  | 2.415981000  | -2.224174000 |
| H  | 1.804078000  | 2.799125000  | -1.514562000 |
| H  | 3.034231000  | 3.263960000  | -2.733927000 |
| H  | 2.052679000  | 1.802245000  | -2.981794000 |
| C  | 5.776865000  | -1.122486000 | 0.468629000  |
| H  | 6.496338000  | -1.941802000 | 0.603258000  |
| H  | 6.213097000  | -0.400930000 | -0.234270000 |
| H  | 5.622372000  | -0.631020000 | 1.445492000  |
| C  | 4.010712000  | -2.869678000 | 0.517751000  |
| H  | 3.083990000  | -3.153396000 | 0.003649000  |
| H  | 4.742941000  | -3.684372000 | 0.423925000  |
| H  | 3.771610000  | -2.717264000 | 1.583192000  |
| H  | 0.402344000  | 0.470755000  | -2.152241000 |
| Si | -0.807077000 | -0.488412000 | -0.228015000 |
| C  | -2.409593000 | -1.649903000 | -0.143051000 |
| C  | -3.758724000 | -1.127992000 | -0.662689000 |
| C  | -1.537210000 | 1.351447000  | -0.543753000 |
| C  | -2.454161000 | 2.145985000  | 0.444802000  |
| C  | 0.362191000  | -0.216827000 | 1.364494000  |
| C  | 0.892936000  | 1.191578000  | 1.687568000  |
| F  | -0.453377000 | 2.152218000  | -0.777121000 |
| F  | -2.196836000 | 1.280950000  | -1.728062000 |
| F  | -1.920545000 | 3.315235000  | 0.766383000  |
| F  | -2.626331000 | 1.441630000  | 1.562708000  |
| F  | -3.637151000 | 2.395803000  | -0.090135000 |
| F  | -2.205237000 | -2.736849000 | -0.916938000 |
| F  | -2.638758000 | -2.048019000 | 1.126277000  |
| F  | -4.689349000 | -2.055061000 | -0.487191000 |
| F  | -4.134730000 | -0.037523000 | -0.010763000 |
| F  | -3.678644000 | -0.856380000 | -1.958473000 |
| F  | -0.079089000 | 2.060567000  | 1.890979000  |
| F  | 1.663849000  | 1.626854000  | 0.684816000  |
| F  | 1.641778000  | 1.147322000  | 2.780791000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| F | -0.296932000 | -0.627160000 | 2.467101000  |
| F | 1.524852000  | -0.916686000 | 1.278818000  |
| C | 0.224638000  | -2.817490000 | 0.135105000  |
| C | -0.099102000 | -3.507754000 | 1.090408000  |
| H | -0.420111000 | -4.113168000 | 1.919393000  |
| H | 0.933183000  | -2.262610000 | -0.873763000 |

**TS-3-Ge (HC≡CH) :** E= -4358.2744070 (-4353.7634476) (i = -630 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.434388000 | 1.255546000  | -1.868038000 |
| N  | -3.563076000 | -1.784381000 | -1.452205000 |
| N  | -4.579787000 | 1.551743000  | -0.155773000 |
| C  | -2.537601000 | 0.650841000  | -1.504093000 |
| C  | -3.351164000 | -0.468777000 | -1.313985000 |
| C  | -3.757149000 | 0.759343000  | -0.841307000 |
| C  | -0.224447000 | 0.484206000  | -1.986473000 |
| H  | 0.437889000  | 0.884368000  | -2.766823000 |
| C  | -4.496610000 | -2.450563000 | -0.566163000 |
| H  | -4.925584000 | -3.325405000 | -1.073873000 |
| H  | -4.004451000 | -2.783714000 | 0.363737000  |
| H  | -5.313691000 | -1.766949000 | -0.306588000 |
| C  | -2.531232000 | -2.606262000 | -2.059812000 |
| H  | -1.791114000 | -2.952819000 | -1.320469000 |
| H  | -3.000900000 | -3.477525000 | -2.537043000 |
| H  | -2.015216000 | -2.028082000 | -2.836484000 |
| C  | -5.778255000 | 1.019115000  | 0.455843000  |
| H  | -6.511244000 | 1.828296000  | 0.576375000  |
| H  | -6.221905000 | 0.255225000  | -0.195692000 |
| H  | -5.578153000 | 0.579421000  | 1.448701000  |
| C  | -4.080641000 | 2.829839000  | 0.331524000  |
| H  | -3.159892000 | 3.097920000  | -0.201239000 |
| H  | -4.837648000 | 3.611444000  | 0.173673000  |
| H  | -3.837848000 | 2.770413000  | 1.405054000  |
| H  | -0.412259000 | -0.577376000 | -2.200291000 |
| Ge | 0.751959000  | 0.500630000  | -0.236489000 |
| C  | 2.477022000  | 1.536868000  | 0.148343000  |
| C  | 3.651583000  | 1.139277000  | -0.758633000 |
| C  | 1.483895000  | -1.429475000 | -0.533353000 |
| C  | 2.443780000  | -2.192611000 | 0.432802000  |
| C  | -0.494002000 | 0.329545000  | 1.389612000  |
| C  | -0.929847000 | -1.079537000 | 1.807332000  |
| F  | 0.390686000  | -2.231777000 | -0.704610000 |
| F  | 2.087600000  | -1.375693000 | -1.749711000 |
| F  | 1.876208000  | -3.294805000 | 0.903223000  |
| F  | 2.758794000  | -1.414224000 | 1.465518000  |
| F  | 3.560750000  | -2.553328000 | -0.178504000 |
| F  | 2.369191000  | 2.860728000  | -0.013357000 |
| F  | 2.850631000  | 1.301321000  | 1.424654000  |
| F  | 4.679604000  | 1.952075000  | -0.584673000 |
| F  | 4.051548000  | -0.098279000 | -0.506522000 |
| F  | 3.264150000  | 1.210923000  | -2.031930000 |
| F  | 0.111370000  | -1.859398000 | 2.039625000  |
| F  | -1.673258000 | -1.625397000 | 0.837626000  |
| F  | -1.670846000 | -1.030181000 | 2.904863000  |
| F  | 0.106537000  | 0.878483000  | 2.462195000  |
| F  | -1.680134000 | 0.962920000  | 1.199765000  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -0.403445000 | 2.901856000 | -0.128999000 |
| C | -0.221816000 | 3.727253000 | 0.755773000  |
| H | -0.022418000 | 4.455745000 | 1.521700000  |
| H | -1.073390000 | 2.192705000 | -1.134904000 |

**TS-3-Sn (HC≡CH):** E= -2495.4986613 (-2491.8111289) (i = -950 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.593753000  | -1.408421000 | -1.767985000 |
| N  | 3.893452000  | 1.513472000  | -1.617681000 |
| N  | 4.641639000  | -1.692105000 | 0.131268000  |
| C  | 2.720622000  | -0.847471000 | -1.424788000 |
| C  | 3.605234000  | 0.233239000  | -1.333356000 |
| C  | 3.903202000  | -0.944816000 | -0.690635000 |
| C  | 0.468610000  | -0.573130000 | -2.094114000 |
| H  | -0.109251000 | -0.962659000 | -2.943132000 |
| C  | 4.774932000  | 2.249523000  | -0.733533000 |
| H  | 5.279334000  | 3.048242000  | -1.294413000 |
| H  | 4.222261000  | 2.698782000  | 0.109918000  |
| H  | 5.539736000  | 1.574211000  | -0.331225000 |
| C  | 2.924585000  | 2.281712000  | -2.380054000 |
| H  | 2.096475000  | 2.651691000  | -1.750783000 |
| H  | 3.431465000  | 3.138536000  | -2.844073000 |
| H  | 2.512879000  | 1.654725000  | -3.181077000 |
| C  | 5.830637000  | -1.149022000 | 0.751284000  |
| H  | 6.509323000  | -1.972497000 | 1.012338000  |
| H  | 6.352507000  | -0.490250000 | 0.044976000  |
| H  | 5.597029000  | -0.583886000 | 1.670832000  |
| C  | 4.046330000  | -2.876506000 | 0.731042000  |
| H  | 3.137027000  | -3.150886000 | 0.181973000  |
| H  | 4.759085000  | -3.713144000 | 0.696209000  |
| H  | 3.761822000  | -2.685234000 | 1.778439000  |
| H  | 0.736971000  | 0.476148000  | -2.290264000 |
| Sn | -0.776226000 | -0.491918000 | -0.280784000 |
| C  | -2.643538000 | -1.703828000 | -0.050356000 |
| C  | -3.917159000 | -0.999306000 | -0.512355000 |
| C  | -1.557196000 | 1.628121000  | -0.564065000 |
| C  | -2.317737000 | 2.370716000  | 0.571152000  |
| C  | 0.619980000  | -0.155378000 | 1.468170000  |
| C  | 1.203240000  | 1.253181000  | 1.582407000  |
| F  | -0.463299000 | 2.386157000  | -0.879850000 |
| F  | -2.350846000 | 1.638394000  | -1.664167000 |
| F  | -1.731784000 | 3.515609000  | 0.892046000  |
| F  | -2.344657000 | 1.600340000  | 1.665730000  |
| F  | -3.565968000 | 2.639283000  | 0.225774000  |
| F  | -2.559581000 | -2.820635000 | -0.800928000 |
| F  | -2.829676000 | -2.075020000 | 1.234963000  |
| F  | -4.982946000 | -1.767492000 | -0.353875000 |
| F  | -4.097448000 | 0.121043000  | 0.177595000  |
| F  | -3.803729000 | -0.690312000 | -1.800894000 |
| F  | 0.258015000  | 2.151678000  | 1.794200000  |
| F  | 1.830502000  | 1.560781000  | 0.436938000  |
| F  | 2.093178000  | 1.338511000  | 2.562398000  |
| F  | 0.011704000  | -0.432257000 | 2.640413000  |
| F  | 1.721296000  | -0.950291000 | 1.379053000  |
| C  | 0.338486000  | -2.880857000 | 0.005090000  |
| C  | -0.172704000 | -3.485089000 | 0.937313000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -0.647282000 | -4.020557000 | 1.741182000  |
| H | 1.102072000  | -2.306570000 | -0.944690000 |

**Adduct-2 (HC≡CH):** E= -2305.3155537 (-2302.2351467)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -2.108574000 | 1.723121000  | -1.195339000 |
| C  | -3.215898000 | 1.140925000  | -1.492859000 |
| C  | -0.762747000 | 1.366298000  | -1.607531000 |
| H  | -0.228456000 | 2.277673000  | -1.911644000 |
| H  | -0.787859000 | 0.645550000  | -2.428441000 |
| Si | 0.135895000  | 0.739566000  | 0.020530000  |
| C  | 2.029015000  | 1.378547000  | 0.214549000  |
| C  | 3.309983000  | 0.579699000  | -0.050198000 |
| C  | 0.486533000  | -1.025393000 | -0.943571000 |
| C  | 1.220652000  | -2.228343000 | -0.298916000 |
| C  | -1.208455000 | -0.031556000 | 1.326665000  |
| C  | -2.021401000 | -1.334600000 | 1.201053000  |
| F  | -0.762674000 | -1.484860000 | -1.298716000 |
| F  | 1.098970000  | -0.758274000 | -2.128650000 |
| F  | 0.601852000  | -3.377292000 | -0.537678000 |
| F  | 1.278087000  | -2.054635000 | 1.023793000  |
| F  | 2.457579000  | -2.333157000 | -0.758167000 |
| F  | 2.104547000  | 2.447543000  | -0.631882000 |
| F  | 2.194255000  | 1.838792000  | 1.476236000  |
| F  | 4.368980000  | 1.355917000  | 0.147849000  |
| F  | 3.386901000  | -0.445747000 | 0.789514000  |
| F  | 3.360996000  | 0.130450000  | -1.294934000 |
| F  | -1.281015000 | -2.413287000 | 1.046009000  |
| F  | -2.870521000 | -1.237309000 | 0.162641000  |
| F  | -2.759210000 | -1.499362000 | 2.291500000  |
| F  | -0.572647000 | -0.108508000 | 2.518654000  |
| F  | -2.226380000 | 0.881525000  | 1.471041000  |
| C  | -3.268235000 | 0.080622000  | -2.539778000 |
| H  | -4.297331000 | -0.262243000 | -2.688932000 |
| H  | -2.868034000 | 0.462480000  | -3.490641000 |
| H  | -2.642984000 | -0.769341000 | -2.227848000 |
| C  | -4.445386000 | 1.497666000  | -0.733162000 |
| H  | -4.273696000 | 2.314149000  | -0.021952000 |
| H  | -5.259685000 | 1.754756000  | -1.424514000 |
| H  | -4.752324000 | 0.600567000  | -0.172465000 |
| C  | -0.293789000 | 2.483606000  | 0.842480000  |
| C  | -0.586243000 | 3.606240000  | 1.214035000  |
| H  | -0.801604000 | 4.594606000  | 1.578893000  |
| H  | -2.112175000 | 2.407615000  | -0.423978000 |

**Adduct-3-Si (HC≡CH):** E= -2570.7911384 (-2567.2499270)

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 0.927358000  | -0.629886000 | -2.417982000 |
| N | 2.256806000  | 2.542542000  | -1.206257000 |
| N | 4.368163000  | -0.502972000 | -1.154679000 |
| C | 1.977508000  | 0.069577000  | -2.005779000 |
| C | 2.466080000  | 1.272946000  | -1.534670000 |
| C | 3.267111000  | 0.139240000  | -1.519964000 |
| C | -0.403030000 | -0.173723000 | -2.002111000 |
| H | -1.146317000 | -0.553183000 | -2.716222000 |
| C | 3.023205000  | 3.165434000  | -0.141286000 |
| H | 3.291584000  | 4.193406000  | -0.423439000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 2.434358000  | 3.184710000  | 0.789765000  |
| H  | 3.937794000  | 2.591825000  | 0.043484000  |
| C  | 1.014642000  | 3.197404000  | -1.589994000 |
| H  | 0.228815000  | 3.057238000  | -0.832314000 |
| H  | 1.208854000  | 4.271180000  | -1.716640000 |
| H  | 0.670748000  | 2.797170000  | -2.551877000 |
| C  | 5.394999000  | 0.187610000  | -0.396957000 |
| H  | 6.361009000  | -0.305346000 | -0.568508000 |
| H  | 5.475380000  | 1.226205000  | -0.741343000 |
| H  | 5.170690000  | 0.172431000  | 0.682334000  |
| C  | 4.377779000  | -1.958555000 | -1.115153000 |
| H  | 3.602776000  | -2.348424000 | -1.784508000 |
| H  | 5.358490000  | -2.323954000 | -1.449859000 |
| H  | 4.168644000  | -2.325608000 | -0.099014000 |
| H  | -0.437922000 | 0.922520000  | -2.061600000 |
| Si | -0.964228000 | -0.786837000 | -0.269127000 |
| C  | -2.972471000 | -0.763740000 | -0.671260000 |
| C  | -3.804923000 | 0.448215000  | -1.128890000 |
| C  | -1.030305000 | 0.903433000  | 0.776221000  |
| C  | -1.602118000 | 0.841923000  | 2.199145000  |
| C  | 0.838782000  | -1.322770000 | 0.822164000  |
| C  | 1.857482000  | -0.557302000 | 1.697328000  |
| F  | 0.243642000  | 1.397379000  | 0.857681000  |
| F  | -1.715901000 | 1.860480000  | 0.095859000  |
| F  | -1.113370000 | 1.801673000  | 2.975689000  |
| F  | -1.301446000 | -0.335540000 | 2.747057000  |
| F  | -2.919449000 | 0.953001000  | 2.166651000  |
| F  | -3.125264000 | -1.629066000 | -1.720334000 |
| F  | -3.646630000 | -1.292794000 | 0.387320000  |
| F  | -4.934352000 | 0.048883000  | -1.709352000 |
| F  | -4.142742000 | 1.248651000  | -0.131534000 |
| F  | -3.121018000 | 1.154312000  | -2.039714000 |
| F  | 1.297723000  | 0.010257000  | 2.751102000  |
| F  | 2.535938000  | 0.390055000  | 1.024481000  |
| F  | 2.790894000  | -1.406369000 | 2.144950000  |
| F  | 0.439503000  | -2.297282000 | 1.684124000  |
| F  | 1.675466000  | -1.951497000 | -0.095339000 |
| C  | -1.053532000 | -2.659507000 | -0.471821000 |
| C  | -1.069679000 | -3.860055000 | -0.652776000 |
| H  | -1.099902000 | -4.923722000 | -0.802467000 |
| H  | 1.051801000  | -1.638610000 | -2.380568000 |

**Adduct-3-Ge (HC≡CH):** E= -4358.3006509 (-4353.7884811)

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 1.163367000  | -1.235217000 | -2.191290000 |
| N | 2.720537000  | 2.031737000  | -1.701188000 |
| N | 4.373344000  | -1.006328000 | -0.388081000 |
| C | 2.212736000  | -0.536438000 | -1.774948000 |
| C | 2.780455000  | 0.709108000  | -1.576526000 |
| C | 3.408699000  | -0.426788000 | -1.087217000 |
| C | -0.155371000 | -0.586460000 | -2.132793000 |
| H | -0.832460000 | -1.081942000 | -2.840203000 |
| C | 3.268246000  | 2.883127000  | -0.658271000 |
| H | 3.700805000  | 3.789411000  | -1.104448000 |
| H | 2.473538000  | 3.164227000  | 0.052058000  |
| H | 4.050207000  | 2.345231000  | -0.110096000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 1.707009000  | 2.627758000  | -2.558757000 |
| H  | 0.787872000  | 2.858868000  | -2.000197000 |
| H  | 2.113372000  | 3.550795000  | -2.995643000 |
| H  | 1.469381000  | 1.935548000  | -3.376044000 |
| C  | 5.399683000  | -0.202018000 | 0.247205000  |
| H  | 6.339410000  | -0.770431000 | 0.275855000  |
| H  | 5.568544000  | 0.711962000  | -0.335237000 |
| H  | 5.113874000  | 0.067127000  | 1.277581000  |
| C  | 4.244821000  | -2.387300000 | 0.049982000  |
| H  | 3.467388000  | -2.890377000 | -0.535367000 |
| H  | 5.203073000  | -2.906171000 | -0.094110000 |
| H  | 3.954459000  | -2.435383000 | 1.110657000  |
| H  | -0.047554000 | 0.461138000  | -2.430505000 |
| Ge | -0.886723000 | -0.821883000 | -0.265381000 |
| C  | -2.893687000 | -1.010863000 | 0.130284000  |
| C  | -3.798923000 | -0.160090000 | -0.765899000 |
| C  | -0.849096000 | 1.354038000  | -0.055761000 |
| C  | -1.403797000 | 2.268058000  | 1.073365000  |
| C  | 0.544304000  | -1.134630000 | 1.231577000  |
| C  | 1.355992000  | -0.102566000 | 2.033442000  |
| F  | 0.518654000  | 1.581386000  | -0.086093000 |
| F  | -1.299885000 | 1.897266000  | -1.229955000 |
| F  | -0.455554000 | 3.079172000  | 1.550271000  |
| F  | -1.867228000 | 1.546295000  | 2.086240000  |
| F  | -2.390413000 | 3.039184000  | 0.636257000  |
| F  | -3.305304000 | -2.281277000 | -0.034557000 |
| F  | -3.160615000 | -0.658460000 | 1.409898000  |
| F  | -5.068034000 | -0.528343000 | -0.677354000 |
| F  | -3.711012000 | 1.120644000  | -0.434831000 |
| F  | -3.413792000 | -0.290783000 | -2.040076000 |
| F  | 0.599622000  | 0.870203000  | 2.504338000  |
| F  | 2.336484000  | 0.434367000  | 1.292507000  |
| F  | 1.951541000  | -0.701490000 | 3.063224000  |
| F  | -0.105237000 | -1.862457000 | 2.170830000  |
| F  | 1.526593000  | -1.941609000 | 0.710244000  |
| C  | -0.725251000 | -2.856672000 | -0.549768000 |
| C  | -0.572152000 | -4.019683000 | -0.882436000 |
| H  | -0.477504000 | -5.058582000 | -1.142253000 |
| H  | 1.145586000  | -2.220872000 | -1.925271000 |

**Adduct-3-Sn (HC≡CH):** E= -2495.5274074 (-2491.8420700)

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 1.492571000  | -1.370691000 | -2.050076000 |
| N | 3.587968000  | 1.628338000  | -1.588179000 |
| N | 4.500485000  | -1.609304000 | -0.011336000 |
| C | 2.590976000  | -0.795640000 | -1.576623000 |
| C | 3.374362000  | 0.332547000  | -1.389029000 |
| C | 3.736546000  | -0.871981000 | -0.806024000 |
| C | 0.242911000  | -0.608252000 | -2.131365000 |
| H | -0.401302000 | -1.033216000 | -2.911548000 |
| C | 4.506072000  | 2.360574000  | -0.736109000 |
| H | 5.054713000  | 3.101139000  | -1.334477000 |
| H | 3.964156000  | 2.878236000  | 0.071219000  |
| H | 5.227205000  | 1.667684000  | -0.288274000 |
| C | 2.608240000  | 2.411277000  | -2.326475000 |
| H | 1.835365000  | 2.818460000  | -1.656511000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | 3.123361000  | 3.234128000  | -2.840590000 |
| H  | 2.128805000  | 1.777172000  | -3.082319000 |
| C  | 5.644702000  | -1.024126000 | 0.659871000  |
| H  | 6.351635000  | -1.822928000 | 0.919694000  |
| H  | 6.156867000  | -0.323311000 | -0.011444000 |
| H  | 5.347852000  | -0.500503000 | 1.584544000  |
| C  | 3.974670000  | -2.857194000 | 0.527538000  |
| H  | 3.037272000  | -3.115879000 | 0.020325000  |
| H  | 4.709897000  | -3.663954000 | 0.395522000  |
| H  | 3.742683000  | -2.739109000 | 1.597082000  |
| H  | 0.461763000  | 0.433240000  | -2.398008000 |
| Sn | -0.720865000 | -0.672612000 | -0.134439000 |
| C  | -2.779311000 | -1.416202000 | 0.380278000  |
| C  | -3.864120000 | -0.975486000 | -0.598632000 |
| C  | -1.361251000 | 1.522882000  | -0.578455000 |
| C  | -2.228999000 | 2.414208000  | 0.345836000  |
| C  | 0.744586000  | -0.214584000 | 1.533818000  |
| C  | 1.228877000  | 1.211336000  | 1.762862000  |
| F  | -0.193878000 | 2.216843000  | -0.813799000 |
| F  | -1.979766000 | 1.459756000  | -1.794143000 |
| F  | -1.580476000 | 3.511543000  | 0.725688000  |
| F  | -2.552203000 | 1.734912000  | 1.448883000  |
| F  | -3.354134000 | 2.798798000  | -0.241018000 |
| F  | -2.798344000 | -2.765171000 | 0.374006000  |
| F  | -3.159393000 | -1.007570000 | 1.613984000  |
| F  | -5.004075000 | -1.624282000 | -0.407450000 |
| F  | -4.095992000 | 0.324991000  | -0.481005000 |
| F  | -3.452372000 | -1.216106000 | -1.848151000 |
| F  | 0.212793000  | 2.034911000  | 1.951058000  |
| F  | 1.926035000  | 1.626901000  | 0.693404000  |
| F  | 2.038673000  | 1.294515000  | 2.814405000  |
| F  | 0.227319000  | -0.637924000 | 2.709257000  |
| F  | 1.898716000  | -0.930604000 | 1.328156000  |
| C  | 0.028442000  | -2.800416000 | 0.070789000  |
| C  | 0.389758000  | -3.968125000 | 0.059084000  |
| H  | 0.664035000  | -5.008145000 | 0.081816000  |
| H  | 1.356863000  | -2.329331000 | -1.721577000 |

#### SiH<sub>4</sub> activation

**TS-2 (SiH<sub>4</sub>):** E= -2519.7969981 (-2516.4333961) (i = -860 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 2.208570000  | 1.239667000  | 1.183894000  |
| C  | 3.404320000  | 0.904722000  | 1.472378000  |
| C  | 0.981663000  | 0.679691000  | 1.654391000  |
| H  | 0.427494000  | 1.403957000  | 2.272286000  |
| H  | 1.119983000  | -0.257025000 | 2.206449000  |
| Si | -0.068595000 | 0.305990000  | 0.073347000  |
| C  | -1.690136000 | 1.150105000  | -0.663801000 |
| C  | -2.556785000 | 1.875312000  | 0.389270000  |
| C  | -0.943042000 | -1.247567000 | 0.957633000  |
| C  | -1.994544000 | -2.167964000 | 0.296909000  |
| C  | 1.052390000  | -0.454896000 | -1.355382000 |
| C  | 1.736282000  | -1.801219000 | -1.063100000 |
| F  | 0.045621000  | -2.071561000 | 1.406761000  |
| F  | -1.523169000 | -0.722238000 | 2.074847000  |



|    |              |              |              |
|----|--------------|--------------|--------------|
| F  | -1.999448000 | -3.357400000 | 0.883539000  |
| F  | -1.711541000 | -2.340780000 | -0.989153000 |
| F  | -3.205762000 | -1.650210000 | 0.407214000  |
| F  | -1.413726000 | 2.036822000  | -1.632813000 |
| F  | -2.456061000 | 0.189040000  | -1.225548000 |
| F  | -3.333700000 | 2.782059000  | -0.171645000 |
| F  | -3.308446000 | 1.007675000  | 1.043690000  |
| F  | -1.760691000 | 2.486370000  | 1.273181000  |
| F  | 0.867952000  | -2.786153000 | -0.947707000 |
| F  | 2.423014000  | -1.687918000 | 0.085070000  |
| F  | 2.592517000  | -2.106092000 | -2.022385000 |
| F  | 0.305711000  | -0.610535000 | -2.465643000 |
| F  | 2.094751000  | 0.358545000  | -1.658611000 |
| C  | 3.720709000  | -0.099720000 | 2.541939000  |
| H  | 3.144123000  | 0.102709000  | 3.454728000  |
| H  | 3.445578000  | -1.104088000 | 2.183698000  |
| H  | 4.790698000  | -0.097264000 | 2.779226000  |
| C  | 4.524462000  | 1.500701000  | 0.681049000  |
| H  | 5.050238000  | 0.688813000  | 0.154339000  |
| H  | 4.153567000  | 2.229307000  | -0.049491000 |
| H  | 5.250770000  | 1.976558000  | 1.355354000  |
| H  | 0.889065000  | 2.845742000  | -2.452281000 |
| Si | 1.073318000  | 3.110109000  | -0.998671000 |
| H  | 2.376194000  | 3.867423000  | -0.921316000 |
| H  | 0.043966000  | 4.104006000  | -0.566290000 |
| H  | 1.817096000  | 1.953167000  | 0.235690000  |

**TS-3-Si (SiH<sub>4</sub>):** E= -2785.2624647 (-2781.4375366) (i = -1038 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.407913000  | -1.275317000 | -1.561157000 |
| N  | 3.511608000  | 1.793305000  | -1.521764000 |
| N  | 4.759104000  | -1.428295000 | -0.167903000 |
| C  | 2.526490000  | -0.650382000 | -1.305572000 |
| C  | 3.338419000  | 0.489016000  | -1.260609000 |
| C  | 3.812488000  | -0.701385000 | -0.762957000 |
| C  | 0.207097000  | -0.504406000 | -1.777025000 |
| H  | -0.410757000 | -0.932126000 | -2.582492000 |
| C  | 4.472523000  | 2.553286000  | -0.747898000 |
| H  | 5.315959000  | 1.911446000  | -0.467075000 |
| H  | 4.856622000  | 3.385923000  | -1.353089000 |
| H  | 4.019596000  | 2.962339000  | 0.172082000  |
| C  | 2.434538000  | 2.537063000  | -2.150893000 |
| H  | 1.937126000  | 1.900834000  | -2.893763000 |
| H  | 1.687443000  | 2.890800000  | -1.421771000 |
| H  | 2.861085000  | 3.402566000  | -2.676145000 |
| C  | 5.991403000  | -0.810188000 | 0.273010000  |
| H  | 6.772832000  | -1.578903000 | 0.339961000  |
| H  | 6.317190000  | -0.059344000 | -0.458931000 |
| H  | 5.888340000  | -0.332344000 | 1.262868000  |
| C  | 4.422884000  | -2.740003000 | 0.360865000  |
| H  | 3.498315000  | -3.097681000 | -0.106714000 |
| H  | 5.234424000  | -3.448433000 | 0.141728000  |
| H  | 4.260070000  | -2.704347000 | 1.450511000  |
| H  | 0.428340000  | 0.540352000  | -2.039797000 |
| Si | -0.850411000 | -0.409012000 | -0.187811000 |
| C  | -2.437396000 | -1.569572000 | 0.017455000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -3.648318000 | -1.238431000 | -0.870005000 |
| C  | -1.624961000 | 1.386798000  | -0.566671000 |
| C  | -2.625917000 | 2.104968000  | 0.395077000  |
| C  | 0.219615000  | -0.141019000 | 1.460000000  |
| C  | 0.800511000  | 1.258557000  | 1.714778000  |
| F  | -0.578868000 | 2.243218000  | -0.752251000 |
| F  | -2.224502000 | 1.277219000  | -1.778788000 |
| F  | -2.141793000 | 3.260530000  | 0.823164000  |
| F  | -2.850302000 | 1.323838000  | 1.450986000  |
| F  | -3.776727000 | 2.359032000  | -0.202359000 |
| F  | -2.154401000 | -2.844333000 | -0.322758000 |
| F  | -2.861842000 | -1.551687000 | 1.295506000  |
| F  | -4.574515000 | -2.174322000 | -0.751694000 |
| F  | -4.185115000 | -0.077129000 | -0.530395000 |
| F  | -3.261863000 | -1.180334000 | -2.142516000 |
| F  | -0.155968000 | 2.154210000  | 1.879602000  |
| F  | 1.565488000  | 1.625902000  | 0.678954000  |
| F  | 1.560028000  | 1.253767000  | 2.798421000  |
| F  | -0.525363000 | -0.444250000 | 2.538613000  |
| F  | 1.329961000  | -0.924953000 | 1.474739000  |
| H  | -0.475674000 | -3.049855000 | 1.679742000  |
| Si | 0.399390000  | -3.397226000 | 0.512044000  |
| H  | 1.679192000  | -3.817276000 | 1.185829000  |
| H  | -0.164583000 | -4.664959000 | -0.047979000 |
| H  | 1.044182000  | -2.201720000 | -0.778821000 |

**TS-3-Ge (SiH<sub>4</sub>):** E= -4572.7874489 (-4567.9945002) (i = -986 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.477911000  | -1.259037000 | -1.609750000 |
| N  | 3.583498000  | 1.801122000  | -1.535929000 |
| N  | 4.793025000  | -1.410133000 | -0.123792000 |
| C  | 2.595207000  | -0.639381000 | -1.330323000 |
| C  | 3.406911000  | 0.497649000  | -1.274415000 |
| C  | 3.865618000  | -0.689694000 | -0.753472000 |
| C  | 0.284112000  | -0.489685000 | -1.848274000 |
| H  | -0.326643000 | -0.925635000 | -2.652236000 |
| C  | 4.520776000  | 2.565837000  | -0.737459000 |
| H  | 5.365092000  | 1.930561000  | -0.444530000 |
| H  | 4.908358000  | 3.405977000  | -1.329671000 |
| H  | 4.045254000  | 2.963767000  | 0.175854000  |
| C  | 2.514207000  | 2.537541000  | -2.187234000 |
| H  | 2.942667000  | 3.416294000  | -2.687936000 |
| H  | 2.049358000  | 1.904073000  | -2.953322000 |
| H  | 1.740375000  | 2.870339000  | -1.475985000 |
| C  | 6.015094000  | -0.789008000 | 0.341318000  |
| H  | 6.794865000  | -1.557138000 | 0.430388000  |
| H  | 6.357096000  | -0.042157000 | -0.387201000 |
| H  | 5.889030000  | -0.306032000 | 1.325899000  |
| C  | 4.440776000  | -2.715335000 | 0.411860000  |
| H  | 3.529949000  | -3.079279000 | -0.077084000 |
| H  | 5.258365000  | -3.426233000 | 0.226341000  |
| H  | 4.245174000  | -2.664160000 | 1.495367000  |
| H  | 0.504002000  | 0.556271000  | -2.105811000 |
| Ge | -0.816528000 | -0.385280000 | -0.192814000 |
| C  | -2.456087000 | -1.577476000 | 0.057903000  |
| C  | -3.661685000 | -1.197050000 | -0.811527000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -1.594553000 | 1.488322000  | -0.562108000 |
| C  | -2.566153000 | 2.187035000  | 0.438260000  |
| C  | 0.336268000  | -0.150675000 | 1.488436000  |
| C  | 0.904512000  | 1.254598000  | 1.720754000  |
| F  | -0.538766000 | 2.329116000  | -0.751587000 |
| F  | -2.217698000 | 1.402090000  | -1.761781000 |
| F  | -2.063466000 | 3.328132000  | 0.883554000  |
| F  | -2.769382000 | 1.382073000  | 1.481872000  |
| F  | -3.731077000 | 2.455638000  | -0.124142000 |
| F  | -2.189119000 | -2.849291000 | -0.291698000 |
| F  | -2.855456000 | -1.556593000 | 1.341868000  |
| F  | -4.620022000 | -2.100605000 | -0.708102000 |
| F  | -4.151354000 | -0.020991000 | -0.447196000 |
| F  | -3.277939000 | -1.123678000 | -2.084838000 |
| F  | -0.064728000 | 2.135574000  | 1.898169000  |
| F  | 1.632548000  | 1.624731000  | 0.658390000  |
| F  | 1.693957000  | 1.275810000  | 2.782104000  |
| F  | -0.369128000 | -0.469175000 | 2.586885000  |
| F  | 1.443227000  | -0.934734000 | 1.448960000  |
| H  | -0.381707000 | -3.064633000 | 1.596960000  |
| Si | 0.471238000  | -3.451921000 | 0.419115000  |
| H  | 1.723150000  | -3.938155000 | 1.104692000  |
| H  | -0.159501000 | -4.703948000 | -0.108892000 |
| H  | 1.141234000  | -2.206682000 | -0.878500000 |

**TS-3-Sn (SiH<sub>4</sub>):** E= -2710.0076373 (-2706.0397929) (I = -1288 cm<sup>-1</sup>)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.609074000  | -1.307412000 | -1.736206000 |
| N  | 3.776283000  | 1.704317000  | -1.564975000 |
| N  | 4.801352000  | -1.500366000 | 0.003429000  |
| C  | 2.724875000  | -0.717687000 | -1.398120000 |
| C  | 3.559702000  | 0.404931000  | -1.308790000 |
| C  | 3.949151000  | -0.777545000 | -0.727126000 |
| C  | 0.479226000  | -0.495668000 | -2.068890000 |
| H  | -0.082959000 | -0.878931000 | -2.930965000 |
| C  | 4.660693000  | 2.453909000  | -0.694376000 |
| H  | 5.507219000  | 1.824450000  | -0.394497000 |
| H  | 5.054182000  | 3.325630000  | -1.234039000 |
| H  | 4.138905000  | 2.801515000  | 0.214271000  |
| C  | 2.752267000  | 2.449381000  | -2.277733000 |
| H  | 2.368937000  | 1.839596000  | -3.105734000 |
| H  | 1.912129000  | 2.741467000  | -1.625025000 |
| H  | 3.204215000  | 3.354665000  | -2.704219000 |
| C  | 5.963759000  | -0.878604000 | 0.600441000  |
| H  | 6.720382000  | -1.649584000 | 0.797977000  |
| H  | 6.396746000  | -0.151051000 | -0.098542000 |
| H  | 5.725643000  | -0.370480000 | 1.551389000  |
| C  | 4.351175000  | -2.772904000 | 0.541509000  |
| H  | 3.556424000  | -3.174180000 | -0.097786000 |
| H  | 5.189529000  | -3.483181000 | 0.557289000  |
| H  | 3.947571000  | -2.663661000 | 1.561894000  |
| H  | 0.720311000  | 0.565934000  | -2.227310000 |
| Sn | -0.794848000 | -0.444976000 | -0.271372000 |
| C  | -2.667807000 | -1.605429000 | 0.131120000  |
| C  | -3.871029000 | -1.060059000 | -0.635878000 |
| C  | -1.579316000 | 1.656612000  | -0.589657000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -2.398155000 | 2.364119000  | 0.525528000  |
| C  | 0.542273000  | -0.152662000 | 1.526080000  |
| C  | 1.133802000  | 1.249787000  | 1.654644000  |
| F  | -0.491068000 | 2.439718000  | -0.855629000 |
| F  | -2.326006000 | 1.655474000  | -1.721694000 |
| F  | -1.826589000 | 3.493752000  | 0.915593000  |
| F  | -2.478658000 | 1.553313000  | 1.587837000  |
| F  | -3.627036000 | 2.645664000  | 0.127573000  |
| F  | -2.519547000 | -2.884000000 | -0.278256000 |
| F  | -2.980257000 | -1.614864000 | 1.440479000  |
| F  | -4.930589000 | -1.840034000 | -0.512640000 |
| F  | -4.180221000 | 0.152668000  | -0.194357000 |
| F  | -3.555742000 | -0.969367000 | -1.929051000 |
| F  | 0.180080000  | 2.144721000  | 1.850301000  |
| F  | 1.776466000  | 1.561363000  | 0.518452000  |
| F  | 2.006389000  | 1.333786000  | 2.647848000  |
| F  | -0.094266000 | -0.423200000 | 2.681167000  |
| F  | 1.627630000  | -0.976509000 | 1.451394000  |
| H  | -0.481029000 | -2.993188000 | 1.449872000  |
| Si | 0.379160000  | -3.394957000 | 0.286458000  |
| H  | 1.606406000  | -3.951136000 | 0.940304000  |
| H  | -0.300399000 | -4.555055000 | -0.358972000 |
| H  | 1.113989000  | -2.241860000 | -0.887137000 |

**Adduct-2 (SiH<sub>4</sub>):** E= -2519.8329373 (-2516.4680358)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | -1.182624000 | -2.257170000 | 0.887317000  |
| C  | -2.268805000 | -2.152333000 | 1.568899000  |
| C  | 0.090946000  | -1.592455000 | 1.102606000  |
| H  | 0.884120000  | -2.353288000 | 1.081616000  |
| H  | 0.101924000  | -1.088326000 | 2.075012000  |
| Si | 0.404981000  | -0.344589000 | -0.374446000 |
| C  | 2.417560000  | -0.066984000 | -0.461991000 |
| C  | 3.270679000  | -0.995555000 | 0.402510000  |
| C  | 0.272905000  | 1.256790000  | 0.860406000  |
| C  | 0.379948000  | 2.704761000  | 0.315844000  |
| C  | -1.470123000 | 0.031217000  | -1.202400000 |
| C  | -2.684857000 | 0.802345000  | -0.674184000 |
| F  | -0.952999000 | 1.154171000  | 1.474875000  |
| F  | 1.171827000  | 1.115797000  | 1.865273000  |
| F  | -0.591559000 | 3.482247000  | 0.777342000  |
| F  | 0.280968000  | 2.667853000  | -1.017736000 |
| F  | 1.529137000  | 3.272206000  | 0.634135000  |
| F  | 2.832960000  | -0.260818000 | -1.743354000 |
| F  | 2.782049000  | 1.196016000  | -0.135668000 |
| F  | 4.565861000  | -0.766246000 | 0.261285000  |
| F  | 2.957608000  | -0.856879000 | 1.689771000  |
| F  | 3.034298000  | -2.271410000 | 0.071544000  |
| F  | -2.406923000 | 2.070469000  | -0.443291000 |
| F  | -3.143423000 | 0.239637000  | 0.459532000  |
| F  | -3.682021000 | 0.753935000  | -1.551669000 |
| F  | -1.207292000 | 0.597584000  | -2.406973000 |
| F  | -2.018398000 | -1.214269000 | -1.474700000 |
| C  | -2.297998000 | -1.396448000 | 2.852763000  |
| H  | -1.528563000 | -1.775974000 | 3.540880000  |
| H  | -2.078190000 | -0.337544000 | 2.649801000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | -3.282613000 | -1.479099000 | 3.324410000  |
| C  | -3.515727000 | -2.770521000 | 1.041652000  |
| H  | -4.253394000 | -1.966192000 | 0.901038000  |
| H  | -3.356411000 | -3.279823000 | 0.083790000  |
| H  | -3.925361000 | -3.472535000 | 1.782052000  |
| H  | 0.030956000  | -1.693560000 | -3.470489000 |
| Si | 0.574392000  | -2.061291000 | -2.137822000 |
| H  | -0.257089000 | -3.235638000 | -1.670827000 |
| H  | 1.934601000  | -2.633665000 | -2.304667000 |
| H  | -1.238846000 | -2.749402000 | -0.011984000 |

**Adduct-3-Si (SiH<sub>4</sub>):** E= -2785.3204351 (-2781.4943604)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.233677000  | 0.080104000  | -1.980329000 |
| N  | 1.823089000  | 3.116805000  | 0.067248000  |
| N  | 4.553389000  | 0.739392000  | -0.615093000 |
| C  | 2.027794000  | 0.868546000  | -1.281536000 |
| C  | 2.257391000  | 2.009740000  | -0.523544000 |
| C  | 3.284421000  | 1.115753000  | -0.757968000 |
| C  | -0.224615000 | 0.180486000  | -1.968625000 |
| H  | -0.607029000 | -0.133015000 | -2.949074000 |
| C  | 2.666609000  | 3.828219000  | 1.005995000  |
| H  | 3.378617000  | 3.136043000  | 1.471247000  |
| H  | 3.216595000  | 4.654031000  | 0.522697000  |
| H  | 2.036038000  | 4.247829000  | 1.801728000  |
| C  | 0.552689000  | 3.725467000  | -0.287340000 |
| H  | 0.083434000  | 3.156477000  | -1.094305000 |
| H  | -0.134156000 | 3.728017000  | 0.569731000  |
| H  | 0.719985000  | 4.758007000  | -0.631815000 |
| C  | 5.458100000  | 1.511441000  | 0.213179000  |
| H  | 6.478377000  | 1.413940000  | -0.182079000 |
| H  | 5.181019000  | 2.572589000  | 0.181045000  |
| H  | 5.454373000  | 1.166563000  | 1.261052000  |
| C  | 5.001104000  | -0.564056000 | -1.075960000 |
| H  | 4.276125000  | -0.971556000 | -1.788847000 |
| H  | 5.973195000  | -0.457803000 | -1.578402000 |
| H  | 5.096860000  | -1.275374000 | -0.241861000 |
| H  | -0.495655000 | 1.240096000  | -1.863976000 |
| Si | -1.147309000 | -0.790530000 | -0.567001000 |
| C  | -2.846394000 | 0.418950000  | -0.785372000 |
| C  | -3.114343000 | 1.892834000  | -0.466194000 |
| C  | -0.551926000 | 0.118273000  | 1.079716000  |
| C  | -1.209235000 | -0.345546000 | 2.373428000  |
| C  | 0.350321000  | -2.325569000 | -0.341137000 |
| C  | 1.693153000  | -2.446197000 | 0.389641000  |
| F  | 0.794409000  | -0.001299000 | 1.258317000  |
| F  | -0.763124000 | 1.461083000  | 0.974776000  |
| F  | -0.714220000 | 0.281606000  | 3.434803000  |
| F  | -1.009104000 | -1.651064000 | 2.523111000  |
| F  | -2.514947000 | -0.120464000 | 2.317805000  |
| F  | -3.056931000 | 0.355765000  | -2.147857000 |
| F  | -3.905052000 | -0.222211000 | -0.200113000 |
| F  | -4.252489000 | 2.301849000  | -1.022035000 |
| F  | -3.207012000 | 2.116707000  | 0.836410000  |
| F  | -2.140213000 | 2.675205000  | -0.962083000 |
| F  | 1.557222000  | -2.385884000 | 1.702178000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| F  | 2.553119000  | -1.481043000 | 0.007301000  |
| F  | 2.291794000  | -3.602527000 | 0.099608000  |
| F  | -0.317738000 | -3.419680000 | 0.142466000  |
| F  | 0.684398000  | -2.639603000 | -1.654787000 |
| H  | -3.159734000 | -3.235132000 | 0.158882000  |
| Si | -2.624210000 | -2.627163000 | -1.087250000 |
| H  | -1.890899000 | -3.659913000 | -1.864922000 |
| H  | -3.760474000 | -2.164216000 | -1.922142000 |
| H  | 1.612087000  | -0.828999000 | -2.227027000 |

**Adduct-3-Ge (SiH<sub>4</sub>):** E= -4572.8356736 (-4568.0394809)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.100087000  | 0.963767000  | -2.262879000 |
| N  | 1.978441000  | 2.957454000  | 0.675512000  |
| N  | 4.525403000  | 0.828270000  | -0.993105000 |
| C  | 2.029904000  | 1.411158000  | -1.434613000 |
| C  | 2.356318000  | 2.158081000  | -0.316000000 |
| C  | 3.319054000  | 1.381161000  | -0.940111000 |
| C  | -0.296567000 | 0.971564000  | -1.846987000 |
| H  | -0.940968000 | 0.975459000  | -2.734424000 |
| C  | 2.688239000  | 2.922725000  | 1.942701000  |
| H  | 3.707823000  | 2.553235000  | 1.785448000  |
| H  | 2.737798000  | 3.933218000  | 2.371039000  |
| H  | 2.177293000  | 2.251150000  | 2.651327000  |
| C  | 0.623311000  | 3.491845000  | 0.686348000  |
| H  | 0.615459000  | 4.409568000  | 1.289020000  |
| H  | 0.322558000  | 3.753159000  | -0.336185000 |
| H  | -0.098652000 | 2.777945000  | 1.108751000  |
| C  | 5.468071000  | 1.071795000  | 0.082991000  |
| H  | 6.485073000  | 0.873426000  | -0.279336000 |
| H  | 5.414857000  | 2.123723000  | 0.391443000  |
| H  | 5.262064000  | 0.420356000  | 0.949053000  |
| C  | 4.691310000  | -0.399833000 | -1.759101000 |
| H  | 3.994230000  | -0.401330000 | -2.605153000 |
| H  | 5.717765000  | -0.448678000 | -2.145982000 |
| H  | 4.484758000  | -1.285991000 | -1.138150000 |
| H  | -0.498742000 | 1.912415000  | -1.319543000 |
| Ge | -0.964456000 | -0.517768000 | -0.666293000 |
| C  | -2.966113000 | 0.281459000  | -0.881808000 |
| C  | -3.507833000 | 1.625676000  | -0.378200000 |
| C  | -0.833091000 | 0.003256000  | 1.310268000  |
| C  | -1.383133000 | -1.046959000 | 2.277803000  |
| C  | 1.043654000  | -1.677713000 | -0.405679000 |
| C  | 2.135479000  | -1.700008000 | 0.670763000  |
| F  | 0.458166000  | 0.270347000  | 1.657556000  |
| F  | -1.510508000 | 1.152748000  | 1.574110000  |
| F  | -1.007314000 | -0.813840000 | 3.529068000  |
| F  | -0.961723000 | -2.260027000 | 1.930778000  |
| F  | -2.707710000 | -1.035743000 | 2.218450000  |
| F  | -3.113030000 | 0.350825000  | -2.249696000 |
| F  | -3.863222000 | -0.652999000 | -0.451727000 |
| F  | -4.538219000 | 2.047925000  | -1.108551000 |
| F  | -3.913858000 | 1.549728000  | 0.878636000  |
| F  | -2.559110000 | 2.576610000  | -0.462977000 |
| F  | 1.657344000  | -2.018272000 | 1.860127000  |
| F  | 2.767833000  | -0.516616000 | 0.779440000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| F  | 3.091042000  | -2.592477000 | 0.371850000  |
| F  | 0.608409000  | -2.980539000 | -0.380429000 |
| F  | 1.775498000  | -1.575678000 | -1.588240000 |
| H  | -2.097303000 | -3.587128000 | -0.607697000 |
| Si | -1.793027000 | -2.585007000 | -1.657881000 |
| H  | -0.773658000 | -3.119490000 | -2.599219000 |
| H  | -3.023600000 | -2.285341000 | -2.430355000 |
| H  | 1.386685000  | 0.173355000  | -2.830822000 |

**Adduct-3-Sn (SiH<sub>4</sub>):** E= -2710.0593374 (-2706.0895174)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 1.609074000  | -1.307412000 | -1.736206000 |
| N  | 3.776283000  | 1.704317000  | -1.564975000 |
| N  | 4.801352000  | -1.500366000 | 0.003429000  |
| C  | 2.724875000  | -0.717687000 | -1.398120000 |
| C  | 3.559702000  | 0.404931000  | -1.308790000 |
| C  | 3.949151000  | -0.777545000 | -0.727126000 |
| C  | 0.479226000  | -0.495668000 | -2.068890000 |
| H  | -0.082959000 | -0.878931000 | -2.930965000 |
| C  | 4.660693000  | 2.453909000  | -0.694376000 |
| H  | 5.507219000  | 1.824450000  | -0.394497000 |
| H  | 5.054182000  | 3.325630000  | -1.234039000 |
| H  | 4.138905000  | 2.801515000  | 0.214271000  |
| C  | 2.752267000  | 2.449381000  | -2.277733000 |
| H  | 2.368937000  | 1.839596000  | -3.105734000 |
| H  | 1.912129000  | 2.741467000  | -1.625025000 |
| H  | 3.204215000  | 3.354665000  | -2.704219000 |
| C  | 5.963759000  | -0.878604000 | 0.600441000  |
| H  | 6.720382000  | -1.649584000 | 0.797977000  |
| H  | 6.396746000  | -0.151051000 | -0.098542000 |
| H  | 5.725643000  | -0.370480000 | 1.551389000  |
| C  | 4.351175000  | -2.772904000 | 0.541509000  |
| H  | 3.556424000  | -3.174180000 | -0.097786000 |
| H  | 5.189529000  | -3.483181000 | 0.557289000  |
| H  | 3.947571000  | -2.663661000 | 1.561894000  |
| H  | 0.720311000  | 0.565934000  | -2.227310000 |
| Sn | -0.794848000 | -0.444976000 | -0.271372000 |
| C  | -2.667807000 | -1.605429000 | 0.131120000  |
| C  | -3.871029000 | -1.060059000 | -0.635878000 |
| C  | -1.579316000 | 1.656612000  | -0.589657000 |
| C  | -2.398155000 | 2.364119000  | 0.525528000  |
| C  | 0.542273000  | -0.152662000 | 1.526080000  |
| C  | 1.133802000  | 1.249787000  | 1.654644000  |
| F  | -0.491068000 | 2.439718000  | -0.855629000 |
| F  | -2.326006000 | 1.655474000  | -1.721694000 |
| F  | -1.826589000 | 3.493752000  | 0.915593000  |
| F  | -2.478658000 | 1.553313000  | 1.587837000  |
| F  | -3.627036000 | 2.645664000  | 0.127573000  |
| F  | -2.519547000 | -2.884000000 | -0.278256000 |
| F  | -2.980257000 | -1.614864000 | 1.440479000  |
| F  | -4.930589000 | -1.840034000 | -0.512640000 |
| F  | -4.180221000 | 0.152668000  | -0.194357000 |
| F  | -3.555742000 | -0.969367000 | -1.929051000 |
| F  | 0.180080000  | 2.144721000  | 1.850301000  |
| F  | 1.776466000  | 1.561363000  | 0.518452000  |
| F  | 2.006389000  | 1.333786000  | 2.647848000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| F  | -0.094266000 | -0.423200000 | 2.681167000  |
| F  | 1.627630000  | -0.976509000 | 1.451394000  |
| H  | -0.481029000 | -2.993188000 | 1.449872000  |
| Si | 0.379160000  | -3.394957000 | 0.286458000  |
| H  | 1.606406000  | -3.951136000 | 0.940304000  |
| H  | -0.300399000 | -4.555055000 | -0.358972000 |
| H  | 1.113989000  | -2.241860000 | -0.887137000 |