

# Supporting Information

## Planar tetracoordinate carbons with a double bond in $CAI_3E$ clusters

Zhong-hua Cui,<sup>a</sup> Yi-hong Ding,<sup>a,\*</sup> José Luis Cabellos,<sup>b</sup> Edison Osorio,<sup>c</sup> Rafael Islas,<sup>d</sup>

Albeiro Restrepo,<sup>e</sup> and Gabriel Merino.<sup>b,\*</sup>

<sup>a</sup>State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical  
Chemistry, Jilin University, Changchun 130023, People's Republic of China.

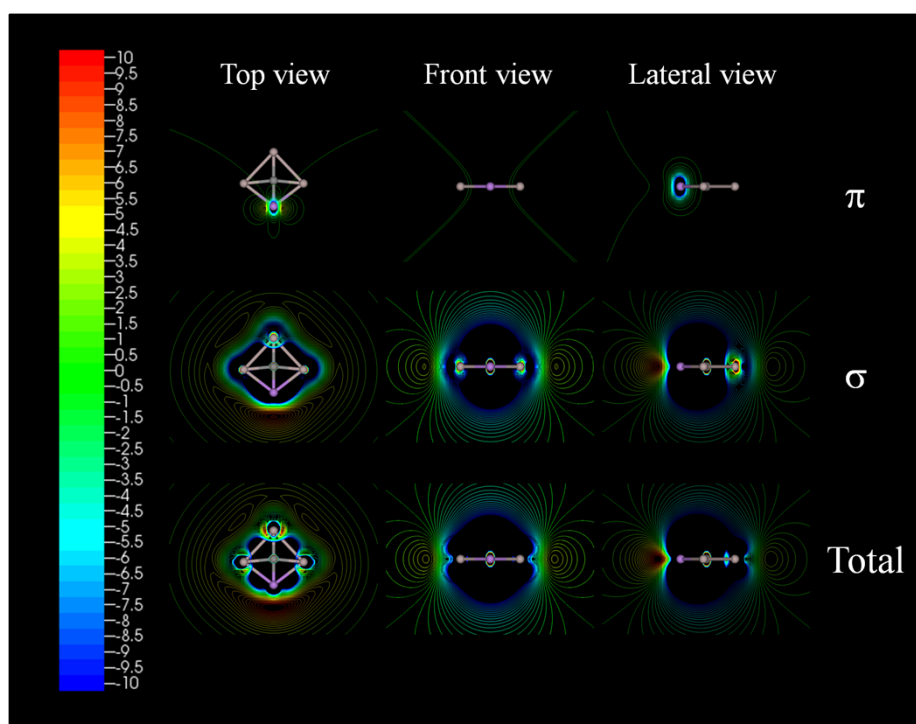
<sup>b</sup>Departamento de Física Aplicada, Centro de Investigación y de Estudios Avanzados Unidad  
Mérida. km 6 Antigua carretera a Progreso. Apdo. Postal 73, Cordemex, 97310, Mérida, Yuc.,  
México.

<sup>c</sup>Departamento de Ciencias Básicas, Fundación Universitaria Luis Amigó, SISCO, Transversal  
51A # 67B 90, Medellín, Colombia.

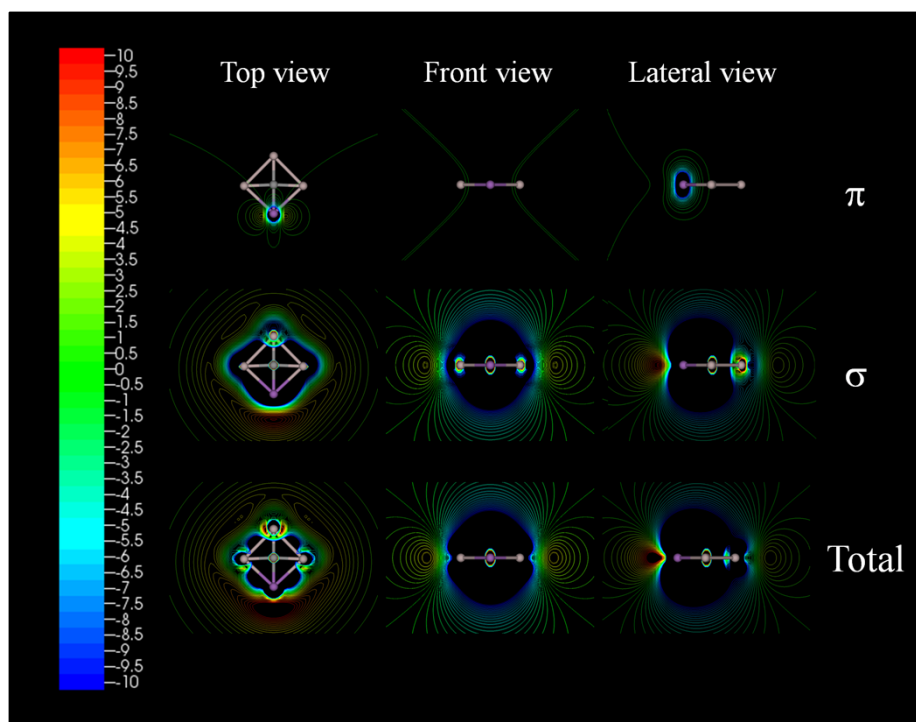
<sup>d</sup>Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello,  
Avenida República 275, Santiago, Chile.

<sup>e</sup>Instituto de Química, Universidad de Antioquia UdeA, Calle 70 No. 52-21, Medellín, Colombia.

(a)

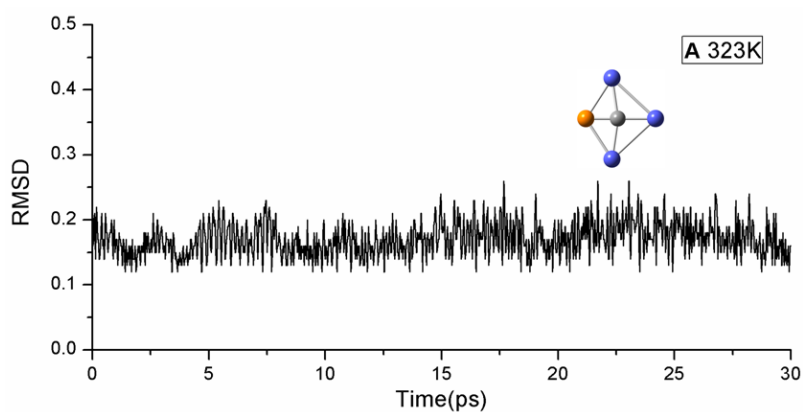


(b)

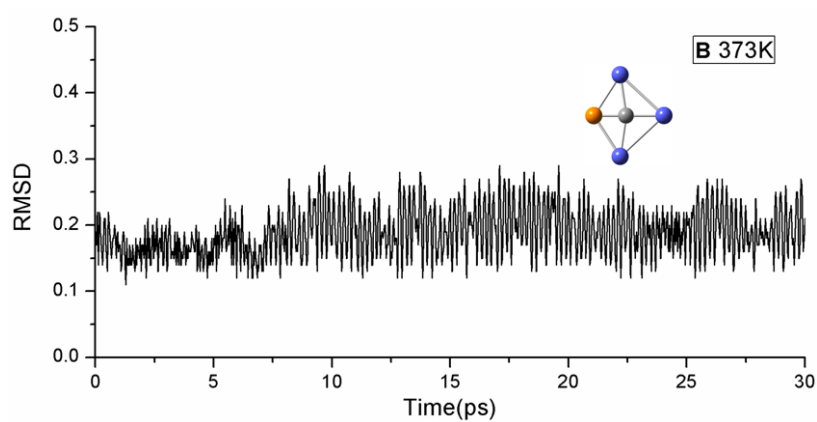


**Figure 1-SI.** Contour lines of z-component of the induced magnetic field ( $B_z^{\text{ind}}$ ) for (a) CAI<sub>3</sub>As and (b) CAI<sub>3</sub>Sb in the molecular plane and perpendicular to the molecular plane through the origin. The scale is given in ppm (or  $\mu\text{T}$  for an external field of 1 T).

(a)



(b)



**Figure 2-SI.** Structural evolution of the global minimum of  $CAI_3P$  via the root-mean-square deviations (RMSD). Born-Oppenheimer molecular dynamics simulations were computed at the B3LYP/6-31G(d) level at (a) 323 and (b) 373 K, respectively, during 30 ps.

Cartesian coordinates and zero-point energies (a.u.) at the B3LYP/aug-cc-pVTZ (aug-cc-pVTZ-PP for Sb and Bi) level for the low-lying isomers and transition states of the  $CA_3E$  ( $E=P,As,Sb,Bi$ ) cluster. The absolute energies (a.u.) are estimated at the CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ level.

<b>1-P</b>	CCSD(T)= -1104.9202427	Zero-Point=0.0069372	
13	0.000000000	2.115280000	0.183158000
6	0.000000000	0.000000000	-0.121284000
13	0.000000000	0.000000000	-2.115080000
13	0.000000000	-2.115280000	0.183158000
15	0.000000000	0.000000000	1.564109000
<b>2-P</b>	CCSD(T)= -1104.8938579	Zero-Point=0.0068967	
13	-2.618701000	0.397056000	0.000000000
13	2.752811000	0.492760000	0.000000000
13	-0.609668000	-1.604788000	0.000000000
6	1.030374000	-0.545310000	0.000000000
15	0.000000000	0.837766000	0.000000000
<b>3-P</b>	CCSD(T)= -1104.8860632	Zero-Point=0.0070539	
6	-1.064334000	-0.600742000	0.000000000
15	-2.287257000	0.502563000	0.000000000
13	0.000000000	1.219201000	0.000000000
13	2.674078000	0.230655000	0.000000000
13	0.456295000	-1.752472000	0.000000000
<b>4-P</b>	CCSD(T)= -1104.8689665	Zero-Point=0.0079516	
13	-0.709624000	1.344157000	-0.036469000
6	1.080999000	0.785364000	0.339133000
13	2.558367000	-0.184282000	-0.169600000
13	0.093120000	-0.990202000	0.155595000
15	-2.115348000	-0.461196000	-0.091909000
<b>5-P</b>	CCSD(T)= -1104.8669544	Zero-Point=0.0071328	
13	-0.571891000	-0.494702000	1.496469000
6	-0.571891000	0.710928000	0.000000000
13	0.444081000	2.429125000	0.000000000
13	-0.571891000	-0.494702000	-1.496469000
15	0.835163000	-1.532130000	0.000000000
<b>6-P</b>	CCSD(T)= -1104.8480065	Zero-Point=0.0081276	
13	0.000000000	1.216814000	0.368288000

6	0.000000000	0.000000000	-1.051555000
13	0.000000000	-1.216814000	0.368288000
13	0.000000000	0.000000000	-2.964232000
15	0.000000000	0.000000000	2.351257000

**7-P** CCSD(T)= -1104.8707539 Zero-Point=0.0075935

6	0.000000000	0.000000000	1.841061000
13	0.000000000	1.215303000	-2.347139000
13	0.000000000	-1.215303000	-2.347139000
13	0.000000000	0.000000000	-0.078098000
15	0.000000000	0.000000000	3.399635000

**8-P** CCSD(T)= -1104.8916879 Zero-Point=0.0067329

13	0.641171000	-2.686116000	0.000000000
6	0.000000000	1.065383000	0.000000000
13	-0.907466000	2.817153000	0.000000000
15	1.256638000	-0.039862000	0.000000000
13	-1.183673000	-0.576757000	0.000000000

**9-P** CCSD(T)= -1104.8830313 Zero-Point=0.0067644

13	0.000000000	1.915729000	0.218396000
6	0.000000000	0.000000000	-0.262410000
13	0.000000000	0.000000000	-2.215777000
13	0.000000000	-1.915729000	0.218396000
15	0.000000000	0.000000000	1.646750000

**10-P** CCSD(T)= -1104.8841898 Zero-Point=0.0070123

13	1.569573000	1.561033000	0.000000000
6	0.000000000	0.326114000	0.000000000
13	1.467199000	-1.055816000	0.000000000
13	-1.146410000	-1.569711000	0.000000000
15	-1.638313000	0.792116000	0.000000000

**11-P** CCSD(T)= -1104.8767876 Zero-Point=0.0075733

13	0.333499000	0.888823000	1.537541000
6	1.124144000	0.000102000	0.000000000
13	0.333499000	-1.776346000	0.000000000
13	0.333499000	0.888823000	-1.537541000
15	-1.316755000	-0.001168000	0.000000000

**12-P** CCSD(T)= -1104.8752388 Zero-Point=0.0069929

13	-0.260582000	-2.540833000	0.000000000
6	0.000000000	0.931459000	0.000000000
13	0.171857000	2.866725000	0.000000000

15	-1.179967000	-0.310403000	0.000000000
13	1.450226000	-0.397638000	0.000000000

**13-P** CCSD(T)=-1104.8731286 Zero-Point=0.0060449

13	0.000000000	2.016124000	-0.550678000
13	-1.746015000	-1.008062000	-0.550678000
6	0.000000000	0.000000000	-0.245095000
13	1.746015000	-1.008062000	-0.550678000
15	0.000000000	0.000000000	1.529800000

**14-P** CCSD(T)=-1104.8691038 Zero-Point=0.0071784

6	0.000000000	0.997344000	0.000000000
15	-1.453408000	1.757114000	0.000000000
13	-1.187451000	-0.719010000	0.000000000
13	1.047046000	-2.138976000	0.000000000
13	1.817413000	0.370233000	0.000000000

**15-P** CCSD(T)=-1104.8629539 Zero-Point=0.0072032

13	-0.670611000	-1.442879000	0.000000000
6	1.050411000	-0.609532000	0.000000000
13	2.726878000	0.263953000	0.000000000
13	0.000000000	1.045365000	0.000000000
15	-2.202263000	0.359566000	0.000000000

**16-P** CCSD(T)=-1104.8576872 Zero-Point=0.0079375

13	-1.271577000	-0.387594000	0.000000000
6	0.000000000	1.056304000	0.000000000
13	-0.043340000	2.897005000	0.000000000
13	1.290407000	-0.370533000	0.000000000
15	0.021242000	-2.276215000	0.000000000

**17-P** CCSD(T)=-1104.8474305 Zero-Point=0.0068653

13	0.000000000	1.686239000	-1.919122000
6	0.000000000	0.000000000	-1.029457000
13	0.000000000	0.000000000	0.810140000
15	0.000000000	0.000000000	3.036139000
13	0.000000000	-1.686239000	-1.919122000

**TS<sub>1-2</sub>-P** CCSD(T)=-1104.8771422 Zero-Point=0.0062327

13	0.960659000	-2.239039000	0.000000000
13	-1.868130000	1.736266000	0.000000000
13	1.944999000	0.762259000	0.000000000
6	0.000000000	0.894928000	0.000000000
15	-0.899191000	-0.582859000	0.000000000

**TS<sub>1-8</sub>-P** CCSD(T)= -1104.8728527 Zero-Point=0.0065537  
6 -0.538313000 -0.504386000 -0.180138000  
15 0.832710000 -1.329230000 0.314035000  
13 -0.363987000 1.390567000 0.451403000  
13 2.120084000 0.563579000 -0.432744000  
13 -2.468464000 -0.187626000 -0.297866000

**TS<sub>1-3</sub>-P** CCSD(T)= -1104.8876245 Zero-Point=0.0070689  
6 -0.488063000 0.705184000 -0.301343000  
15 -2.059420000 0.194287000 -0.341040000  
13 -0.425223000 -1.217458000 0.688369000  
13 1.899564000 -0.841420000 -0.530789000  
13 1.127172000 1.509232000 0.375009000

**TS<sub>1-5</sub>-P** CCSD(T)= -1104.85974 Zero-Point=0.0065715  
13 -1.008148000 1.524814000 -0.377904000  
6 0.502657000 0.378325000 -0.041853000  
13 2.415111000 0.344683000 0.306884000  
13 0.204013000 -1.470040000 -0.537481000  
15 -1.597241000 -0.497526000 0.544109000

**TS<sub>2-7</sub>-P** CCSD(T)= -1104.8219735 Zero-Point=0.0055106  
6 1.497246000 -0.206963000 -0.065842000  
13 3.432408000 0.052207000 -0.120882000  
15 -0.062133000 -0.310883000 0.323636000  
13 -1.744995000 1.546762000 -0.051346000  
13 -2.306757000 -1.144736000 -0.170810000

**TS<sub>2-4</sub>-P** CCSD(T)= -1104.8096805 Zero-Point=0.0066448  
6 2.337821000 0.048818000 -0.031916000  
13 0.923926000 -1.071791000 0.481400000  
15 -1.139632000 -1.069544000 -0.448653000  
13 -1.622115000 1.017821000 0.409953000  
13 0.934154000 1.265528000 -0.358946000

**TS<sub>2-5</sub>-P** CCSD(T)= -1104.8415314 Zero-Point=0.0064508  
6 -0.739722000 1.021150000 -0.726771000  
13 0.784670000 1.574771000 0.155388000  
15 -0.076553000 -0.577951000 1.056884000  
13 1.605158000 -1.021376000 -0.649068000  
13 -1.960088000 -0.357828000 -0.390369000

**TS<sub>3-7</sub>-P** CCSD(T)= -1104.8448955 Zero-Point=0.0062831

6	-1.374683000	-0.422657000	0.122589000
13	1.148001000	1.623208000	0.193067000
13	2.352140000	-0.697136000	-0.738718000
13	0.330169000	-0.811805000	0.951097000
15	-2.769729000	0.070032000	-0.400422000

**TS<sub>4-5-P</sub>** CCSD(T)= -1104.8583279 Zero-Point=0.0067899

13	-0.722435000	1.458065000	-0.172719000
6	0.855107000	0.483882000	0.366979000
13	2.644527000	0.003357000	0.028493000
13	0.052540000	-1.237433000	-0.188327000
15	-2.053391000	-0.387677000	0.141421000

**1-As** CCSD(T)= -2998.4743783 Zero-Point=0.0062955

6	0.000000000	0.000000000	-0.511757000
13	0.000000000	2.107827000	-0.285756000
13	0.000000000	0.000000000	-2.512928000
13	0.000000000	-2.107827000	-0.285756000
33	0.000000000	0.000000000	1.308129000

**2-As** CCSD(T)= -2998.4495039 Zero-Point=0.0065838

13	2.774011000	0.277788000	0.000000000
6	1.080494000	-0.809581000	0.000000000
13	-0.596103000	-1.802912000	0.000000000
13	-2.676598000	0.073059000	0.000000000
33	0.000000000	0.719222000	0.000000000

**3-As** CCSD(T)= -2998.4386572 Zero-Point=0.0063883

13	-0.086281000	-1.201198000	0.000000000
13	1.896938000	1.027153000	0.000000000
6	0.000000000	0.885871000	0.000000000
33	-1.763261000	0.642340000	0.000000000
13	2.665313000	-1.865375000	0.000000000

**4-As** CCSD(T)= -2998.4358663 Zero-Point=0.0074154

6	1.680478000	0.745820000	0.347465000
13	-0.040171000	1.490804000	-0.014255000
13	3.076300000	-0.323175000	-0.210459000
33	-1.719782000	-0.227489000	-0.059209000
13	0.553865000	-0.934381000	0.214645000

**5-As** CCSD(T)= -2998.434773 Zero-Point=0.0066945

13	0.557622000	0.561298000	1.510243000
----	-------------	-------------	-------------



13	-2.350929000	1.621946000	0.000000000
6	-0.389606000	1.270961000	0.000000000
33	0.557622000	-1.312267000	0.000000000
13	0.557622000	0.561298000	-1.510243000

**6-As** CCSD(T)= -2998.4179767 Zero-Point=0.0077054

13	0.000000000	1.234096000	-0.225984000
6	0.000000000	0.000000000	-1.627414000
13	0.000000000	-1.234096000	-0.225984000
13	0.000000000	0.000000000	-3.543516000
33	0.000000000	0.000000000	1.869872000

**7-As** CCSD(T)= -2998.4163672 Zero-Point=0.0068913

13	0.000000000	1.216376000	-3.180063000
13	0.000000000	0.000000000	-0.906494000
6	0.000000000	0.000000000	1.006952000
33	0.000000000	0.000000000	2.679526000
13	0.000000000	-1.216376000	-3.180063000

**9-As** CCSD(T)= -2998.4462894 Zero-Point=0.0063721

6	0.000000000	0.000000000	-0.702708000
13	0.000000000	1.916371000	-0.243605000
13	0.000000000	0.000000000	-2.661011000
13	0.000000000	-1.916371000	-0.243605000
33	0.000000000	0.000000000	1.367974000

**10-As** CCSD(T)= -2998.4406716 Zero-Point=0.0064245

13	1.580261000	-1.076350000	0.000000000
13	-0.885671000	2.208693000	0.000000000
6	0.000000000	0.453713000	0.000000000
33	-0.931437000	-1.147041000	0.000000000
13	1.669826000	1.569970000	0.000000000

**11-As** CCSD(T)= -2998.4435784 Zero-Point=0.0070877

13	-0.488223000	-1.028782000	1.554083000
13	1.918426000	0.171260000	0.000000000
6	0.644275000	-1.293989000	0.000000000
33	-0.488223000	0.978360000	0.000000000
13	-0.488223000	-1.028782000	-1.554083000

**12-As** CCSD(T)= -2998.4317085 Zero-Point=0.0064246

13	2.775286000	-1.156607000	0.000000000
6	0.915194000	-0.610361000	0.000000000
13	-0.736736000	-1.626204000	0.000000000

13	-2.460947000	0.487105000	0.000000000
33	0.000000000	1.015344000	0.000000000
<b>13-As</b>	CCSD(T)= -2998.4365724	Zero-Point=0.0059012	
13	0.000000000	1.995037000	-0.994321000
13	-1.727753000	-0.997518000	-0.994321000
6	0.000000000	0.000000000	-0.636591000
13	1.727753000	-0.997518000	-0.994321000
33	0.000000000	0.000000000	1.290850000
<b>14-As</b>	CCSD(T)= -2998.4212661	Zero-Point=0.0064583	
13	0.028635000	-1.411011000	0.000000000
13	1.809476000	1.240826000	0.000000000
6	0.000000000	0.638081000	0.000000000
33	-1.773053000	0.447284000	0.000000000
13	2.662717000	-1.259727000	0.000000000
<b>15-As</b>	CCSD(T)= -2998.433242	Zero-Point=0.0067055	
13	2.778165000	1.776492000	0.000000000
6	1.728483000	0.202484000	0.000000000
13	0.681502000	-1.392773000	0.000000000
33	-1.677169000	-0.627013000	0.000000000
13	0.000000000	1.114475000	0.000000000
<b>16-As</b>	CCSD(T)= -2998.4369783	Zero-Point=0.0066703	
13	0.008627000	0.214452000	1.270019000
6	0.008627000	1.648272000	0.000000000
13	0.008627000	0.214452000	-1.270019000
13	-0.470630000	3.526869000	0.000000000
33	0.177034000	-1.858020000	0.000000000
<b>17-As</b>	CCSD(T)= -2998.4199667	Zero-Point=0.006579	
13	0.000000000	1.688761000	-2.664302000
6	0.000000000	0.000000000	-1.772383000
13	0.000000000	0.000000000	0.064534000
33	0.000000000	0.000000000	2.395977000
13	0.000000000	-1.688761000	-2.664302000
<b>TS<sub>1-2</sub>-As</b>	CCSD(T)= -2998.4325355	Zero-Point=0.0056519	
13	-2.444699000	0.073259000	0.000000000
13	2.547352000	0.181345000	0.000000000
13	-0.444980000	-2.304416000	0.000000000
6	0.741707000	-0.764823000	0.000000000
33	0.000000000	0.946560000	0.000000000

**TS<sub>1-3</sub>-As**      CCSD(T)= -2998.4395574      Zero-Point=0.0063887  
6      -0.017082000      0.672394000      -0.205915000  
33      -1.694961000      0.059874000      -0.159189000  
13      0.224604000      -1.246898000      0.711409000  
13      2.497485000      -0.773551000      -0.560071000  
13      1.588388000      1.558124000      0.347796000

**TS<sub>1-5</sub>-As**      CCSD(T)= -2998.4271058      Zero-Point=0.0061384  
13      0.334919000      1.783999000      0.458306000  
6      -0.942148000      0.397443000      0.059872000  
13      -2.796869000      0.099244000      -0.451267000  
13      -0.551060000      -1.393153000      0.703137000  
33      1.358243000      -0.265328000      -0.290652000

**TS<sub>2-4</sub>-As**      CCSD(T)= -2998.3760688      Zero-Point=0.0062289  
6      2.543716000      -0.699093000      -0.091488000  
13      0.883107000      -1.174349000      0.617016000  
33      -1.215933000      -0.476014000      -0.227144000  
13      -0.654851000      1.781875000      0.488046000  
13      1.684320000      0.923475000      -0.486241000

**TS<sub>2-5</sub>-As**      CCSD(T)= -2998.4091588      Zero-Point=0.0060626  
6      0.450030000      1.592048000      0.271848000  
13      -1.057152000      1.423501000      -0.780542000  
33      0.217466000      -0.852692000      -0.531063000  
13      -1.577864000      -0.472959000      1.258255000  
13      1.875282000      0.479194000      0.744902000

**TS<sub>2-7</sub>-As**      CCSD(T)= -2998.3672965      Zero-Point=0.0047914  
6      1.623536000      -0.252903000      -0.238562000  
13      3.513472000      0.198576000      -0.187156000  
33      -0.031171000      -0.297190000      0.263183000  
13      -1.764439000      1.672832000      -0.060999000  
13      -2.419231000      -1.000280000      -0.309819000

**TS<sub>3-7</sub>-As**      CCSD(T)= -2998.3916056      Zero-Point=0.0056736  
6      -0.692136000      -0.517567000      0.202843000  
13      1.795995000      1.596799000      0.257695000  
13      3.122994000      -0.580936000      -0.760956000  
13      1.069543000      -0.894430000      0.876003000  
33      -2.233276000      0.046266000      -0.183719000

**TS<sub>4-5</sub>-As**      CCSD(T)= -2998.4255545      Zero-Point=0.0063044

13	-0.066636000	1.586278000	-0.178993000
6	1.408818000	0.474787000	0.374550000
13	3.160970000	-0.134098000	0.040076000
13	0.499971000	-1.184920000	-0.202076000
33	-1.672087000	-0.191609000	0.066230000

**1-Sb** CCSD(T)= -1003.5042163 Zero-Point=0.0059668

6	0.000000000	0.000000000	-0.838223000
13	0.000000000	2.085146000	-0.734352000
13	0.000000000	0.000000000	-2.859631000
13	0.000000000	-2.085146000	-0.734352000
51	0.000000000	0.000000000	1.201916000

**2-Sb** CCSD(T)= -1003.4807986 Zero-Point=0.0060527

13	-2.857584000	-0.315435000	0.000000000
6	1.087341000	-1.007877000	0.000000000
13	2.943551000	-0.304893000	0.000000000
51	0.000000000	0.776302000	0.000000000
13	-0.587817000	-1.959991000	0.000000000

**3-Sb** CCSD(T)= -1003.46715 Zero-Point=0.0061025

13	1.022958000	-0.928479000	0.000000000
13	1.532115000	1.973914000	0.000000000
6	0.000000000	0.860801000	0.000000000
51	-1.596438000	-0.347836000	0.000000000
13	3.707877000	-0.078142000	0.000000000

**4-Sb** CCSD(T)= -1003.4777044 Zero-Point=0.0070443

6	2.133433000	0.694746000	0.339842000
13	0.476525000	1.573612000	0.016283000
13	3.504146000	-0.399378000	-0.262784000
51	-1.510128000	-0.144440000	-0.050840000
13	0.959017000	-0.928235000	0.289100000

**5-Sb** CCSD(T)= -1003.4768505 Zero-Point=0.0064616

13	-0.992104000	-0.197858000	1.534939000
13	-0.310505000	-3.203505000	0.000000000
6	-0.992104000	-1.338984000	0.000000000
51	0.701645000	1.074976000	0.000000000
13	-0.992104000	-0.197858000	-1.534939000

**6-Sb** CCSD(T)= -1003.4640046 Zero-Point=0.0074524

13	0.000000000	1.260179000	-0.699681000
6	0.000000000	0.000000000	-2.073789000

13	0.000000000	-1.260179000	-0.699681000
13	0.000000000	0.000000000	-3.995699000
51	0.000000000	0.000000000	1.619187000

**7-Sb** CCSD(T)= -1003.432398 Zero-Point=0.0063761

13	0.000000000	1.217637000	-3.793200000
13	0.000000000	0.000000000	-1.508980000
6	0.000000000	0.000000000	0.392468000
51	0.000000000	0.000000000	2.272258000
13	0.000000000	-1.217637000	-3.793200000

**9-Sb** CCSD(T)= -1003.4552012 Zero-Point=0.0061716

6	0.000000000	0.000000000	-1.058007000
13	0.000000000	1.926706000	-0.682468000
13	0.000000000	0.000000000	-3.027745000
13	0.000000000	-1.926706000	-0.682468000
51	0.000000000	0.000000000	1.244174000

**10-Sb** CCSD(T)= -1003.4429193 Zero-Point=0.0060579

13	2.010276000	0.058888000	0.000000000
13	-1.521376000	1.990508000	0.000000000
6	0.000000000	0.793795000	0.000000000
51	-0.394785000	-1.257594000	0.000000000
13	1.059871000	2.517876000	0.000000000

**11-Sb** CCSD(T)= -1003.4513151 Zero-Point=0.0067319

13	-0.408244000	-1.340956000	1.585464000
13	2.102801000	-0.230721000	0.000000000
6	0.683058000	-1.546793000	0.000000000
51	-0.408244000	0.924412000	0.000000000
13	-0.408244000	-1.340956000	-1.585464000

**12-Sb** CCSD(T)= -1003.4344624 Zero-Point=0.0061631

13	-2.582793000	0.043384000	0.000000000
6	0.958236000	-0.929787000	0.000000000
13	2.829078000	-1.406954000	0.000000000
51	0.000000000	0.940723000	0.000000000
13	-0.688548000	-1.897824000	0.000000000

**13-Sb** CCSD(T)= -1003.4499366 Zero-Point=0.0058979

13	0.000000000	1.969944000	-1.397186000
13	-1.706022000	-0.984972000	-1.397186000
6	0.000000000	0.000000000	-0.981330000
13	1.706022000	-0.984972000	-1.397186000

51	0.000000000	0.000000000	1.183887000
<b>16-Sb</b>	CCSD(T)= -1003.4788034		Zero-Point=0.0064336
13	0.000000000	1.300400000	-0.698686000
6	0.000000000	0.000000000	-2.082033000
13	0.000000000	-1.300400000	-0.698686000
13	0.000000000	0.000000000	-4.032587000
51	0.000000000	0.000000000	1.629052000
<b>17-Sb</b>	CCSD(T)= -1003.4400461		Zero-Point=0.0064358
13	0.000000000	1.692427000	-3.229504000
6	0.000000000	0.000000000	-2.331413000
13	0.000000000	0.000000000	-0.501881000
51	0.000000000	0.000000000	2.048628000
13	0.000000000	-1.692427000	-3.229504000
<b>TS<sub>1-2</sub>-Sb</b>	CCSD(T)= -1003.4641169		Zero-Point=0.0054821
13	-2.455457000	-0.217792000	0.442830000
13	2.412126000	1.054295000	0.308396000
13	-1.120670000	2.155188000	-0.373912000
6	0.405569000	1.138701000	0.254297000
51	0.248992000	-0.896553000	-0.126095000
<b>TS<sub>1-3</sub>-Sb</b>	CCSD(T)= -1003.4665339		Zero-Point=0.0059891
6	0.412402000	0.654224000	-0.160891000
51	-1.503570000	0.027270000	-0.092387000
13	0.698455000	-1.253944000	0.657202000
13	3.014686000	-0.758929000	-0.523192000
13	1.995138000	1.603942000	0.302688000
<b>TS<sub>1-5</sub>-Sb</b>	CCSD(T)= -1003.469933		Zero-Point=0.0058857
13	-0.240868000	1.907187000	0.500454000
6	-1.283647000	0.350750000	0.062325000
13	-3.087767000	-0.044382000	-0.569536000
13	-0.896283000	-1.419977000	0.777046000
51	1.227957000	-0.154142000	-0.187794000
<b>TS<sub>2-5</sub>-Sb</b>	CCSD(T)= -1003.4502125		Zero-Point=0.0058304
6	-1.181401000	1.380815000	-0.297231000
13	-1.761437000	-0.100779000	-1.236274000
51	0.863371000	-0.422668000	-0.156893000
13	-1.395437000	-0.966739000	1.423520000
13	0.315064000	2.088376000	0.565441000

**TS<sub>2-7-Sb</sub>** CCSD(T)= -1003.3958469 Zero-Point=0.0044901  
 6 -1.857794000 -0.369251000 0.428613000  
 13 -3.460639000 0.568246000 -0.035684000  
 51 0.020829000 -0.491125000 -0.064476000  
 13 1.455225000 1.932302000 0.002452000  
 13 2.781142000 -0.403402000 0.088353000

**TS<sub>4-5-Sb</sub>** CCSD(T)= -1003.4671036 Zero-Point=0.0058458  
 13 0.455693000 1.658420000 -0.149577000  
 6 1.856694000 0.448991000 0.375120000  
 13 3.591478000 -0.207597000 0.016961000  
 13 0.903728000 -1.195193000 -0.156949000  
 51 -1.480429000 -0.117983000 0.029679000

**TS<sub>4-6-Sb</sub>** CCSD(T)= -1003.4606681 Zero-Point=0.0064389  
 13 1.318288000 -0.715183000 0.000000000  
 6 1.903839000 1.094906000 0.000000000  
 13 3.007110000 2.630626000 0.000000000  
 13 0.000000000 1.323016000 0.000000000  
 51 -1.326533000 -0.954302000 0.000000000

**TS<sub>3-7-Sb</sub>** CCSD(T)= -1003.4099345 Zero-Point=0.0052607  
 6 -0.184657000 -0.633974000 0.145344000  
 13 2.276068000 1.548982000 0.287324000  
 13 3.824615000 -0.444701000 -0.658828000  
 13 1.602332000 -0.974830000 0.696733000  
 51 -1.941789000 0.041588000 -0.100001000

**1-Bi** CCSD(T)= -977.825095 Zero-Point=0.0058192  
 6 0.000000000 0.000000000 -1.200541000  
 13 0.000000000 2.071575000 -1.125598000  
 13 0.000000000 0.000000000 -3.227433000  
 13 0.000000000 -2.071575000 -1.125598000  
 83 0.000000000 0.000000000 0.944885000

**2-Bi** CCSD(T)= -977.8064762 Zero-Point=0.0068036  
 6 2.571017000 0.655437000 0.344241000  
 13 0.954438000 1.610456000 0.040208000  
 13 3.937661000 -0.429542000 -0.304553000  
 83 -1.166489000 -0.086930000 -0.037560000  
 13 1.368864000 -0.928409000 0.345273000

**3-Bi** CCSD(T)= -977.7865197 Zero-Point=0.0058435  
 13 1.682245000 -0.079663000 0.000000000

13	0.888985000	2.750701000	0.000000000
6	0.000000000	1.080112000	0.000000000
83	-0.988455000	-0.781859000	0.000000000
13	3.739672000	1.822317000	0.000000000

**4-Bi** CCSD(T)= -977.8013339      Zero-Point=0.005932

13	-2.895028000	-0.634738000	0.000000000
6	1.107654000	-1.273929000	0.000000000
13	2.963635000	-0.589627000	0.000000000
83	0.000000000	0.626781000	0.000000000
13	-0.579832000	-2.189423000	0.000000000

**5-Bi** CCSD(T)= -977.8047662      Zero-Point=0.0063445

13	-1.211789000	-0.506306000	1.538788000
13	-0.568372000	-3.513012000	0.000000000
6	-1.211789000	-1.638387000	0.000000000
83	0.556218000	0.827270000	0.000000000
13	-1.211789000	-0.506306000	-1.538788000

**6-Bi** CCSD(T)= -977.7926942      Zero-Point=0.0072824

13	0.000000000	1.271261000	-1.164349000
6	0.000000000	0.000000000	-2.527521000
13	0.000000000	-1.271261000	-1.164349000
13	0.000000000	0.000000000	-4.451804000
83	0.000000000	0.000000000	1.244719000

**7-Bi** CCSD(T)= -977.7483324      Zero-Point=0.0060963

13	0.000000000	1.217906000	-4.418174000
13	0.000000000	0.000000000	-2.129998000
6	0.000000000	0.000000000	-0.231055000
83	0.000000000	0.000000000	1.734323000
13	0.000000000	-1.217906000	-4.418174000

**9-Bi** CCSD(T)= -977.8126751      Zero-Point=0.0060824

6	0.000000000	0.000000000	-1.443214000
13	0.000000000	1.923870000	-1.079871000
13	0.000000000	0.000000000	-3.413796000
13	0.000000000	-1.923870000	-1.079871000
83	0.000000000	0.000000000	0.977292000

**11-Bi** CCSD(T)= -977.8088639      Zero-Point=0.006571

13	-0.309116000	-1.639603000	1.596018000
13	2.237399000	-0.565080000	0.000000000
6	0.767915000	-1.823108000	0.000000000



83	-0.309116000	0.733908000	0.000000000
13	-0.309116000	-1.639603000	-1.596018000

**12-Bi** CCSD(T)= -977.7865257 Zero-Point=0.0059501

13	-2.619928000	-0.301022000	0.000000000
6	0.974805000	-1.250151000	0.000000000
13	2.849754000	-1.695709000	0.000000000
83	0.000000000	0.744607000	0.000000000
13	-0.679736000	-2.180302000	0.000000000

**13-Bi** CCSD(T)= -977.8086839 Zero-Point=0.0058324

13	0.000000000	1.960786000	-1.772921000
13	-1.698090000	-0.980393000	-1.772921000
6	0.000000000	0.000000000	-1.360006000
13	1.698090000	-0.980393000	-1.772921000
83	0.000000000	0.000000000	0.931373000

**16-Bi** CCSD(T)= -977.8094614 Zero-Point=0.0063978

13	0.000000000	1.312532000	-1.171455000
6	0.000000000	0.000000000	-2.536894000
13	0.000000000	-1.312532000	-1.171455000
13	0.000000000	0.000000000	-4.485727000
83	0.000000000	0.000000000	1.252936000

**17-Bi** CCSD(T)= -977.8027725 ZeroPoint=0.0063558

13	0.000000000	1.694808000	-3.797107000
6	0.000000000	0.000000000	-2.898011000
13	0.000000000	0.000000000	-1.071513000
83	0.000000000	0.000000000	1.566777000
13	0.000000000	-1.694808000	-3.797107000

**TS<sub>1-2</sub>-Bi** CCSD(T)= -977.7845952 Zero-Point=0.0053826

13	2.455903000	-0.664355000	0.542613000
13	-1.730583000	2.096927000	0.367065000
13	1.886722000	1.851100000	-0.499653000
6	0.157048000	1.453063000	0.273639000
83	-0.420468000	-0.619351000	-0.084002000

**TS<sub>1-5</sub>-Bi** CCSD(T)= -977.7976204 Zero-Point=0.0057325

13	-0.704294000	1.963756000	0.512778000
6	-1.627305000	0.334131000	0.070084000
13	-3.400195000	-0.107760000	-0.621165000
13	-1.260412000	-1.439474000	0.798410000
83	0.957922000	-0.089392000	-0.113142000

**TS<sub>1-3</sub>-Bi** CCSD(T)= -977.7856455 Zero-Point=0.0057433  
 6 0.848731000 0.657588000 -0.142356000  
 83 -1.175203000 0.011355000 -0.052422000  
 13 1.158493000 -1.243155000 0.613226000  
 13 3.525950000 -0.761537000 -0.483622000  
 13 2.427055000 1.628696000 0.270796000

**TS<sub>4-6</sub>-Bi** CCSD(T)= -977.7883254 Zero-Point=0.0063925  
 13 1.395092000 -1.113432000 0.000000000  
 6 0.272331000 -2.647442000 0.000000000  
 13 -0.467529000 -4.381141000 0.000000000  
 13 -1.053254000 -1.256294000 0.000000000  
 83 0.000000000 1.248746000 0.000000000

**TS<sub>2-5</sub>-Bi** CCSD(T)= -977.7763784 Zero-Point=0.0057039  
 6 -1.734845000 1.072101000 -0.414294000  
 13 -1.929557000 -0.552073000 -1.275687000  
 83 0.752184000 -0.155511000 -0.071197000  
 13 -1.523350000 -1.145458000 1.433296000  
 13 -0.548798000 2.195591000 0.488168000

**TS<sub>2-7</sub>-Bi** CCSD(T)= -977.7016754 Zero-Point=0.0042846  
 6 -1.982042000 -0.274073000 0.364426000  
 13 -3.470742000 0.836307000 -0.076840000  
 83 0.012866000 -0.422039000 -0.020178000  
 13 1.432224000 2.093183000 0.027277000  
 13 2.871159000 -0.108441000 0.010195000

**TS<sub>3-7</sub>-Bi** CCSD(T)= -977.726866 ZeroPoint=0.0050558  
 6 0.350305000 -0.691365000 0.122235000  
 13 2.800481000 1.533511000 0.284459000  
 13 4.420803000 -0.400530000 -0.616076000  
 13 2.149599000 -0.995787000 0.636365000  
 83 -1.493052000 0.028490000 -0.056568000

