Supporting Information for

Mechanism and Origin of Stereoselectivity of Manganese catalyzed Hydrosilylation of Alkynes: A DFT study

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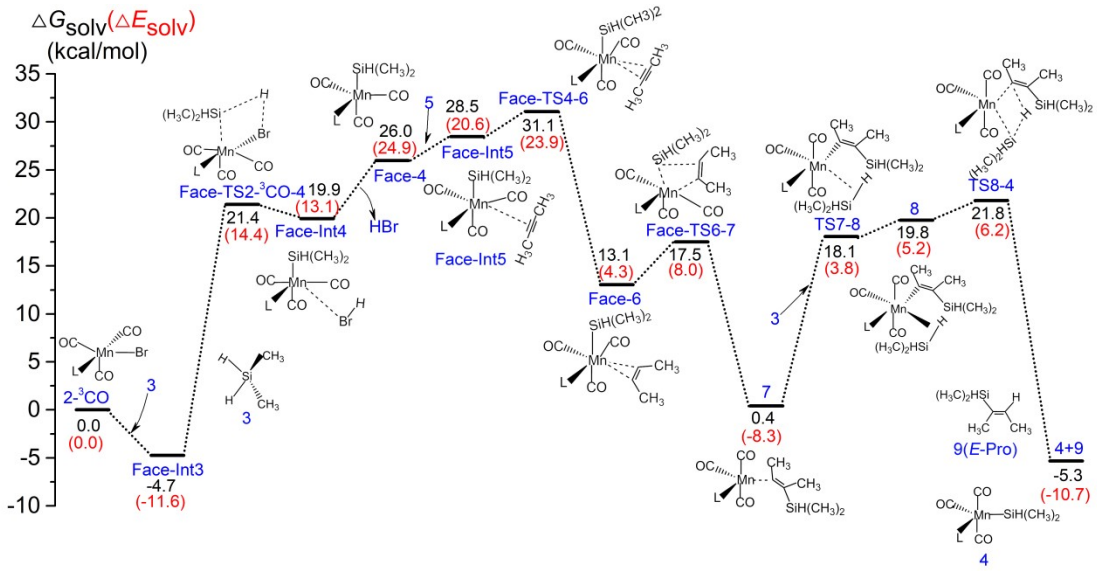

Fig. S1 Gibbs energy (kcal/mol) profile for the transformation from facial direction of 2-^{3}CO to the products (electronic energies are given in parentheses)

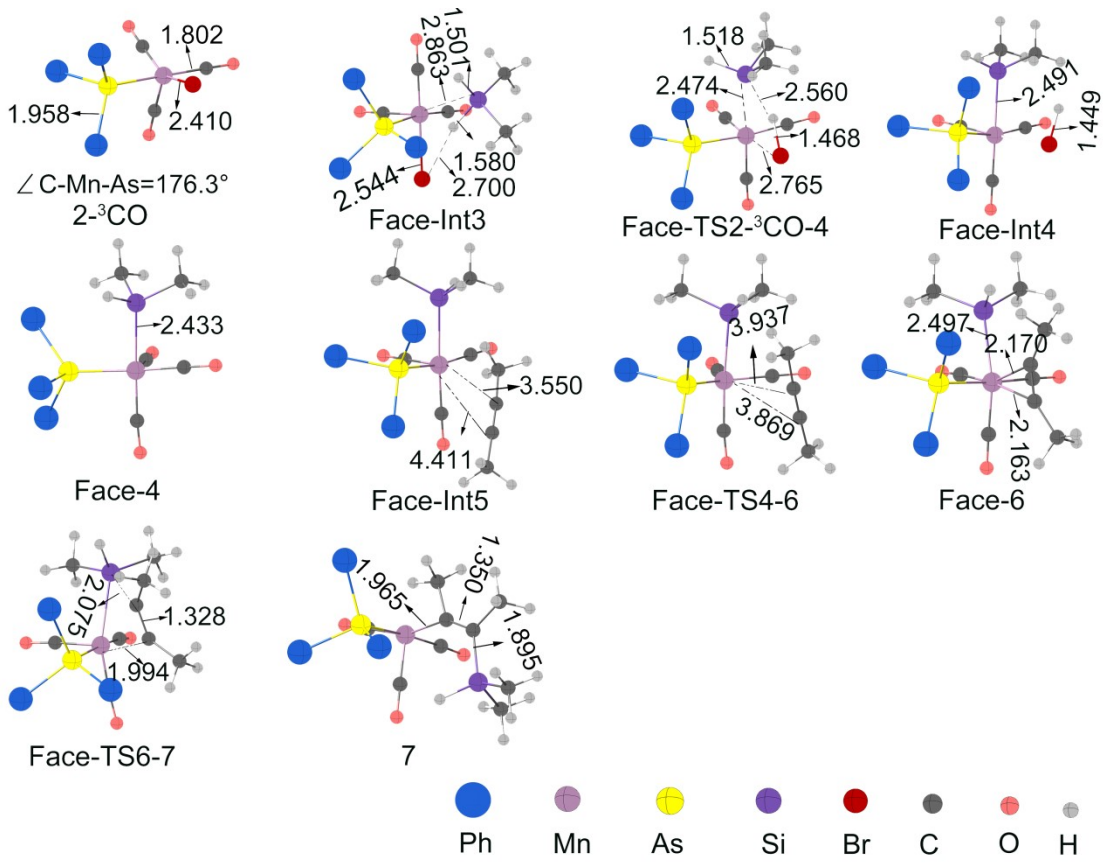

Fig.S2 Geometries and key bonds (in Å) of stationary points from facial direction 2-^{3}CO to *E*-Pro

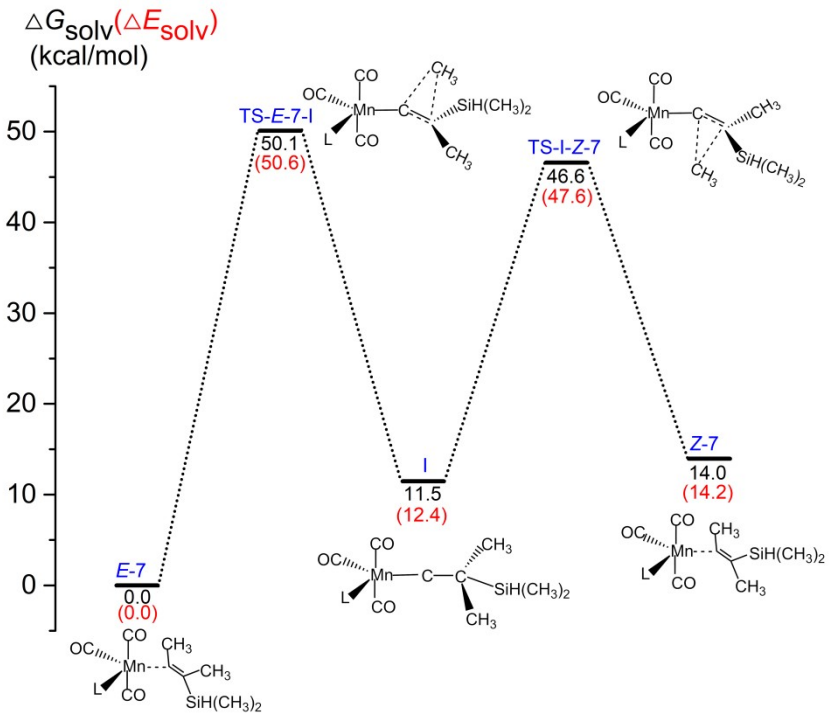

Fig. S3 Gibbs energy (kcal/mol) profile for the transformation from ***E*-7** to the **Z-7**

(electronic energies are given in parentheses)

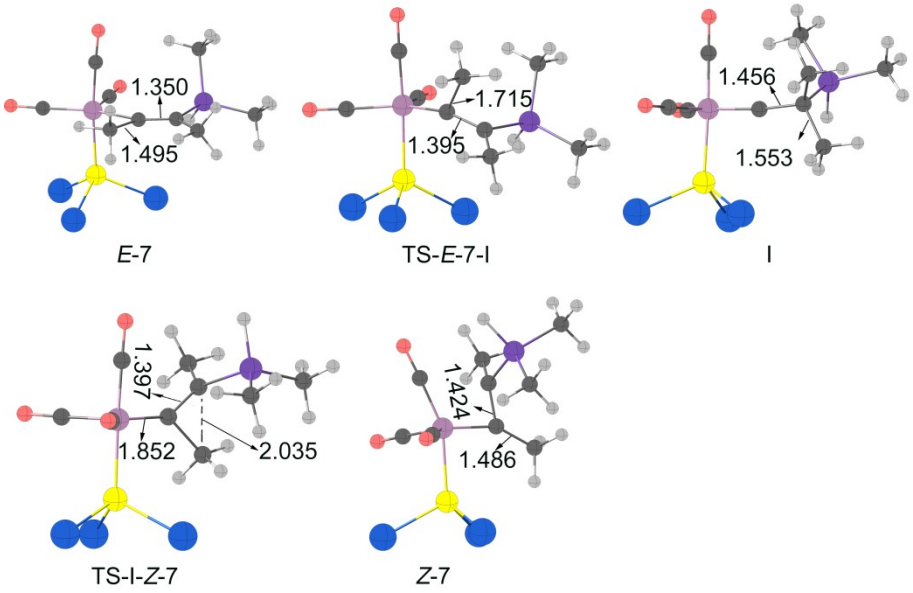

Fig. S4 Geometries and key bonds (in Å) of stationary points for the transformation from ***E-7*** to the ***Z-7***

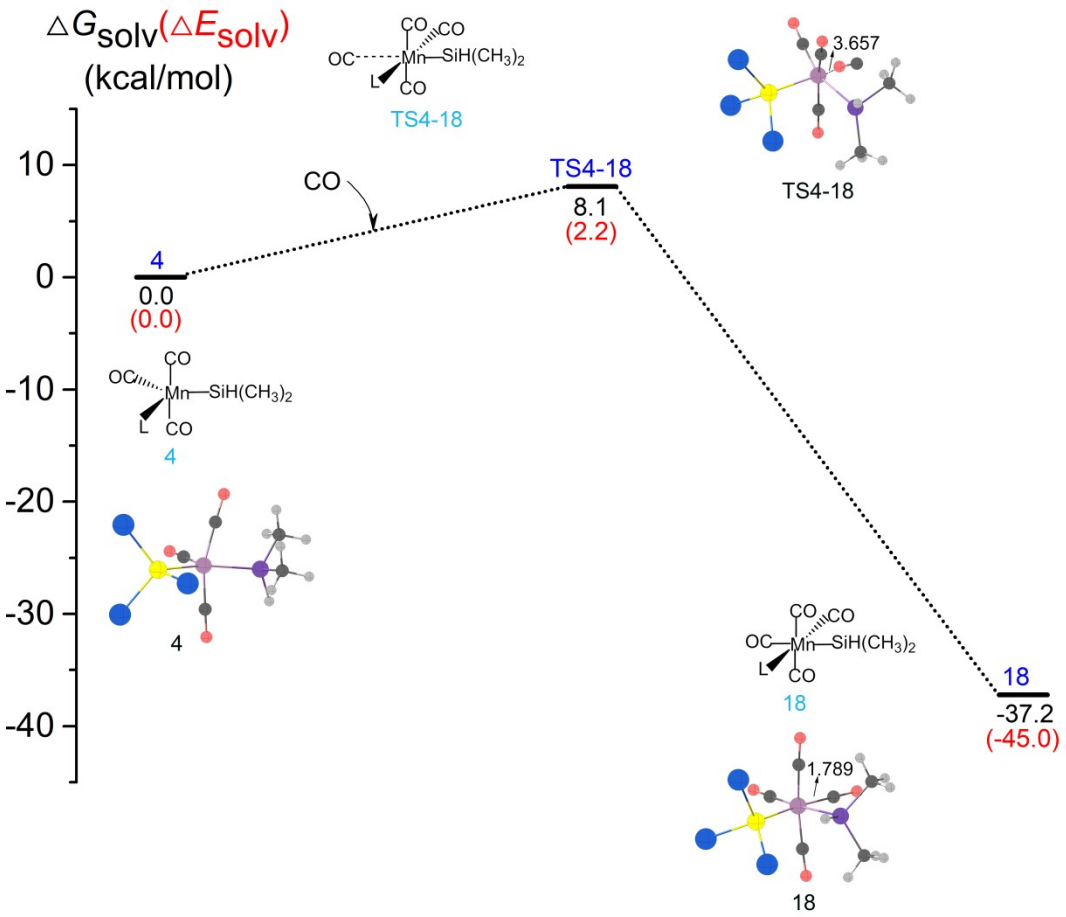

Fig. S5 Gibbs energy (kcal/mol) profile (electronic energies are given in parentheses) and geometries and key bonds (in Å) of stationary points for the transformation from **4** to the **18**

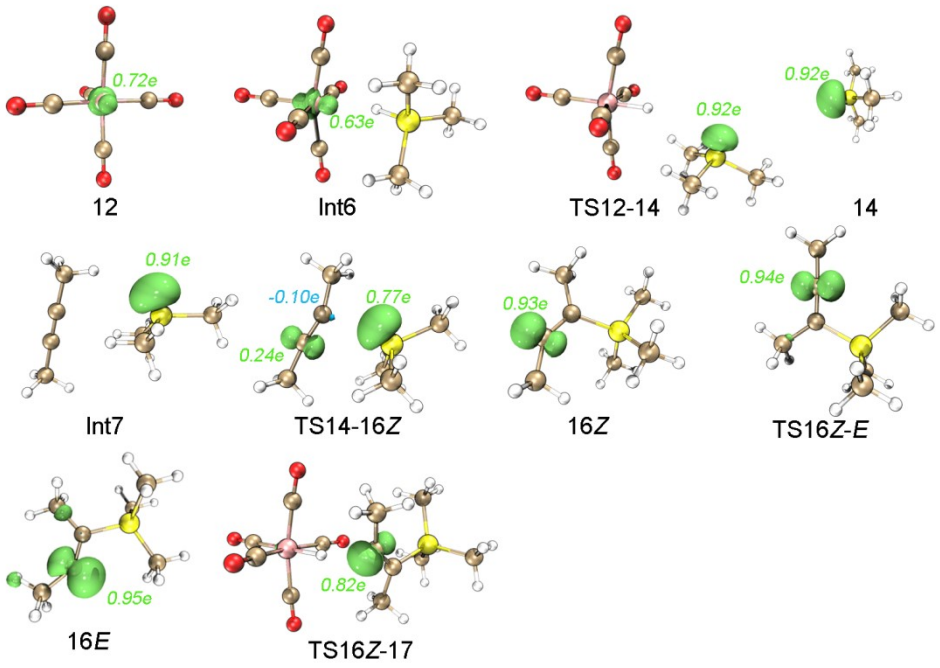

Fig. S6 Spin density isosurface graphs of of stationary points on the PES of radical mechanism (alpha electron density is green and beta density is blue, and spin population of selected atoms are shown in italics).

1-18

1	E= -4290.988550	G= -4291.030532	
Br	2.04000	0.00100	-0.00100
C	-0.36500	1.01000	1.55300
C	-0.36900	1.55300	-1.00900
C	-0.36600	-1.01000	-1.55200
C	-2.30200	-0.00100	0.00100
C	-0.36600	-1.55300	1.01000
Mn	-0.50300	0.00000	0.00000
O	-0.26300	1.63500	2.51600
O	-3.46200	-0.00200	0.00100
O	-0.27100	2.51600	-1.63400
O	-0.26500	-1.63600	-2.51400
O	-0.26500	-2.51500	1.63500
L	E= -2929.576604	G= -2929.620569	
As	0.00000	-0.00200	-1.26200
C	-0.04800	1.73300	-0.31400
C	0.78600	2.75900	-0.80800
C	-0.86400	1.99300	0.80500
C	0.81500	4.01700	-0.18500
C	-0.84100	3.25600	1.42200
C	-0.00000	4.26800	0.93200
C	1.52500	-0.82300	-0.30600
C	2.04800	-2.01900	-0.84100
C	2.10600	-0.27900	0.85700
C	3.12500	-2.66900	-0.21700
C	3.18900	-0.92700	1.47600
C	3.69900	-2.12200	0.94300
C	-1.47900	-0.90700	-0.31000
C	-2.78300	-0.70700	-0.81100

C	-1.29600	-1.74200	0.81100
C	-3.88700	-1.31500	-0.19200
C	-2.40100	-2.35900	1.42300
C	-3.69700	-2.14500	0.92600
H	1.42300	2.57500	-1.68900
H	-1.52200	1.20300	1.20100
H	1.47400	4.80700	-0.57600
H	-1.48300	3.44700	2.29600
H	0.01700	5.25600	1.41800
H	1.60800	-2.45200	-1.75500
H	1.71000	0.65400	1.28700
H	3.52100	-3.60400	-0.64300
H	3.63600	-0.49300	2.38400
H	4.54800	-2.62700	1.43000
H	-2.94200	-0.06600	-1.69400
H	-0.28400	-1.91100	1.21100
H	-4.90000	-1.14600	-0.59000
H	-2.24600	-3.01000	2.29800
H	-4.56100	-2.62800	1.40800
Int1	E= -7220.572611	G= -7220.639896	
As	1.48100	-0.01500	-0.01400
Br	-4.55100	1.45500	-0.10100
C	-4.06900	-1.33700	-1.20900
C	-2.03700	0.31300	-1.36100
C	-2.00400	0.51200	1.24800
C	-1.80900	-1.90100	0.11500
C	-4.03300	-1.13700	1.40300
C	2.44800	-0.40500	1.66500
C	1.92100	0.14300	2.85500
C	3.60500	-1.20600	1.73100

C	2.55200	-0.09500	4.08700
C	4.22900	-1.44900	2.96600
C	3.70700	-0.89300	4.14600
C	2.26200	1.75300	-0.41900
C	1.66600	2.49500	-1.46100
C	3.35700	2.30200	0.27800
C	2.16600	3.76100	-1.80900
C	3.85100	3.57100	-0.06800
C	3.25900	4.30200	-1.11200
C	2.54100	-1.12400	-1.25900
C	2.10800	-2.45100	-1.46900
C	3.68200	-0.65500	-1.94000
C	2.81700	-3.30000	-2.33500
C	4.38500	-1.50500	-2.81100
C	3.95600	-2.82800	-3.00900
H	1.01300	0.76500	2.82300
H	4.02700	-1.63900	0.81100
H	2.13500	0.34300	5.00800
H	5.13400	-2.07600	3.00600
H	4.19800	-1.08400	5.11200
H	0.80200	2.08400	-2.00800
H	3.83000	1.73400	1.09400
H	1.69400	4.32900	-2.62600
H	4.70800	3.99100	0.48200
H	3.64800	5.29600	-1.38000
H	1.21200	-2.82700	-0.95100
H	4.02900	0.37900	-1.78600
H	2.47300	-4.33500	-2.48800
H	5.27600	-1.12900	-3.33800
H	4.50800	-3.49200	-3.69200

Mn	-2.95000	-0.51700	0.02600
O	-4.77200	-1.83300	-1.97600
O	-1.07100	-2.79600	0.16900
O	-1.49000	0.84300	-2.22600
O	-1.43900	1.16500	2.01200
O	-4.71300	-1.50900	2.25500

TS1-2 E= -7220.531515 G= -7220.598680 imaginary eigenvalue= -123.05

As	1.19700	0.12900	-0.22200
Br	-3.26200	0.67300	1.43000
C	-3.69000	1.10200	-1.80700
C	-1.52200	1.79600	-0.68600
C	-1.36500	-2.06600	0.73900
C	-1.60500	-0.32400	-2.31400
C	-3.64300	-1.24500	-0.85900
C	1.16700	-0.60800	1.59900
C	1.86900	-1.77000	1.97800
C	0.32100	0.03100	2.53300
C	1.72400	-2.28500	3.27600
C	0.18600	-0.48400	3.83100
C	0.88300	-1.64600	4.20300
C	2.41200	1.65500	0.02200
C	2.46700	2.60800	-1.01700
C	3.19400	1.84600	1.18000
C	3.30600	3.72800	-0.90800
C	4.02700	2.97100	1.28800
C	4.08700	3.91100	0.24600
C	2.38300	-1.16100	-1.11600
C	1.78400	-2.29900	-1.69700
C	3.77900	-0.99100	-1.20200
C	2.57500	-3.26400	-2.34100

C	4.56600	-1.95400	-1.85400
C	3.96700	-3.09200	-2.42100
H	2.52700	-2.27700	1.25500
H	-0.25500	0.92300	2.24100
H	2.27300	-3.19500	3.56600
H	-0.48100	0.01700	4.54900
H	0.76700	-2.05700	5.21700
H	1.84700	2.47700	-1.91900
H	3.15300	1.11200	2.00000
H	3.34500	4.46500	-1.72500
H	4.63600	3.11300	2.19400
H	4.74000	4.79300	0.33500
H	0.69100	-2.43400	-1.64900
H	4.25500	-0.10400	-0.75500
H	2.10000	-4.15000	-2.78800
H	5.65700	-1.81500	-1.91700
H	4.58700	-3.84500	-2.93200
Mn	-2.50200	0.21700	-0.85900
O	-4.48900	1.69900	-2.40700
O	-1.02200	-0.68400	-3.25400
O	-1.02800	2.83800	-0.60700
O	-1.53100	-2.87100	1.53400
O	-4.41100	-2.10800	-0.88600
CO	E= -113.229850	G= -113.248995	
C	0.00000	0.00000	-0.65200
O	0.00000	0.00000	0.48900
2	E= -7107.337985	G= -7107.397813	
As	-0.55100	-0.04200	-0.00000
Br	2.67600	-1.58100	-0.00000
C	3.49000	1.33600	-0.00000

C	1.74200	0.71600	-1.84200
C	1.17400	2.49700	0.00000
C	1.74200	0.71600	1.84200
C	-1.76700	1.48900	0.00000
C	-2.12200	2.10000	-1.21900
C	-2.12200	2.10000	1.21900
C	-2.85000	3.30100	-1.21600
C	-2.85000	3.30100	1.21600
C	-3.21600	3.90100	0.00000
C	-1.18000	-1.11600	-1.51800
C	-2.54900	-1.12200	-1.85700
C	-0.27700	-1.93100	-2.22600
C	-3.00500	-1.92900	-2.91000
C	-0.74200	-2.73700	-3.27900
C	-2.10300	-2.73500	-3.62400
C	-1.18000	-1.11600	1.51800
C	-0.27700	-1.93100	2.22600
C	-2.54900	-1.12200	1.85700
C	-0.74200	-2.73700	3.27900
C	-3.00500	-1.92900	2.91000
C	-2.10300	-2.73500	3.62400
H	-1.82800	1.64500	-2.17700
H	-1.82800	1.64500	2.17700
H	-3.12700	3.77200	-2.17100
H	-3.12700	3.77200	2.17100
H	-3.78400	4.84400	0.00000
H	-3.26700	-0.49300	-1.30800
H	0.78800	-1.95600	-1.94600
H	-4.07400	-1.92600	-3.17400
H	-0.03100	-3.37100	-3.82900

H	-2.46300	-3.36600	-4.45100
H	0.78800	-1.95600	1.94600
H	-3.26700	-0.49300	1.30800
H	-0.03100	-3.37100	3.82900
H	-4.07400	-1.92600	3.17400
H	-2.46300	-3.36600	4.45100
Mn	1.75900	0.81200	-0.00000
O	4.59900	1.67500	-0.00000
O	0.82200	3.60800	0.00000
O	1.74600	0.67600	-2.99900
O	1.74700	0.67500	2.99900
3	E= -370.208420	G= -370.235467	
C	-1.56400	-0.51400	0.00000
C	1.56400	-0.51400	-0.00000
H	-0.00000	1.44800	-1.21400
H	0.00000	1.44800	1.21400
H	-2.47700	0.11600	-0.00000
H	-1.59600	-1.16500	-0.89800
H	-1.59600	-1.16500	0.89800
H	2.47700	0.11600	-0.00000
H	1.59700	-1.16500	0.89800
H	1.59600	-1.16500	-0.89700
Si	0.00000	0.55000	-0.00000
int2	E= -7477.551296	G= -7477.620466	
As	-1.11700	0.18500	-0.07300
Br	1.70400	-0.38400	2.04000
C	2.04200	-2.68100	0.11800
C	-0.36100	-2.50000	1.15200
C	-0.02200	-2.35100	-1.43200
C	1.67200	-0.40100	-1.09000

C	5.92500	0.52800	-2.02400
C	4.53000	1.94100	0.38800
C	-2.36600	-0.25500	-1.51100
C	-3.47800	-1.08000	-1.25200
C	-2.05200	0.10100	-2.83900
C	-4.28600	-1.52200	-2.31300
C	-2.86500	-0.34200	-3.89400
C	-3.98300	-1.15100	-3.63300
C	-0.61600	2.04300	-0.45300
C	-1.49100	2.89900	-1.15200
C	0.60600	2.53900	0.04200
C	-1.13300	4.24000	-1.36800
C	0.95700	3.88100	-0.17900
C	0.09200	4.73100	-0.88600
C	-2.29600	0.41700	1.47800
C	-1.87100	0.03300	2.76400
C	-3.55400	1.03300	1.30600
C	-2.71000	0.25200	3.87000
C	-4.38500	1.24700	2.41600
C	-3.96600	0.85400	3.69900
H	4.64400	-0.83200	0.03700
H	6.73200	0.24800	0.63400
H	6.53800	1.42900	-2.22500
H	6.49700	-0.36100	-2.35800
H	5.00100	0.59400	-2.63500
H	3.67300	2.13500	-0.28700
H	4.13100	1.79700	1.41200
H	5.18700	2.83500	0.38200
H	-3.71800	-1.38500	-0.22200
H	-1.17000	0.72300	-3.05700

H	-5.15500	-2.16300	-2.10300
H	-2.61800	-0.05700	-4.92800
H	-4.61700	-1.49900	-4.46200
H	-2.45200	2.52700	-1.53800
H	1.27900	1.88100	0.61400
H	-1.81800	4.90200	-1.91900
H	1.91600	4.25800	0.20700
H	0.37000	5.78200	-1.06000
H	-0.87400	-0.40900	2.91000
H	-3.89500	1.34400	0.30700
H	-2.37100	-0.05000	4.87300
H	-5.36700	1.72400	2.27600
H	-4.62000	1.02300	4.56800
Mn	0.66800	-1.51000	-0.01800
O	2.92300	-3.42800	0.20400
O	-0.45200	-2.91900	-2.35400
O	-0.99600	-3.14700	1.87100
O	2.30400	0.27200	-1.79000
Si	5.47500	0.40600	-0.18900

TS2-10 E= -7477.474853 G= -7477.541697 imaginary eigenvalue=-241.12

As	1.16700	0.08500	0.00100
Br	-2.46700	0.00300	-0.91100
C	-1.90100	-2.67400	0.69600
C	-0.28400	-2.17000	-1.26400
C	0.64400	-2.69800	1.29100
C	-0.99400	-0.52600	1.84600
C	-5.88100	-0.32300	-0.34200
C	-4.28600	2.07800	1.08700
C	2.67000	-0.40400	-1.16400
C	3.41800	0.58000	-1.84200

C	3.03700	-1.75800	-1.27000
C	4.52000	0.20600	-2.62600
C	4.14300	-2.12700	-2.05300
C	4.88400	-1.14800	-2.73300
C	2.11600	0.86400	1.53600
C	2.76100	2.11200	1.42300
C	2.19400	0.14400	2.74300
C	3.47500	2.63400	2.51300
C	2.91300	0.66900	3.82900
C	3.55300	1.91300	3.71600
C	0.42000	1.67100	-0.86500
C	0.27200	1.70700	-2.26600
C	-0.19400	2.66100	-0.07100
C	-0.47100	2.73600	-2.86700
C	-0.93700	3.68600	-0.67700
C	-1.08000	3.72400	-2.07500
H	-3.94000	-0.62700	1.60300
H	-3.78400	1.10700	-1.64700
H	-6.24600	0.36900	-1.12400
H	-5.69700	-1.31900	-0.79400
H	-6.66300	-0.43900	0.43900
H	-3.29000	2.30600	1.51500
H	-4.50700	2.79400	0.27300
H	-5.04400	2.19500	1.89100
H	3.14000	1.64300	-1.76800
H	2.46200	-2.53100	-0.73900
H	5.09800	0.97700	-3.15800
H	4.42400	-3.18900	-2.13200
H	5.74800	-1.43900	-3.35000
H	2.69800	2.68900	0.48800

H	1.69600	-0.83200	2.83700
H	3.97300	3.61200	2.42000
H	2.97000	0.10000	4.77000
H	4.11400	2.32500	4.57000
H	0.72500	0.92300	-2.89200
H	-0.10800	2.62500	1.02600
H	-0.58400	2.75800	-3.96200
H	-1.41700	4.45400	-0.05100
H	-1.67000	4.52400	-2.54800
Mn	-0.48500	-1.59500	0.45900
O	-2.81500	-3.38400	0.85700
O	1.34000	-3.46100	1.84500
O	-0.15700	-2.54100	-2.36400
O	-1.31600	0.17800	2.72400
Si	-4.32200	0.30300	0.48700
10	E= -7477.475172	G= -7477.542683	
As	1.18900	0.06000	0.02100
Br	-2.55400	0.02200	-1.02600
C	-1.85300	-2.62300	0.89400
C	-0.32000	-2.15400	-1.10900
C	0.69400	-2.60400	1.51600
C	-1.02000	-0.35500	1.81900
C	-5.85500	-0.23100	-0.29000
C	-4.13400	1.98000	1.20600
C	2.69000	-0.50700	-1.11700
C	3.43500	0.42100	-1.87200
C	3.04600	-1.86800	-1.13400
C	4.52800	-0.01400	-2.63700
C	4.14300	-2.29900	-1.89800
C	4.88500	-1.37300	-2.65000

C	2.12600	0.99500	1.47600
C	2.80900	2.20700	1.24500
C	2.13900	0.41900	2.75900
C	3.49800	2.83400	2.29400
C	2.83400	1.04900	3.80600
C	3.51300	2.25600	3.57500
C	0.43000	1.55500	-0.99300
C	0.25200	1.44100	-2.38700
C	-0.17700	2.62200	-0.30000
C	-0.51700	2.39100	-3.08000
C	-0.94600	3.56900	-0.99600
C	-1.12100	3.45400	-2.38600
H	-3.86600	-0.80800	1.60800
H	-3.59200	0.92800	-1.92500
H	-6.09600	0.49600	-1.08900
H	-5.78400	-1.24600	-0.72900
H	-6.68300	-0.23000	0.45000
H	-3.16100	2.12800	1.71200
H	-4.23100	2.69900	0.36800
H	-4.94700	2.17600	1.93700
H	3.15900	1.48600	-1.87700
H	2.46300	-2.59500	-0.54800
H	5.10400	0.71400	-3.22900
H	4.41600	-3.36500	-1.90700
H	5.74200	-1.71200	-3.25200
H	2.79700	2.67300	0.24800
H	1.60400	-0.52500	2.94100
H	4.02700	3.78200	2.10900
H	2.84000	0.59200	4.80700
H	4.05400	2.75000	4.39600

H	0.69900	0.59700	-2.93600
H	-0.06700	2.70500	0.79200
H	-0.65100	2.29400	-4.16800
H	-1.41700	4.39800	-0.44500
H	-1.72800	4.19400	-2.93000
Mn	-0.43700	-1.56500	0.60700
O	-2.77800	-3.31700	1.08400
O	1.39100	-3.32400	2.12900
O	-0.24700	-2.52400	-2.22000
O	-1.39100	0.44100	2.60500
Si	-4.27600	0.21700	0.60700

TS10-18 E= -7477.466040 G= -7477.532309 imaginary eigenvalue=-180.78

As	1.06200	0.04300	0.05300
Br	-2.70400	0.80900	-1.06800
C	-2.04000	-2.62000	-0.70500
C	-0.49100	-1.11900	-2.10200
C	0.54100	-3.00700	-0.37600
C	-0.95500	-1.59600	1.42400
C	-5.53700	0.06600	0.38800
C	-3.22300	0.87100	2.34400
C	2.60100	0.11500	-1.17700
C	3.46500	1.22900	-1.17100
C	2.87000	-0.97100	-2.02900
C	4.58700	1.25300	-2.01400
C	3.99500	-0.94400	-2.87000
C	4.85400	0.16600	-2.86500
C	2.01300	0.00100	1.77500
C	2.58000	1.16100	2.34100
C	2.19000	-1.24200	2.41300
C	3.30800	1.07700	3.53800

C	2.92200	-1.32200	3.60900
C	3.48000	-0.16400	4.17500
C	0.41500	1.89100	-0.04500
C	0.36900	2.54200	-1.29500
C	-0.20000	2.49000	1.07200
C	-0.28300	3.77800	-1.42200
C	-0.84600	3.73000	0.94200
C	-0.89500	4.37400	-0.30600
H	-3.67600	-1.72900	1.28500
H	-3.54300	2.04300	-1.50500
H	-5.72500	1.13900	0.19000
H	-5.77000	-0.51700	-0.52600
H	-6.22500	-0.27500	1.19200
H	-2.22000	0.60200	2.72100
H	-3.22400	1.92600	2.00800
H	-3.95000	0.76200	3.17800
H	3.26400	2.08700	-0.51200
H	2.20400	-1.84600	-2.03500
H	5.25700	2.12700	-2.00500
H	4.19800	-1.79800	-3.53400
H	5.73400	0.18700	-3.52500
H	2.45200	2.14000	1.85300
H	1.75900	-2.15500	1.97500
H	3.74400	1.98800	3.97600
H	3.05400	-2.29800	4.10100
H	4.05000	-0.22800	5.11400
H	0.82900	2.07300	-2.17900
H	-0.18400	1.98400	2.05000
H	-0.31600	4.27800	-2.40300
H	-1.32000	4.19200	1.82200

H	-1.40600	5.34300	-0.40800
Mn	-0.58500	-1.63500	-0.35500
O	-2.97100	-3.29300	-0.93800
O	1.23300	-3.95600	-0.38400
O	-0.38900	-0.82100	-3.23100
O	-1.14100	-1.63600	2.58500
Si	-3.78000	-0.27100	0.97000
HBr	E= -2574.363297	G= -2574.382538	
Br	0.00000	0.00000	0.04000
H	0.00000	0.00000	-1.39600
18	E= -4903.168706	G= -4903.230882	
As	0.58700	0.00400	-0.00300
C	-1.62600	-0.89400	-1.85400
C	-1.68000	-0.99200	1.77300
C	-3.30000	-1.62600	-0.10500
C	-0.93400	-2.77400	-0.09200
C	-4.08300	1.19500	1.38400
C	-3.44700	1.68800	-1.57700
C	1.28500	0.47200	1.77400
C	2.57600	0.09300	2.18800
C	0.47400	1.23900	2.63600
C	3.04400	0.46900	3.45800
C	0.94900	1.61700	3.90000
C	2.23400	1.22900	4.31600
C	0.80200	1.71800	-0.94900
C	1.39300	2.82700	-0.31400
C	0.36600	1.83400	-2.28500
C	1.53200	4.04300	-1.00400
C	0.51300	3.05100	-2.97100
C	1.09000	4.15900	-2.33100

C	2.06900	-1.04800	-0.75000
C	2.88200	-0.55700	-1.79000
C	2.31900	-2.32900	-0.21700
C	3.92900	-1.34700	-2.29500
C	3.37200	-3.10900	-0.71800
C	4.17600	-2.62100	-1.76200
H	-1.69800	2.19200	0.47600
H	-4.53600	2.20800	1.39400
H	-4.88300	0.46200	1.15400
H	-3.70200	0.97600	2.40200
H	-3.98100	2.65100	-1.43800
H	-2.66600	1.83100	-2.34900
H	-4.17300	0.93900	-1.95600
H	3.22600	-0.49300	1.52100
H	-0.53000	1.55600	2.31700
H	4.05400	0.16500	3.77600
H	0.30900	2.21700	4.56400
H	2.60400	1.52100	5.31100
H	1.74500	2.75100	0.72500
H	-0.08100	0.98000	-2.80900
H	1.99000	4.90500	-0.49500
H	0.16900	3.12900	-4.01400
H	1.19700	5.11400	-2.86800
H	2.70600	0.44400	-2.21000
H	1.69900	-2.72400	0.60200
H	4.55700	-0.95700	-3.11100
H	3.56100	-4.10600	-0.29200
H	4.99800	-3.23700	-2.15900
Mn	-1.59300	-1.09500	-0.04600
O	-4.41500	-1.96600	-0.15600

O	-1.69700	-0.81000	-3.01500
O	-0.59800	-3.89100	-0.12200
O	-1.78400	-0.95900	2.93300
Si	-2.69800	1.12100	0.07800

2-^{3}CO-4

2-^{3}CO E= -6994.059784 G= -6994.118255

As	-0.41900	0.02600	-0.01700
Br	2.61700	1.48600	0.11300
C	1.64100	-1.91900	1.00500
C	1.32000	-1.98200	-1.46500
C	3.60300	-1.24800	-0.49200
C	-0.88900	1.64500	-1.00500
C	-0.30200	1.83900	-2.27000
C	-1.80800	2.58300	-0.50000
C	-0.64800	2.96300	-3.03600
C	-2.14600	3.70900	-1.26900
C	-1.57000	3.89800	-2.53600
C	-1.81400	-1.23100	-0.57600
C	-2.77000	-0.89600	-1.55300
C	-1.82300	-2.51700	0.00300
C	-3.73300	-1.84200	-1.94500
C	-2.79000	-3.45600	-0.38800
C	-3.74500	-3.12000	-1.36400
C	-0.95200	0.40500	1.82900
C	-2.28600	0.22100	2.24300
C	0.01500	0.86000	2.74600
C	-2.65100	0.50400	3.56900
C	-0.35700	1.14000	4.07100
C	-1.68800	0.96400	4.48300
H	0.43500	1.11600	-2.65500
H	-2.26000	2.44200	0.49400
H	-0.18900	3.11200	-4.02500
H	-2.86200	4.44500	-0.87200
H	-1.83600	4.78200	-3.13500

H	-2.76800	0.10600	-2.01000
H	-1.08000	-2.79200	0.76800
H	-4.47800	-1.57600	-2.71000
H	-2.79500	-4.45600	0.07000
H	-4.50000	-3.85900	-1.67200
H	-3.04200	-0.15000	1.53400
H	1.05900	1.00000	2.42300
H	-3.69500	0.36100	3.88900
H	0.40100	1.49500	4.78500
H	-1.97700	1.18100	5.52300
Mn	1.87600	-0.77000	-0.29800
O	0.96100	-2.76000	-2.25800
O	1.48800	-2.64400	1.91000
O	4.70900	-1.58500	-0.60800

TS2-CO E= -6994.024974 G= -6994.083100 imaginary eigenvalue=-315.15

As	0.40400	0.00900	0.07100
Br	-2.90900	1.21800	-0.21000
C	-1.07800	-0.00200	-2.42300
C	-0.82700	-2.20900	-1.35000
C	-2.99900	-1.88600	-0.29800
C	0.19800	-0.05100	2.01400
C	-0.32700	-1.22800	2.58800
C	0.50400	1.05700	2.82600
C	-0.52200	-1.30100	3.97600
C	0.30000	0.97800	4.21400
C	-0.20900	-0.19800	4.78900
C	1.96900	-1.10900	-0.28200
C	2.67500	-1.75600	0.74900
C	2.37700	-1.26200	-1.62200
C	3.79000	-2.55200	0.43600

C	3.49200	-2.05600	-1.92700
C	4.19900	-2.70300	-0.89800
C	1.13200	1.78900	-0.29700
C	2.49100	2.05000	-0.02100
C	0.31600	2.79400	-0.84800
C	3.02400	3.32100	-0.28800
C	0.86000	4.06200	-1.11600
C	2.21000	4.32700	-0.83600
H	-0.58400	-2.08800	1.95100
H	0.90100	1.98200	2.37900
H	-0.92600	-2.22200	4.42300
H	0.54200	1.84400	4.84900
H	-0.36800	-0.25400	5.87700
H	2.36200	-1.64000	1.79800
H	1.82500	-0.76300	-2.43600
H	4.34200	-3.05700	1.24400
H	3.80800	-2.17400	-2.97500
H	5.07100	-3.33000	-1.14000
H	3.13700	1.26200	0.39600
H	-0.74600	2.59200	-1.05700
H	4.08500	3.52300	-0.07100
H	0.22000	4.84600	-1.54800
H	2.63300	5.32100	-1.05000
Mn	-1.59800	-0.68400	-0.88900
O	-0.34200	-3.22500	-1.67400
O	-0.80300	0.43400	-3.47600
O	-3.76700	-2.71400	-0.06300
2-^{1}CO	E= -6994.048450	G= -6994.107315	
As	-0.46800	-0.00600	0.02800
Br	3.73300	0.09200	0.15100

C	1.70400	-1.75400	-1.05600
C	0.92000	0.12500	-2.62000
C	1.67200	1.91900	-0.96600
C	-1.14800	1.69400	0.71900
C	-1.44900	2.72300	-0.19600
C	-1.29900	1.91400	2.10100
C	-1.90800	3.96300	0.27100
C	-1.75500	3.16000	2.56300
C	-2.06100	4.18300	1.65100
C	-1.99700	-0.68100	-0.99300
C	-3.28500	-0.13700	-0.82200
C	-1.80200	-1.75100	-1.89000
C	-4.37000	-0.66300	-1.54400
C	-2.89000	-2.27400	-2.60500
C	-4.17400	-1.73000	-2.43500
C	-0.46900	-1.15800	1.61500
C	-1.65700	-1.76400	2.07000
C	0.73900	-1.35700	2.31100
C	-1.63200	-2.56000	3.22600
C	0.75500	-2.15300	3.46800
C	-0.42900	-2.75400	3.92600
H	-1.32600	2.56100	-1.27900
H	-1.06500	1.11400	2.82000
H	-2.14500	4.76300	-0.44700
H	-1.87200	3.33000	3.64400
H	-2.41700	5.15900	2.01600
H	-3.44800	0.70100	-0.12700
H	-0.80200	-2.18500	-2.03700
H	-5.37400	-0.23200	-1.40800
H	-2.73000	-3.10900	-3.30400

H -5.02500 -2.13800 -3.00200

H -2.60200 -1.62000 1.52300

H 1.67200 -0.89600 1.94500

H -2.56000 -3.03500 3.58000

H 1.70100 -2.30700 4.00900

H -0.41400 -3.38100 4.83000

Mn 1.62500 0.07900 -1.00700

O 0.50700 0.15900 -3.71600

O 1.75300 -2.91200 -1.12600

O 1.71300 3.07800 -0.97900

3 E= -370.208420 G= -370.235467

C -1.56400 -0.51400 0.00000

C 1.56400 -0.51400 -0.00000

H -0.00000 1.44800 -1.21400

H 0.00000 1.44800 1.21400

H -2.47700 0.11600 -0.00000

H -1.59600 -1.16500 -0.89800

H -1.59600 -1.16500 0.89800

H 2.47700 0.11600 -0.00000

H 1.59700 -1.16500 0.89800

H 1.59600 -1.16500 -0.89700

Si 0.00000 0.55000 -0.00000

INT3 E= -7364.280083 G= -7364.344196

As 0.83800 0.12300 -0.00500

Br -1.45800 -2.41000 0.05800

C -1.68900 0.16100 1.74300

C -1.64700 1.91900 -0.15600

C -1.57000 0.01500 -1.91700

C -5.38500 -0.68200 -0.77800

C -4.67800 1.65500 1.15600

C	1.84300	-1.24700	-0.99200
C	1.29300	-1.90000	-2.11100
C	3.16300	-1.53700	-0.59200
C	2.06400	-2.82800	-2.83000
C	3.92800	-2.46700	-1.31300
C	3.38000	-3.11300	-2.43300
C	1.68400	1.76400	-0.66400
C	2.44800	1.75600	-1.84800
C	1.46800	2.97900	0.01900
C	2.99300	2.95300	-2.34000
C	2.02500	4.17100	-0.47200
C	2.78700	4.16000	-1.65300
C	1.60900	-0.09600	1.78700
C	1.17100	-1.19500	2.55500
C	2.59300	0.77000	2.30100
C	1.71100	-1.41700	3.83100
C	3.12600	0.54400	3.58200
C	2.68700	-0.54700	4.34800
H	-3.05100	-0.46100	-0.01400
H	-4.03400	1.57600	-1.58800
H	-6.37300	-0.23900	-1.02000
H	-5.03800	-1.27100	-1.65100
H	-5.50500	-1.37200	0.08100
H	-4.62800	1.00600	2.05300
H	-4.04100	2.54500	1.32700
H	-5.72700	1.99500	1.03100
H	0.25900	-1.70400	-2.42200
H	3.60000	-1.03800	0.28700
H	1.62500	-3.33600	-3.70200
H	4.95800	-2.68900	-0.99300

H	3.98000	-3.84600	-2.99600
H	2.62100	0.81400	-2.38900
H	0.86300	3.00500	0.93800
H	3.58700	2.93800	-3.26600
H	1.85600	5.11400	0.07000
H	3.21800	5.09600	-2.03900
H	0.40700	-1.88100	2.15100
H	2.95500	1.62200	1.70700
H	1.36500	-2.27600	4.42500
H	3.89400	1.22600	3.97900
H	3.10600	-0.72200	5.35100
Mn	-1.58100	0.15100	-0.09100
O	-1.69700	3.08900	-0.19200
O	-1.81100	0.18200	2.89600
O	-1.61400	-0.04900	-3.07700
Si	-4.14800	0.69600	-0.37500

TS2-^{1}CO-4 E= -7364.245369 G= -7364.309395 imaginary eigenvalue=-525.85

As	-0.86400	0.12800	0.00300
Br	1.72400	-2.32900	0.01200
C	1.64000	0.26200	-2.02600
C	1.36200	2.18200	-0.41500
C	1.92400	0.65900	1.53000
C	4.52400	2.35500	0.40200
C	4.94500	-0.66600	0.42600
C	-2.02000	1.55700	-0.68000
C	-2.95100	1.34100	-1.71300
C	-1.88700	2.84300	-0.11700
C	-3.74000	2.40500	-2.18100
C	-2.68300	3.90100	-0.58300
C	-3.60900	3.68500	-1.61800

C	-1.57800	-0.09900	1.82100
C	-2.82600	0.43200	2.20200
C	-0.82400	-0.84100	2.75100
C	-3.30900	0.22700	3.50500
C	-1.31400	-1.05100	4.05000
C	-2.55500	-0.51400	4.43000
C	-1.60900	-1.46500	-0.88300
C	-2.49800	-2.33500	-0.22300
C	-1.21600	-1.74300	-2.20800
C	-2.99500	-3.46900	-0.88800
C	-1.72300	-2.87200	-2.87200
C	-2.61100	-3.73800	-2.21200
H	2.96700	-1.55100	0.11800
H	4.37100	0.76000	-1.83100
H	4.29700	2.37500	1.48700
H	5.62200	2.44800	0.27200
H	4.04000	3.23500	-0.06600
H	4.85400	-1.66200	-0.05900
H	6.01400	-0.38100	0.33400
H	4.71700	-0.77500	1.50700
H	-3.06900	0.33900	-2.15500
H	-1.16300	3.02700	0.69200
H	-4.46500	2.22900	-2.99100
H	-2.57400	4.90100	-0.13700
H	-4.22900	4.51600	-1.98600
H	-3.42600	1.01000	1.48200
H	0.15000	-1.26600	2.46400
H	-4.28300	0.64900	3.79700
H	-0.71900	-1.63200	4.77000
H	-2.93600	-0.67200	5.45100

H	-2.80700	-2.13100	0.81300
H	-0.51300	-1.07800	-2.73100
H	-3.68800	-4.14600	-0.36500
H	-1.41500	-3.07800	-3.90800
H	-3.00200	-4.62700	-2.73000
Mn	1.49900	0.45000	-0.22200
O	1.28400	3.34600	-0.55100
O	1.78600	0.18000	-3.18200
O	2.26200	0.83000	2.63800
Si	3.90100	0.73800	-0.38900
INT4	E= -7364.248008	G= -7364.312034	
As	-0.87100	-0.13900	0.03600
Br	1.80700	2.29700	0.00200
C	2.04200	-0.54500	1.52100
C	1.28200	-2.18700	-0.27500
C	1.54100	-0.29200	-2.01300
C	4.97500	0.60600	0.13600
C	4.49100	-2.40900	0.33500
C	-1.49200	1.72600	0.16500
C	-1.35200	2.54900	-0.97500
C	-1.99000	2.27400	1.36200
C	-1.71600	3.90400	-0.91600
C	-2.34900	3.63200	1.41600
C	-2.21400	4.44800	0.28100
C	-2.00500	-0.77200	-1.44100
C	-3.24600	-0.16200	-1.72100
C	-1.57800	-1.86200	-2.22500
C	-4.04500	-0.63600	-2.77300
C	-2.38200	-2.33500	-3.27500
C	-3.61400	-1.72200	-3.55300

C	-1.75000	-0.95600	1.59300
C	-1.10800	-0.87100	2.84500
C	-2.98800	-1.61800	1.49000
C	-1.70900	-1.42700	3.98600
C	-3.58100	-2.18300	2.63200
C	-2.94500	-2.08500	3.88100
H	3.24800	2.23900	0.14600
H	4.22900	-0.95600	-1.97100
H	6.04000	0.30500	0.05000
H	4.87500	1.53600	-0.46600
H	4.78200	0.83600	1.20600
H	4.34900	-2.35900	1.43400
H	3.94500	-3.29900	-0.03900
H	5.57300	-2.55200	0.12900
H	-0.96800	2.12900	-1.91900
H	-2.10600	1.64100	2.25400
H	-1.61000	4.53600	-1.81000
H	-2.74200	4.05300	2.35500
H	-2.49700	5.51000	0.32700
H	-3.59300	0.69200	-1.11800
H	-0.61700	-2.35500	-2.01900
H	-5.01000	-0.15000	-2.98600
H	-2.03700	-3.18700	-3.88100
H	-4.24000	-2.09100	-4.38000
H	-0.13000	-0.37400	2.93600
H	-3.49500	-1.69900	0.51700
H	-1.20200	-1.35200	4.96000
H	-4.54600	-2.70400	2.54200
H	-3.41200	-2.52900	4.77400
Mn	1.47900	-0.45100	-0.20000

O	1.15700	-3.35600	-0.32000
O	2.48500	-0.61100	2.60500
O	1.61600	-0.20700	-3.17600
Si	3.85900	-0.82000	-0.50400
HBr	E= -2574.363297	G= -2574.382538	
Br	0.00000	0.00000	0.04000
H	0.00000	0.00000	-1.39600
4	E= -4789.867139	G= -4789.929596	
As	-0.71700	0.04500	-0.09900
C	1.64200	-1.99500	-0.33000
C	1.51800	-0.46600	-2.30300
C	2.10600	1.50400	-0.85700
C	3.95200	0.16800	1.70700
C	5.15700	0.51900	-1.15700
C	-0.56100	0.26300	1.84600
C	-0.07100	-0.82600	2.60300
C	-0.77700	1.50800	2.47000
C	0.18300	-0.66900	3.97400
C	-0.52100	1.65600	3.84300
C	-0.04000	0.57100	4.59500
C	-1.91400	-1.48800	-0.28800
C	-2.84600	-1.84200	0.70800
C	-1.81000	-2.26000	-1.46100
C	-3.67400	-2.96100	0.52300
C	-2.64500	-3.37400	-1.64300
C	-3.57600	-3.72500	-0.65200
C	-1.83900	1.55900	-0.63300
C	-1.21000	2.75800	-1.01800
C	-3.24500	1.47100	-0.63300
C	-1.98500	3.87100	-1.38400

C	-4.01500	2.58500	-1.00500
C	-3.38700	3.78500	-1.37800
H	4.38500	-1.87000	-0.11300
H	4.95700	-0.03200	2.13600
H	3.76200	1.25900	1.76600
H	3.20100	-0.34500	2.34200
H	6.18100	0.34900	-0.76300
H	5.13300	0.16600	-2.20800
H	4.95300	1.60800	-1.15600
H	0.10200	-1.80300	2.12400
H	-1.15000	2.36300	1.88500
H	0.55900	-1.52200	4.56000
H	-0.69900	2.62900	4.32700
H	0.16200	0.69300	5.67000
H	-2.92000	-1.25000	1.63400
H	-1.07100	-1.99500	-2.23500
H	-4.39800	-3.23900	1.30500
H	-2.56100	-3.97500	-2.56200
H	-4.22500	-4.60300	-0.79300
H	-0.11200	2.82800	-1.03700
H	-3.74500	0.53300	-0.34600
H	-1.48800	4.80700	-1.68200
H	-5.11300	2.51200	-1.00600
H	-3.99400	4.65600	-1.67200
Mn	1.56400	-0.20100	-0.58300
O	1.46500	-0.65200	-3.46200
O	2.51300	2.58200	-1.07200
O	1.71900	-3.15500	-0.20700
Si	3.88600	-0.43600	-0.11300

5	E= -155.736538	G= -155.763309	
C	0.61300	-0.00100	-0.00000
C	-0.61300	-0.00000	-0.00000
C	-2.07200	0.00000	0.00000
C	2.07200	0.00000	0.00000
H	-2.48000	0.95700	-0.39000
H	-2.48100	-0.81600	-0.63300
H	-2.48000	-0.14000	1.02300
H	2.48000	1.02300	-0.14200
H	2.48000	-0.38800	0.95700
H	2.48100	-0.63400	-0.81500
INT5	E= -4945.613978	G= -4945.679953	
As	-0.65600	0.31700	-0.01900
C	1.62000	-1.55400	-1.52200
C	1.91400	0.93900	-1.52900
C	2.24400	0.90000	1.02600
C	4.75500	-1.53500	1.11200
C	5.05700	1.00100	-0.60800
C	-0.56200	-3.73400	0.48600
C	0.29100	-3.03100	1.01400
C	1.27800	-2.13900	1.59300
C	-1.59100	-4.53700	-0.16000
C	-2.06400	-0.73300	-0.89900
C	-3.37200	-0.82600	-0.38100
C	-1.75200	-1.37500	-2.11200
C	-4.35100	-1.56300	-1.06800
C	-2.73500	-2.10500	-2.80000
C	-4.03500	-2.20300	-2.27800
C	-1.09100	2.13300	-0.65000
C	-2.30100	2.41300	-1.31600

C	-0.16700	3.17500	-0.42700
C	-2.58400	3.72100	-1.74300
C	-0.45900	4.48300	-0.84600
C	-1.66700	4.75800	-1.50700
C	-1.30100	0.41400	1.84400
C	-1.76100	-0.74700	2.50100
C	-1.19100	1.61900	2.56600
C	-2.11600	-0.69600	3.85900
C	-1.54500	1.66400	3.92400
C	-2.00900	0.50900	4.57400
H	4.40900	-1.46000	-1.61200
H	5.86000	-1.60600	1.03300
H	4.51200	-0.99700	2.05200
H	4.35500	-2.56600	1.18800
H	6.13800	0.76800	-0.70300
H	4.74000	1.55400	-1.51500
H	4.91900	1.66800	0.26700
H	0.82700	-1.33700	2.20900
H	2.01000	-2.66900	2.24000
H	2.01700	-1.72400	0.80900
H	-2.54900	-3.97800	-0.22000
H	-1.29900	-4.79600	-1.20000
H	-1.78000	-5.48500	0.38500
H	-3.63500	-0.32100	0.56100
H	-0.73500	-1.31600	-2.52500
H	-5.36900	-1.63200	-0.65500
H	-2.47900	-2.60400	-3.74800
H	-4.80400	-2.78100	-2.81400
H	-3.02800	1.61100	-1.50800
H	0.79200	2.97300	0.07400

H	-3.53000	3.92800	-2.26600
H	0.26900	5.28700	-0.66300
H	-1.89200	5.78200	-1.84300
H	-1.83700	-1.70000	1.95500
H	-0.83400	2.53400	2.07000
H	-2.47800	-1.60700	4.36000
H	-1.45800	2.61200	4.47600
H	-2.28700	0.54700	5.63800
Mn	1.66700	-0.24200	-0.26000
O	2.09400	1.71700	-2.38900
O	2.66400	1.63200	1.83800
O	1.65900	-2.38300	-2.34400
Si	4.05400	-0.60800	-0.40600

TS4-6 E= -4945.603541 G= -4945.671398 imaginary eigenvalue=-116.49

As	0.92400	-0.01700	0.02900
C	-1.78500	0.69400	-1.35700
C	-1.62500	-1.38400	1.52500
C	-2.09600	-1.81500	-0.96400
C	-4.80100	-1.45700	0.86900
C	-4.66800	1.24900	-0.47900
C	-1.62600	3.41800	0.98800
C	-1.20900	2.72700	1.91300
C	-0.73000	1.93500	3.04000
C	-2.11300	4.25400	-0.10400
C	1.14300	-1.64500	-1.04700
C	0.86600	-1.59000	-2.43100
C	1.46500	-2.87800	-0.44300
C	0.91800	-2.76100	-3.20200
C	1.51500	-4.04500	-1.22200
C	1.24100	-3.98900	-2.59900

C	1.80300	1.34400	-1.06000
C	2.91200	1.04300	-1.87700
C	1.29300	2.65600	-1.01800
C	3.50400	2.05600	-2.64900
C	1.89200	3.66500	-1.79000
C	2.99500	3.36600	-2.60700
C	2.15300	-0.26800	1.53400
C	1.72400	-1.03400	2.63800
C	3.43700	0.31200	1.54000
C	2.58700	-1.23900	3.72700
C	4.29000	0.11100	2.63700
C	3.87000	-0.66700	3.72900
H	-3.56300	0.75000	1.98200
H	-5.79600	-1.13700	1.24300
H	-4.94900	-1.98000	-0.09800
H	-4.37600	-2.18400	1.58900
H	-5.66900	1.39600	-0.02200
H	-4.18400	2.23900	-0.58400
H	-4.81000	0.82700	-1.49500
H	-1.36000	1.03400	3.19400
H	0.31300	1.58800	2.88500
H	-0.74800	2.52200	3.98100
H	-3.16100	4.57600	0.06900
H	-1.49800	5.17100	-0.21900
H	-2.08900	3.70900	-1.07100
H	0.60700	-0.63200	-2.90800
H	1.68000	-2.93100	0.63500
H	0.69900	-2.71300	-4.27900
H	1.76900	-5.00400	-0.74800
H	1.27500	-4.90700	-3.20500

H	3.31000	0.01800	-1.92000
H	0.42900	2.88600	-0.37600
H	4.36800	1.82000	-3.28900
H	1.48800	4.68800	-1.75600
H	3.46000	4.15600	-3.21600
H	0.71400	-1.46800	2.65900
H	3.77500	0.92500	0.69100
H	2.24800	-1.84200	4.58300
H	5.29200	0.56700	2.63600
H	4.54200	-0.82200	4.58700
Mn	-1.44700	-0.49000	-0.03500
O	-2.03500	1.46400	-2.20400
O	-2.44600	-2.72900	-1.61500
O	-1.82400	-1.93900	2.54000
Si	-3.67000	0.06000	0.63000
6	E= -4945.637415	G= -4945.702628	
As	-0.80700	-0.02700	0.02600
C	1.80800	-1.26900	-1.40400
C	1.62000	-1.20800	1.20300
C	1.69000	1.36100	1.07100
C	1.27000	1.15500	-1.95400
C	2.31000	1.62400	-1.39300
C	3.36000	2.65300	-1.27900
C	0.32400	1.08200	-3.08200
C	4.45200	-2.23200	0.32100
C	4.81000	0.59300	1.40900
C	-1.76200	1.69300	0.08600
C	-1.09700	2.88100	-0.27300
C	-3.10200	1.75100	0.52400
C	-1.77100	4.11300	-0.21200

C	-3.77200	2.98300	0.58200
C	-3.10800	4.16500	0.21300
C	-1.54400	-0.82200	1.66900
C	-1.11800	-0.28100	2.89900
C	-2.46300	-1.88700	1.65700
C	-1.61200	-0.79800	4.10600
C	-2.95200	-2.40500	2.87000
C	-2.52900	-1.86300	4.09300
C	-1.78200	-1.02200	-1.35900
C	-2.85000	-0.46600	-2.08900
C	-1.35500	-2.33600	-1.64200
C	-3.48500	-1.21900	-3.09200
C	-1.99900	-3.08800	-2.63800
C	-3.06200	-2.53000	-3.36700
H	4.62200	-0.04300	-1.27800
H	3.21700	3.27200	-0.36900
H	4.37300	2.20600	-1.22000
H	3.32900	3.32200	-2.16400
H	0.22900	0.04800	-3.47200
H	-0.69500	1.40600	-2.78400
H	0.66400	1.74000	-3.90800
H	4.03200	-2.90000	-0.45800
H	5.55800	-2.31600	0.28500
H	4.10900	-2.59800	1.30900
H	4.64900	1.68400	1.30400
H	4.41200	0.28900	2.39900
H	5.90200	0.39700	1.40100
H	-0.04600	2.84600	-0.60000
H	-3.62500	0.83100	0.83200
H	-1.24300	5.03700	-0.49300

H	-4.81800	3.01900	0.92400
H	-3.63400	5.13100	0.26300
H	-0.39600	0.55100	2.92100
H	-2.80400	-2.31800	0.70400
H	-1.27400	-0.36900	5.06100
H	-3.67000	-3.24000	2.85400
H	-2.91300	-2.27100	5.04000
H	-3.19100	0.56000	-1.88100
H	-0.51600	-2.77900	-1.08400
H	-4.31600	-0.77500	-3.66100
H	-1.66100	-4.11500	-2.84900
H	-3.56100	-3.11800	-4.15200
Mn	1.56500	-0.00800	-0.11300
O	1.65600	-1.99900	2.06700
O	1.83600	2.24500	1.82300
O	1.97800	-2.04300	-2.26300
Si	3.95100	-0.41300	0.03500

TS6-7 E= -4945.615608 G= -4945.679493 imaginary eigenvalue=-119.66

As	-0.85800	0.02200	-0.07400
C	1.40300	1.20200	1.26000
C	1.73600	1.26500	-1.36900
C	1.49300	-1.23700	-1.46400
C	1.84000	-1.44000	1.25200
C	3.08400	-1.24300	0.82400
C	4.07300	-2.36000	0.55300
C	1.16100	-2.54900	1.95700
C	4.08400	2.35400	0.59300
C	4.88500	0.18600	-1.44700
C	-1.71900	-0.82600	1.48500
C	-1.43300	-0.28800	2.75800

C	-2.58200	-1.93100	1.37900
C	-1.99700	-0.85900	3.90900
C	-3.14000	-2.50500	2.53600
C	-2.84700	-1.97400	3.80100
C	-1.75400	1.77400	0.01100
C	-3.08300	1.86000	0.47700
C	-1.08500	2.94300	-0.39900
C	-3.73400	3.10300	0.52600
C	-1.74100	4.18500	-0.34700
C	-3.06300	4.26700	0.11500
C	-1.79800	-0.82900	-1.57400
C	-2.66200	-0.09700	-2.41100
C	-1.56800	-2.19600	-1.83600
C	-3.29600	-0.73100	-3.49400
C	-2.21200	-2.82700	-2.91200
C	-3.07600	-2.09500	-3.74400
H	5.17900	0.06800	1.27900
H	3.93300	-2.77000	-0.47100
H	5.13300	-2.04500	0.65200
H	3.89300	-3.18800	1.26900
H	0.54600	-2.17200	2.80100
H	0.44200	-3.05800	1.27900
H	1.87600	-3.30200	2.35400
H	3.76900	2.58700	1.62900
H	5.13500	2.69700	0.47600
H	3.44500	2.92000	-0.11000
H	4.86700	-0.87800	-1.75100
H	4.33800	0.77200	-2.21200
H	5.94200	0.52600	-1.44000
H	-0.76900	0.58300	2.86000

H	-2.83300	-2.35200	0.39400
H	-1.76900	-0.43000	4.89600
H	-3.81200	-3.37200	2.44100
H	-3.28500	-2.42400	4.70500
H	-3.61500	0.95400	0.80700
H	-0.05100	2.89400	-0.76700
H	-4.77100	3.16000	0.89100
H	-1.20800	5.09300	-0.66900
H	-3.57400	5.24200	0.15700
H	-2.84600	0.97100	-2.22000
H	-0.88200	-2.77800	-1.20200
H	-3.96700	-0.15000	-4.14500
H	-2.03100	-3.89500	-3.10500
H	-3.57600	-2.58800	-4.59100
Mn	1.50200	0.00700	-0.12100
O	1.92100	2.10100	-2.17600
O	1.56600	-2.00300	-2.34000
O	1.24200	1.96200	2.13300
Si	4.11500	0.47400	0.26700
7	E= -4945.654667	G= -4945.719296	
As	0.90300	0.08900	-0.00200
C	0.79200	-2.96400	0.32200
C	-1.82400	-3.07000	0.60800
C	-1.00400	-1.74800	-1.30600
C	-1.84900	-0.53200	1.24800
C	-2.90700	0.29700	1.11600
C	-3.49300	1.06000	2.29100
C	-1.07700	-0.93200	2.46400
C	-4.86400	1.99600	-0.60100
C	-4.69400	-1.06700	-1.03900

C	1.95400	0.66000	1.55900
C	2.48600	-0.35200	2.38600
C	2.21500	2.01100	1.85800
C	3.27200	-0.01400	3.49800
C	3.00000	2.34500	2.97500
C	3.52700	1.33500	3.79700
C	2.33100	-0.16800	-1.32700
C	3.40700	0.74200	-1.38400
C	2.27500	-1.24100	-2.23500
C	4.41500	0.57800	-2.34700
C	3.28600	-1.40000	-3.19900
C	4.35600	-0.49300	-3.25600
C	0.08600	1.74900	-0.63100
C	0.15100	2.09700	-1.99400
C	-0.68100	2.53500	0.25500
C	-0.53900	3.22500	-2.46600
C	-1.36000	3.66800	-0.22100
C	-1.29500	4.01200	-1.58200
H	-2.65000	0.70300	-1.64200
H	-3.44200	2.16000	2.12800
H	-4.57000	0.82600	2.43900
H	-2.97000	0.83900	3.24400
H	-1.68000	-1.47500	3.21900
H	-0.22900	-1.70000	2.23000
H	-0.50900	-0.10600	2.94000
H	-4.30700	2.92600	-0.36800
H	-5.32900	2.12100	-1.60100
H	-5.68100	1.88700	0.14200
H	-5.15900	-0.96800	-2.04200
H	-4.03900	-1.96100	-1.05100

H	-5.50100	-1.24700	-0.30000
H	2.29400	-1.41200	2.15600
H	1.80900	2.81100	1.21900
H	3.68500	-0.81000	4.13600
H	3.19900	3.40300	3.20300
H	4.13900	1.60000	4.67300
H	3.46600	1.58000	-0.67400
H	1.44400	-1.95800	-2.20300
H	5.25400	1.29000	-2.38400
H	3.23500	-2.24100	-3.90600
H	5.14800	-0.62000	-4.00900
H	0.73900	1.48400	-2.69500
H	-0.75200	2.27000	1.31900
H	-0.48500	3.49000	-3.53300
H	-1.95100	4.28000	0.47800
H	-1.83500	4.89600	-1.95300
Mn	-0.59100	-1.78900	0.41300
O	-2.65000	-3.89000	0.68300
O	-1.28600	-1.75000	-2.44400
O	1.65600	-3.75100	0.27300
Si	-3.70800	0.49100	-0.59000
3	E= -370.208420	G= -370.235467	
C	-1.56400	-0.51400	0.00000
C	1.56400	-0.51400	-0.00000
H	-0.00000	1.44800	-1.21400
H	0.00000	1.44800	1.21400
H	-2.47700	0.11600	-0.00000
H	-1.59600	-1.16500	-0.89800
H	-1.59600	-1.16500	0.89800
H	2.47700	0.11600	-0.00000

H	1.59700	-1.16500	0.89800
H	1.59600	-1.16500	-0.89700
Si	0.00000	0.55000	-0.00000

TS7-8 E= -5315.843796 G= -5315.915552 imaginary eigenvalue=-70.21

As	-1.34000	0.22900	0.04400
C	1.66100	0.18000	1.12000
C	1.01600	2.17800	-0.17200
C	0.60200	1.06400	-2.23000
C	2.78600	-0.06800	-1.26900
C	4.10000	0.19400	-0.99800
C	5.18600	-0.59100	-1.74000
C	2.47100	-1.11100	-2.33900
C	5.65100	0.30000	1.64100
C	3.97200	2.81200	1.01600
C	2.85800	-3.35200	0.46000
C	-0.00200	-4.38600	-0.40700
C	-2.44400	-0.71600	-1.28100
C	-1.81800	-1.57100	-2.20600
C	-3.84500	-0.56100	-1.31200
C	-2.58200	-2.27700	-3.14900
C	-4.60700	-1.26500	-2.25900
C	-3.97800	-2.12400	-3.17600
C	-1.74100	-0.77200	1.68200
C	-2.50500	-1.95500	1.67200
C	-1.16100	-0.32700	2.88800
C	-2.67900	-2.68900	2.85800
C	-1.34700	-1.05700	4.07100
C	-2.10100	-2.24300	4.05700
C	-2.39100	1.86900	0.28000
C	-2.28000	2.86700	-0.71000

C	-3.24200	2.07000	1.38300
C	-3.02100	4.05300	-0.59800
C	-3.97700	3.26300	1.49300
C	-3.86800	4.25500	0.50500
H	6.07900	1.98000	-0.50600
H	5.09800	-0.47700	-2.84400
H	6.21000	-0.26400	-1.46700
H	5.13000	-1.68300	-1.53000
H	3.02500	-2.05900	-2.16900
H	1.39900	-1.38800	-2.41700
H	2.76600	-0.73400	-3.34400
H	6.26300	-0.53000	1.23400
H	6.29400	0.90600	2.31300
H	4.83200	-0.13900	2.24700
H	3.54000	3.48500	0.25200
H	3.15800	2.48900	1.69200
H	4.69900	3.39500	1.61800
H	0.51900	-2.88400	1.90900
H	0.69300	-1.72500	-0.20100
H	3.39700	-2.41700	0.71500
H	3.13900	-4.13300	1.19600
H	3.19500	-3.68300	-0.54200
H	-1.08500	-4.15300	-0.37100
H	0.30600	-4.44800	-1.47000
H	0.15800	-5.38000	0.06000
H	-0.72400	-1.68600	-2.19000
H	-4.34300	0.11300	-0.59900
H	-2.08200	-2.94400	-3.86800
H	-5.70000	-1.13900	-2.28100
H	-4.57800	-2.67300	-3.91800

H	-2.96500	-2.31100	0.73700
H	-0.55200	0.59100	2.90700
H	-3.27200	-3.61700	2.84100
H	-0.89200	-0.70200	5.00900
H	-2.23700	-2.82100	4.98300
H	-1.61800	2.72200	-1.57700
H	-3.33600	1.29600	2.16000
H	-2.93000	4.82700	-1.37500
H	-4.64000	3.41600	2.35800
H	-4.44400	5.18900	0.59400
Mn	0.97300	0.47600	-0.53400
O	0.98600	3.33100	0.05300
O	0.40400	1.57800	-3.25900
O	2.16000	0.04900	2.16800
Si	4.91400	1.36500	0.24700
Si	0.99600	-3.06200	0.49400
8	E= -5315.841578	G= -5315.912819	
As	-1.30900	0.10400	-0.01400
C	1.59000	-0.02100	0.97900
C	1.13300	1.60400	-1.06900
C	0.42400	-0.29600	-2.46600
C	2.95200	-0.43600	-1.34000
C	4.11500	0.16800	-0.93100
C	5.45400	-0.29600	-1.52700
C	3.05600	-1.48900	-2.43800
C	5.32100	0.65200	1.85500
C	3.32100	2.83500	0.98000
C	3.06100	-3.11900	0.72300
C	0.09000	-3.14200	1.75700
C	-2.66000	-1.19600	-0.62000

C	-2.25700	-2.37200	-1.28000
C	-4.03500	-0.94500	-0.42600
C	-3.21500	-3.29800	-1.72600
C	-4.99000	-1.87300	-0.87100
C	-4.58100	-3.05200	-1.51900
C	-1.62700	0.16400	1.92400
C	-2.45600	-0.75600	2.59200
C	-0.93300	1.14200	2.66700
C	-2.58700	-0.69900	3.99100
C	-1.07300	1.20200	4.06100
C	-1.89800	0.27800	4.72600
C	-2.20600	1.76500	-0.58400
C	-2.93600	2.57400	0.30900
C	-2.12800	2.12800	-1.94400
C	-3.57600	3.73600	-0.15600
C	-2.77300	3.28600	-2.40400
C	-3.49600	4.09400	-1.51100
H	5.62800	2.32400	-0.31400
H	5.50400	-0.12300	-2.62500
H	6.32200	0.23800	-1.08800
H	5.63300	-1.38200	-1.36500
H	3.99800	-2.07600	-2.40400
H	2.22000	-2.21600	-2.44200
H	3.03500	-0.99400	-3.43500
H	6.07500	-0.09700	1.53900
H	5.82100	1.38800	2.51800
H	4.54000	0.12900	2.44300
H	2.97300	3.48800	0.15800
H	2.43500	2.44600	1.51600
H	3.89500	3.46100	1.69600

H	0.81000	-1.95200	-0.67400
H	0.92000	-4.24400	-0.67400
H	3.69900	-3.06300	-0.17800
H	3.31600	-2.27100	1.38700
H	3.28200	-4.06700	1.25700
H	-0.97100	-3.12700	1.44100
H	0.26600	-4.07000	2.33900
H	0.27100	-2.27500	2.42200
H	-1.19000	-2.56500	-1.46500
H	-4.36400	-0.01800	0.06800
H	-2.88900	-4.21400	-2.24400
H	-6.06000	-1.67000	-0.71500
H	-5.33200	-3.77600	-1.86900
H	-3.00300	-1.52400	2.02500
H	-0.27900	1.86600	2.15500
H	-3.23500	-1.42500	4.50600
H	-0.52900	1.97000	4.63200
H	-2.00200	0.32100	5.82100
H	-3.00900	2.30300	1.37300
H	-1.56800	1.50600	-2.65800
H	-4.14200	4.36300	0.55000
H	-2.70500	3.55900	-3.46800
H	-3.99600	5.00600	-1.87200
Mn	0.97400	-0.11100	-0.72900
O	1.22700	2.73200	-1.37300
O	0.05800	-0.36900	-3.57100
O	1.98200	-0.02100	2.08000
Si	4.53100	1.51400	0.35100
Si	1.24000	-3.11500	0.27300

TS8-4 E= -5315.839941 G= -5315.909560 imaginary eigenvalue=-88.27

As	1.29500	-0.11900	0.02100
C	-1.45000	0.16000	0.99200
C	-1.36700	-1.46800	-1.17500
C	-0.10100	0.47900	-2.33800
C	-2.94600	0.15000	-1.54700
C	-4.10600	-0.20500	-0.91500
C	-5.45900	0.14800	-1.55100
C	-2.97900	0.67900	-2.96800
C	-4.97200	-0.05500	2.09900
C	-3.30200	-2.57500	1.25800
C	-3.08600	3.21700	0.24000
C	-0.33500	3.06700	1.61500
C	2.41700	-1.24900	-1.14500
C	1.86100	-2.39900	-1.74100
C	3.76800	-0.92900	-1.38200
C	2.65300	-3.22200	-2.55900
C	4.55300	-1.75200	-2.20700
C	3.99900	-2.90000	-2.79600
C	1.49500	-1.02800	1.75100
C	1.25300	-0.31500	2.94300
C	1.79000	-2.40400	1.81300
C	1.31700	-0.97000	4.18300
C	1.84400	-3.05700	3.05600
C	1.60900	-2.34300	4.24200
C	2.48600	1.43700	0.22000
C	2.36800	2.47800	-0.72300
C	3.45200	1.53100	1.24100
C	3.19900	3.60500	-0.64000
C	4.27700	2.66500	1.32500

C	4.15100	3.70400	0.38900
H	-5.73400	-1.95200	0.28100
H	-5.77500	-0.60000	-2.31200
H	-6.26900	0.17000	-0.79300
H	-5.45300	1.14400	-2.03900
H	-3.98400	0.64700	-3.43500
H	-2.60600	1.72500	-3.03900
H	-2.30500	0.07800	-3.61300
H	-5.68600	0.71900	1.75000
H	-5.46300	-0.63500	2.90700
H	-4.08800	0.45400	2.53000
H	-3.14300	-3.31600	0.45100
H	-2.31400	-2.23400	1.61600
H	-3.80700	-3.09200	2.10200
H	-1.48600	1.65400	-1.14500
H	-0.65200	3.77800	-1.01700
H	-3.64600	3.18800	-0.71600
H	-3.54300	2.46900	0.91900
H	-3.20000	4.22400	0.69100
H	0.73600	2.80200	1.54700
H	-0.40900	4.14800	1.85800
H	-0.80700	2.49200	2.43500
H	0.80900	-2.66600	-1.57300
H	4.21600	-0.03300	-0.92900
H	2.20900	-4.11900	-3.01700
H	5.60600	-1.48900	-2.39000
H	4.61600	-3.54200	-3.44300
H	1.01500	0.75900	2.91300
H	1.98400	-2.97400	0.89200
H	1.13000	-0.40300	5.10700

H	2.07500	-4.13300	3.09400
H	1.65300	-2.85600	5.21400
H	1.62100	2.41500	-1.52800
H	3.56500	0.72000	1.97700
H	3.09700	4.41300	-1.38100
H	5.02500	2.73500	2.13000
H	4.79700	4.59200	0.46000
Mn	-0.96000	0.21400	-0.75300
O	-1.64300	-2.55700	-1.50900
O	0.49600	0.66100	-3.32500
O	-1.68000	0.14300	2.14000
Si	-4.47400	-1.20300	0.66900
Si	-1.25800	2.81900	-0.01900
4	E= -4789.867139	G= -4789.929596	
As	-0.71700	0.04500	-0.09900
C	1.64200	-1.99500	-0.33000
C	1.51800	-0.46600	-2.30300
C	2.10600	1.50400	-0.85700
C	3.95200	0.16800	1.70700
C	5.15700	0.51900	-1.15700
C	-0.56100	0.26300	1.84600
C	-0.07100	-0.82600	2.60300
C	-0.77700	1.50800	2.47000
C	0.18300	-0.66900	3.97400
C	-0.52100	1.65600	3.84300
C	-0.04000	0.57100	4.59500
C	-1.91400	-1.48800	-0.28800
C	-2.84600	-1.84200	0.70800
C	-1.81000	-2.26000	-1.46100
C	-3.67400	-2.96100	0.52300

C	-2.64500	-3.37400	-1.64300
C	-3.57600	-3.72500	-0.65200
C	-1.83900	1.55900	-0.63300
C	-1.21000	2.75800	-1.01800
C	-3.24500	1.47100	-0.63300
C	-1.98500	3.87100	-1.38400
C	-4.01500	2.58500	-1.00500
C	-3.38700	3.78500	-1.37800
H	4.38500	-1.87000	-0.11300
H	4.95700	-0.03200	2.13600
H	3.76200	1.25900	1.76600
H	3.20100	-0.34500	2.34200
H	6.18100	0.34900	-0.76300
H	5.13300	0.16600	-2.20800
H	4.95300	1.60800	-1.15600
H	0.10200	-1.80300	2.12400
H	-1.15000	2.36300	1.88500
H	0.55900	-1.52200	4.56000
H	-0.69900	2.62900	4.32700
H	0.16200	0.69300	5.67000
H	-2.92000	-1.25000	1.63400
H	-1.07100	-1.99500	-2.23500
H	-4.39800	-3.23900	1.30500
H	-2.56100	-3.97500	-2.56200
H	-4.22500	-4.60300	-0.79300
H	-0.11200	2.82800	-1.03700
H	-3.74500	0.53300	-0.34600
H	-1.48800	4.80700	-1.68200
H	-5.11300	2.51200	-1.00600
H	-3.99400	4.65600	-1.67200

Mn	1.56400	-0.20100	-0.58300
O	1.46500	-0.65200	-3.46200
O	2.51300	2.58200	-1.07200
O	1.71900	-3.15500	-0.20700
Si	3.88600	-0.43600	-0.11300
9	E= -525.999815	G= -526.033908	
C	1.51700	0.69400	0.14900
C	0.67700	-0.32400	-0.17900
C	1.12400	-1.75400	-0.39500
C	3.00300	0.64400	0.36200
C	-1.60400	1.83900	-0.13700
C	-2.16700	-1.06100	0.83800
H	-1.57600	-0.40300	-1.77900
H	0.69000	-2.43000	0.37300
H	0.76900	-2.14000	-1.37500
H	2.22500	-1.88400	-0.36400
H	3.44000	-0.36000	0.19500
H	3.52200	1.36000	-0.31200
H	3.26300	0.95800	1.39700
H	-1.05900	2.48400	-0.85700
H	-2.69100	1.99900	-0.29200
H	-1.35500	2.17900	0.89000
H	-1.94900	-2.13800	0.69300
H	-1.91300	-0.79800	1.88500
H	-3.25800	-0.91300	0.69900
H	1.07800	1.70000	0.28600
Si	-1.17800	0.01100	-0.37600

E-7-Z

E-7 E= -4945.654667 G= -4945.719296

As	0.90300	0.08900	-0.00200
C	0.79200	-2.96400	0.32200
C	-1.82400	-3.07000	0.60800
C	-1.00400	-1.74800	-1.30600
C	-1.84900	-0.53200	1.24800
C	-2.90700	0.29700	1.11600
C	-3.49300	1.06000	2.29100
C	-1.07700	-0.93200	2.46400
C	-4.86400	1.99600	-0.60100
C	-4.69400	-1.06700	-1.03900
C	1.95400	0.66000	1.55900
C	2.48600	-0.35200	2.38600
C	2.21500	2.01100	1.85800
C	3.27200	-0.01400	3.49800
C	3.00000	2.34500	2.97500
C	3.52700	1.33500	3.79700
C	2.33100	-0.16800	-1.32700
C	3.40700	0.74200	-1.38400
C	2.27500	-1.24100	-2.23500
C	4.41500	0.57800	-2.34700
C	3.28600	-1.40000	-3.19900
C	4.35600	-0.49300	-3.25600
C	0.08600	1.74900	-0.63100
C	0.15100	2.09700	-1.99400
C	-0.68100	2.53500	0.25500
C	-0.53900	3.22500	-2.46600
C	-1.36000	3.66800	-0.22100

C	-1.29500	4.01200	-1.58200
H	-2.65000	0.70300	-1.64200
H	-3.44200	2.16000	2.12800
H	-4.57000	0.82600	2.43900
H	-2.97000	0.83900	3.24400
H	-1.68000	-1.47500	3.21900
H	-0.22900	-1.70000	2.23000
H	-0.50900	-0.10600	2.94000
H	-4.30700	2.92600	-0.36800
H	-5.32900	2.12100	-1.60100
H	-5.68100	1.88700	0.14200
H	-5.15900	-0.96800	-2.04200
H	-4.03900	-1.96100	-1.05100
H	-5.50100	-1.24700	-0.30000
H	2.29400	-1.41200	2.15600
H	1.80900	2.81100	1.21900
H	3.68500	-0.81000	4.13600
H	3.19900	3.40300	3.20300
H	4.13900	1.60000	4.67300
H	3.46600	1.58000	-0.67400
H	1.44400	-1.95800	-2.20300
H	5.25400	1.29000	-2.38400
H	3.23500	-2.24100	-3.90600
H	5.14800	-0.62000	-4.00900
H	0.73900	1.48400	-2.69500
H	-0.75200	2.27000	1.31900
H	-0.48500	3.49000	-3.53300
H	-1.95100	4.28000	0.47800
H	-1.83500	4.89600	-1.95300
Mn	-0.59100	-1.78900	0.41300

O	-2.65000	-3.89000	0.68300
O	-1.28600	-1.75000	-2.44400
O	1.65600	-3.75100	0.27300
Si	-3.70800	0.49100	-0.59000

TS-E-7-I E= -4945.574077 G= -4945.639480 imaginary eigenvalue=-420.11

As	-0.85000	-0.11400	0.01400
C	-1.15000	2.64700	0.93600
C	1.27900	3.38300	0.80500
C	0.43500	2.25400	-1.35200
C	1.78000	0.80900	0.97200
C	2.58100	-0.33000	0.89600
C	2.65700	-1.41700	1.93800
C	3.09800	1.28500	1.96100
C	4.54900	-2.06900	-0.84700
C	4.61900	1.04800	-1.01200
C	-1.15300	-1.22000	1.61000
C	-0.85700	-0.63900	2.85900
C	-1.65600	-2.53800	1.55900
C	-1.06600	-1.36300	4.04400
C	-1.85800	-3.26100	2.74700
C	-1.56500	-2.67500	3.99000
C	-2.67800	0.15900	-0.68300
C	-3.77900	-0.61700	-0.27100
C	-2.87400	1.18500	-1.63000
C	-5.05300	-0.38100	-0.81500
C	-4.14700	1.41000	-2.17900
C	-5.23900	0.62800	-1.77400
C	-0.16300	-1.41900	-1.29300
C	-0.23200	-1.07500	-2.65900
C	0.50700	-2.59800	-0.91400

C	0.35600	-1.90200	-3.62800
C	1.09600	-3.42500	-1.88800
C	1.02400	-3.07800	-3.24500
H	2.45800	-0.47600	-1.84900
H	2.18100	-2.32000	1.50100
H	3.70300	-1.70300	2.17900
H	2.10300	-1.16300	2.86300
H	3.27300	2.31000	1.59400
H	2.70200	1.26500	2.99100
H	4.09000	0.78300	1.95200
H	3.91000	-2.96300	-0.70500
H	5.05000	-2.16500	-1.83300
H	5.33500	-2.06700	-0.06500
H	5.08200	1.03100	-2.02000
H	4.00700	1.96900	-0.93100
H	5.43300	1.08800	-0.26100
H	-0.44600	0.38300	2.88700
H	-1.88600	-3.01200	0.59200
H	-0.83500	-0.89900	5.01600
H	-2.24700	-4.29000	2.69900
H	-1.72500	-3.24400	4.91800
H	-3.65800	-1.40400	0.48600
H	-2.03300	1.82400	-1.93900
H	-5.90700	-0.99100	-0.48100
H	-4.28400	2.21200	-2.92100
H	-6.23900	0.81000	-2.19800
H	-0.73300	-0.14700	-2.97400
H	0.56600	-2.89000	0.14400
H	0.29400	-1.62200	-4.69100
H	1.61300	-4.34600	-1.57800

H	1.48800	-3.72300	-4.00700
Mn	0.40900	1.89400	0.38600
O	1.87800	4.35600	1.07300
O	0.51000	2.47000	-2.50700
O	-2.13000	3.17800	1.30400
Si	3.52800	-0.47900	-0.79800
I	E= -4945.634846	G= -4945.701001	
As	-1.02600	0.00800	0.03400
C	-0.24700	-2.29100	-1.59100
C	2.01200	-2.78200	-0.55100
C	0.41300	-2.22000	1.40500
C	1.87100	-0.32600	-0.51700
C	2.96100	0.60000	-0.79600
C	2.42600	2.05800	-0.83200
C	3.64800	0.22900	-2.13300
C	5.73500	1.48300	0.37400
C	4.66700	-1.33500	1.10900
C	-1.04800	1.49700	-1.24300
C	-0.77200	1.21000	-2.59500
C	-1.28600	2.82400	-0.84100
C	-0.74000	2.24900	-3.53900
C	-1.24100	3.86100	-1.78800
C	-0.96800	3.57600	-3.13600
C	-2.85900	-0.67700	-0.11700
C	-3.89100	0.09000	-0.69100
C	-3.13300	-1.96700	0.37800
C	-5.19500	-0.43000	-0.75600
C	-4.43900	-2.47900	0.31500
C	-5.47100	-1.71100	-0.25200
C	-1.06600	0.92200	1.76800

C	-2.26600	1.40500	2.32600
C	0.15000	1.09600	2.45500
C	-2.24000	2.07600	3.56000
C	0.17000	1.77000	3.68600
C	-1.02400	2.26200	4.23900
H	3.44600	1.03700	1.89700
H	1.87600	2.32300	0.09200
H	3.27000	2.76700	-0.95000
H	1.73800	2.19800	-1.69000
H	4.02200	-0.81500	-2.12600
H	2.92600	0.32400	-2.97000
H	4.50500	0.90500	-2.33200
H	5.49000	2.53600	0.13000
H	6.39000	1.48500	1.26900
H	6.31500	1.05600	-0.46900
H	5.45200	-1.34500	1.89300
H	3.79500	-1.90600	1.48200
H	5.06700	-1.85700	0.21700
H	-0.56600	0.17600	-2.91000
H	-1.49400	3.05600	0.21500
H	-0.52600	2.02000	-4.59400
H	-1.41800	4.90000	-1.46800
H	-0.93100	4.39100	-3.87500
H	-3.68000	1.09400	-1.09300
H	-2.32100	-2.57500	0.80600
H	-6.00000	0.17200	-1.20800
H	-4.64900	-3.48700	0.70400
H	-6.49200	-2.11700	-0.30700
H	-3.22300	1.25700	1.80300
H	1.07900	0.68800	2.02700

H	-3.17900	2.45100	3.99600
H	1.12500	1.90300	4.21800
H	-1.00900	2.78600	5.20700
Mn	0.74300	-1.54400	-0.25700
O	2.83700	-3.57900	-0.76900
O	0.31500	-2.60300	2.50700
O	-0.82000	-2.72700	-2.51500
Si	4.18800	0.44700	0.72300

TS-I-Z-7 E= -4945.578794 G= -4945.645014 imaginary eigenvalue=-312.46

As	-0.99500	0.04900	0.02000
C	0.27700	-1.32000	-2.26300
C	2.11400	-2.52800	-0.96400
C	-0.20400	-2.84200	0.04600
C	2.03600	-0.54600	0.45800
C	3.38700	-0.54600	0.81300
C	3.91800	-1.42500	1.90700
C	2.02200	0.87100	1.33100
C	5.62000	1.66400	0.69800
C	3.76200	1.16700	-1.78900
C	-1.67400	-0.01400	1.86700
C	-0.92100	-0.72900	2.81900
C	-2.88800	0.59300	2.24500
C	-1.36800	-0.81700	4.14800
C	-3.33200	0.50300	3.57400
C	-2.57100	-0.19900	4.52600
C	-2.68200	-0.12100	-0.97500
C	-3.35500	0.99400	-1.51300
C	-3.22300	-1.41100	-1.14600
C	-4.56100	0.81700	-2.21300
C	-4.43000	-1.58200	-1.84100

C	-5.10100	-0.46900	-2.37700
C	-0.60900	1.96200	-0.25000
C	-0.86600	2.95700	0.71200
C	0.03000	2.31000	-1.45800
C	-0.49200	4.29000	0.46400
C	0.39600	3.64200	-1.70600
C	0.13800	4.63400	-0.74300
H	5.55700	-0.71700	-0.75800
H	4.20400	-2.37300	1.39700
H	4.82500	-1.03000	2.40800
H	3.13500	-1.68300	2.64700
H	1.88200	1.71000	0.62600
H	1.14200	0.73200	1.98700
H	2.85300	1.13900	2.02300
H	6.08300	1.20000	1.59200
H	6.43100	2.10500	0.08200
H	4.96000	2.49000	1.03300
H	4.49600	1.48400	-2.55700
H	3.06600	0.42700	-2.23300
H	3.16800	2.05400	-1.49000
H	0.00800	-1.23100	2.49600
H	-3.49600	1.12700	1.49700
H	-0.77900	-1.37900	4.88800
H	-4.28200	0.97700	3.86700
H	-2.92500	-0.27100	5.56600
H	-2.93900	2.00500	-1.39100
H	-2.70400	-2.28900	-0.73200
H	-5.08000	1.69200	-2.63300
H	-4.84700	-2.59300	-1.96800
H	-6.04400	-0.60600	-2.92700

H	-1.35000	2.69600	1.66600
H	0.25000	1.53100	-2.20600
H	-0.69200	5.06200	1.22300
H	0.89000	3.90500	-2.65300
H	0.43200	5.67800	-0.93400
Mn	0.76600	-1.45700	-0.53600
O	3.02100	-3.22300	-1.23500
O	-0.79800	-3.77600	0.44600
O	0.01000	-1.22500	-3.40300
Si	4.64700	0.40300	-0.31900
Z-7	E= -4945.632092	G= -4945.697038	
As	-0.94500	0.01700	-0.00400
C	1.02700	-0.21500	-2.03600
C	2.44800	-1.99100	-1.13000
C	0.37200	-2.47500	0.05400
C	1.85200	0.10100	0.97900
C	3.05800	-0.58100	0.65000
C	3.58400	-1.68200	1.57400
C	1.63500	1.09600	2.06100
C	5.75400	0.91800	1.01100
C	3.76100	1.94500	-1.12300
C	-2.46200	-0.95500	-0.79000
C	-2.26900	-1.64000	-2.00500
C	-3.73000	-0.96400	-0.17500
C	-3.34100	-2.31400	-2.60900
C	-4.79900	-1.64400	-0.78200
C	-4.60700	-2.31700	-2.00000
C	-1.21100	1.82900	-0.71200
C	-2.47400	2.28800	-1.13700
C	-0.09200	2.67900	-0.79600

C	-2.61200	3.59700	-1.62800
C	-0.23600	3.98700	-1.28600
C	-1.49700	4.44800	-1.70000
C	-1.55400	0.19600	1.85800
C	-1.28900	-0.86300	2.74900
C	-2.23100	1.34300	2.31500
C	-1.70800	-0.77700	4.08600
C	-2.64300	1.42600	3.65700
C	-2.38300	0.36800	4.54200
H	5.07300	-0.50600	-1.27100
H	4.23800	-2.39600	1.02800
H	4.19100	-1.24500	2.39800
H	2.75000	-2.25600	2.02600
H	0.63200	1.56200	2.07300
H	1.78900	0.60300	3.04900
H	2.40200	1.90100	2.00400
H	6.21800	0.03500	1.49600
H	6.56000	1.49800	0.51600
H	5.31300	1.55500	1.80600
H	4.59500	2.48500	-1.61700
H	3.01000	1.69100	-1.89600
H	3.29200	2.64000	-0.39700
H	-1.27300	-1.65500	-2.47400
H	-3.88600	-0.44400	0.78300
H	-3.18400	-2.84800	-3.55900
H	-5.78700	-1.65000	-0.29600
H	-5.44600	-2.85100	-2.47200
H	-3.35100	1.62400	-1.09500
H	0.89800	2.30100	-0.50000
H	-3.60000	3.95100	-1.96300

H	0.64500	4.64300	-1.35300
H	-1.60900	5.47100	-2.09000
H	-0.74900	-1.75700	2.40200
H	-2.43400	2.18000	1.63000
H	-1.50000	-1.60900	4.77600
H	-3.16800	2.32700	4.01000
H	-2.70400	0.43600	5.59300
Mn	1.20400	-0.93200	-0.38800
O	3.22200	-2.72000	-1.62000
O	-0.15800	-3.47800	0.34900
O	0.93600	0.26800	-3.10200
Si	4.43300	0.40700	-0.25300

18-4

4	E= -4789.867139	G= -4789.929596	
As	-0.71700	0.04500	-0.09900
C	1.64200	-1.99500	-0.33000
C	1.51800	-0.46600	-2.30300
C	2.10600	1.50400	-0.85700
C	3.95200	0.16800	1.70700
C	5.15700	0.51900	-1.15700
C	-0.56100	0.26300	1.84600
C	-0.07100	-0.82600	2.60300
C	-0.77700	1.50800	2.47000
C	0.18300	-0.66900	3.97400
C	-0.52100	1.65600	3.84300
C	-0.04000	0.57100	4.59500
C	-1.91400	-1.48800	-0.28800
C	-2.84600	-1.84200	0.70800
C	-1.81000	-2.26000	-1.46100
C	-3.67400	-2.96100	0.52300
C	-2.64500	-3.37400	-1.64300
C	-3.57600	-3.72500	-0.65200
C	-1.83900	1.55900	-0.63300
C	-1.21000	2.75800	-1.01800
C	-3.24500	1.47100	-0.63300
C	-1.98500	3.87100	-1.38400
C	-4.01500	2.58500	-1.00500
C	-3.38700	3.78500	-1.37800
H	4.38500	-1.87000	-0.11300
H	4.95700	-0.03200	2.13600
H	3.76200	1.25900	1.76600

H	3.20100	-0.34500	2.34200
H	6.18100	0.34900	-0.76300
H	5.13300	0.16600	-2.20800
H	4.95300	1.60800	-1.15600
H	0.10200	-1.80300	2.12400
H	-1.15000	2.36300	1.88500
H	0.55900	-1.52200	4.56000
H	-0.69900	2.62900	4.32700
H	0.16200	0.69300	5.67000
H	-2.92000	-1.25000	1.63400
H	-1.07100	-1.99500	-2.23500
H	-4.39800	-3.23900	1.30500
H	-2.56100	-3.97500	-2.56200
H	-4.22500	-4.60300	-0.79300
H	-0.11200	2.82800	-1.03700
H	-3.74500	0.53300	-0.34600
H	-1.48800	4.80700	-1.68200
H	-5.11300	2.51200	-1.00600
H	-3.99400	4.65600	-1.67200
Mn	1.56400	-0.20100	-0.58300
O	1.46500	-0.65200	-3.46200
O	2.51300	2.58200	-1.07200
O	1.71900	-3.15500	-0.20700
Si	3.88600	-0.43600	-0.11300

TS4-18 E= -4903.093460 G= -4903.158690 imaginary eigenvalue=-182.19

As	-0.60900	-0.04900	-0.00200
C	2.03900	-0.51200	0.86800
C	0.96700	0.69200	-2.28800
C	4.25100	-2.64100	-0.36500
C	1.26800	-1.93100	-1.46200

C	4.13300	1.18600	-1.36300
C	2.98800	2.50600	1.26900
C	-2.10800	0.07100	-1.26400
C	-2.08800	-0.75200	-2.40800
C	-3.20900	0.91700	-1.02900
C	-3.16400	-0.72800	-3.30800
C	-4.28200	0.93900	-1.93600
C	-4.26100	0.11900	-3.07500
C	-0.77900	1.59000	1.05700
C	-0.81100	2.83000	0.38600
C	-0.69800	1.55300	2.46200
C	-0.78700	4.02500	1.12100
C	-0.66600	2.75400	3.19200
C	-0.71400	3.98900	2.52500
C	-1.26700	-1.43300	1.22700
C	-0.49600	-2.57800	1.49800
C	-2.53800	-1.28700	1.81900
C	-0.99200	-3.56800	2.36300
C	-3.02800	-2.27700	2.68400
C	-2.25500	-3.41900	2.95700
H	2.05800	3.05000	-1.23100
H	5.02300	1.69200	-0.93200
H	4.31200	0.09500	-1.23800
H	4.08600	1.40500	-2.44800
H	3.66000	3.38500	1.18500
H	2.06300	2.83000	1.79000
H	3.48200	1.73700	1.89500
H	-1.23200	-1.41800	-2.60000
H	-3.23500	1.56900	-0.14300
H	-3.14200	-1.37200	-4.20000

H	-5.13800	1.60600	-1.75000
H	-5.10100	0.14000	-3.78600
H	-0.84700	2.86700	-0.71400
H	-0.65000	0.59000	2.99200
H	-0.81700	4.99000	0.59300
H	-0.59900	2.72100	4.29100
H	-0.68700	4.92700	3.10000
H	0.49400	-2.70600	1.03700
H	-3.15400	-0.39900	1.60700
H	-0.38500	-4.46200	2.57100
H	-4.02100	-2.15700	3.14500
H	-2.64200	-4.19600	3.63400
Mn	1.52100	-0.25700	-0.84800
O	3.91900	-3.54500	0.24800
O	2.33000	-0.64300	1.99700
O	1.12600	-3.01400	-1.88800
O	0.57900	1.32600	-3.19200
Si	2.56600	1.85000	-0.46100
18	E= -4903.168706	G= -4903.230882	
As	0.58700	0.00400	-0.00300
C	-1.62600	-0.89400	-1.85400
C	-1.68000	-0.99200	1.77300
C	-3.30000	-1.62600	-0.10500
C	-0.93400	-2.77400	-0.09200
C	-4.08300	1.19500	1.38400
C	-3.44700	1.68800	-1.57700
C	1.28500	0.47200	1.77400
C	2.57600	0.09300	2.18800
C	0.47400	1.23900	2.63600
C	3.04400	0.46900	3.45800

C	0.94900	1.61700	3.90000
C	2.23400	1.22900	4.31600
C	0.80200	1.71800	-0.94900
C	1.39300	2.82700	-0.31400
C	0.36600	1.83400	-2.28500
C	1.53200	4.04300	-1.00400
C	0.51300	3.05100	-2.97100
C	1.09000	4.15900	-2.33100
C	2.06900	-1.04800	-0.75000
C	2.88200	-0.55700	-1.79000
C	2.31900	-2.32900	-0.21700
C	3.92900	-1.34700	-2.29500
C	3.37200	-3.10900	-0.71800
C	4.17600	-2.62100	-1.76200
H	-1.69800	2.19200	0.47600
H	-4.53600	2.20800	1.39400
H	-4.88300	0.46200	1.15400
H	-3.70200	0.97600	2.40200
H	-3.98100	2.65100	-1.43800
H	-2.66600	1.83100	-2.34900
H	-4.17300	0.93900	-1.95600
H	3.22600	-0.49300	1.52100
H	-0.53000	1.55600	2.31700
H	4.05400	0.16500	3.77600
H	0.30900	2.21700	4.56400
H	2.60400	1.52100	5.31100
H	1.74500	2.75100	0.72500
H	-0.08100	0.98000	-2.80900
H	1.99000	4.90500	-0.49500
H	0.16900	3.12900	-4.01400

H	1.19700	5.11400	-2.86800
H	2.70600	0.44400	-2.21000
H	1.69900	-2.72400	0.60200
H	4.55700	-0.95700	-3.11100
H	3.56100	-4.10600	-0.29200
H	4.99800	-3.23700	-2.15900
Mn	-1.59300	-1.09500	-0.04600
O	-4.41500	-1.96600	-0.15600
O	-1.69700	-0.81000	-3.01500
O	-0.59800	-3.89100	-0.12200
O	-1.78400	-0.95900	2.93300
Si	-2.69800	1.12100	0.07800

Radical mechanism

13	E= -409.467789	G= -409.496877	
C	-1.73600	-0.46200	-0.22400
C	0.46800	1.73300	-0.22400
C	1.26800	-1.27200	-0.22400
H	-0.00000	-0.00000	1.89300
H	-2.03100	-1.46800	0.13700
H	-2.49100	0.26600	0.13700
H	-1.77400	-0.47200	-1.33300
H	-0.25700	2.49200	0.13700
H	1.47600	2.02500	0.13800
H	0.47900	1.77200	-1.33300
H	2.28700	-1.02200	0.13600
H	1.01800	-2.29000	0.13700
H	1.29600	-1.30000	-1.33300
Si	-0.00000	-0.00000	0.37900
12	E= -1717.164107	G= -1717.202309	
C	0.00000	1.83200	0.41300
C	1.83200	0.00000	0.41300
C	0.00000	-1.83200	0.41300
C	0.00000	0.00000	-1.60900
C	-1.83200	0.00000	0.41300
Mn	0.00000	0.00000	0.19300
O	0.00000	2.98500	0.53400
O	0.00000	0.00000	-2.77100
O	2.98500	0.00000	0.53400
O	0.00000	-2.98500	0.53400
O	-2.98500	0.00000	0.53400

Int6 E= -2126.639280 G= -2126.689448

C	1.34200	-0.00200	1.86900
C	0.84600	-1.82400	0.08100
C	0.57200	0.00200	-1.72200
C	2.88100	0.00000	-0.34400
C	0.84600	1.82400	0.08500
C	-2.78000	1.56000	-0.89200
C	-2.78000	-1.55900	-0.89300
C	-3.86500	-0.00100	1.59400
H	-1.21100	-0.00000	0.75400
H	-2.56800	2.47100	-0.29500
H	-2.06600	1.53200	-1.73900
H	-3.80300	1.65300	-1.31100
H	-2.06600	-1.53000	-1.74100
H	-2.56800	-2.47100	-0.29800
H	-3.80300	-1.65200	-1.31300
H	-3.73900	-0.90000	2.23100
H	-3.73800	0.89600	2.23300
H	-4.90500	-0.00000	1.20400
Mn	1.12000	-0.00000	0.03500
O	1.50800	-0.00400	3.01600
O	4.01800	0.00100	-0.59100
O	0.67200	-2.97100	0.10200
O	0.24000	0.00400	-2.83500
O	0.67200	2.97100	0.10900
Si	-2.62700	-0.00000	0.16600

TS12-14 E= -2126.595841 G= -2126.647422 imaginary eigenvalue=-33.86

C	1.97700	0.01500	1.77100
C	1.13400	-1.81000	0.16400
C	0.41100	-0.00800	-1.52000

C	3.05200	-0.03500	-0.75800
C	1.18500	1.81900	0.11300
C	-2.81100	1.59000	-0.42800
C	-2.82000	-1.56300	-0.47300
C	-5.25700	0.00300	0.63200
H	-0.02700	0.03100	0.71600
H	-3.26900	2.48000	0.04900
H	-1.71200	1.72400	-0.40900
H	-3.13400	1.56400	-1.49200
H	-1.72700	-1.73100	-0.42100
H	-3.32000	-2.45800	-0.04900
H	-3.10200	-1.48600	-1.54700
H	-5.61700	-0.89900	1.16900
H	-5.61600	0.89800	1.18100
H	-5.72700	0.01000	-0.37700
Mn	1.39600	-0.00100	0.02900
O	2.29200	0.02600	2.88300
O	4.09900	-0.05700	-1.25600
O	0.90700	-2.94000	0.27200
O	-0.25900	-0.01200	-2.46300
O	0.98900	2.95700	0.19000
Si	-3.36500	0.00200	0.46100
15	E= -1717.762507	G= -1717.800055	
C	0.26939	1.68618	0.73502
C	1.84240	-0.11279	-0.22107
C	-0.03981	-1.85832	-0.03343
C	-0.51215	0.38401	-1.56516
C	-1.61283	-0.05934	0.92266
H	0.52093	-0.39059	1.59200
Mn	0.04331	-0.03247	0.13236

O 0.42702 2.74966 1.16152

O 2.98446 -0.17516 -0.39292

O -0.86318 0.64720 -2.63791

O -2.63314 -0.08826 1.46659

O -0.07569 -3.01308 -0.08785

14 E= -408.829501 G= -408.859220

C 1.25100 -1.29700 0.17600

C 0.49900 1.73200 0.17600

C -1.74900 -0.43400 0.17600

H 0.98300 -2.31400 -0.17800

H 2.27500 -1.06800 -0.18100

H 1.27500 -1.32000 1.28900

H 1.51200 2.00800 -0.17900

H -0.21300 2.50500 -0.18000

H 0.50700 1.76300 1.28900

H -2.49500 0.30600 -0.17900

H -2.06300 -1.43700 -0.17900

H -1.78000 -0.44200 1.28900

Si -0.00000 -0.00000 -0.42600

5 E= -155.736538 G= -155.763309

C 0.61300 -0.00100 -0.00000

C -0.61300 -0.00000 -0.00000

C -2.07200 0.00000 0.00000

C 2.07200 0.00000 0.00000

H -2.48000 0.95700 -0.39000

H -2.48100 -0.81600 -0.63300

H -2.48000 -0.14000 1.02300

H 2.48000 1.02300 -0.14200

H 2.48000 -0.38800 0.95700

H 2.48100 -0.63400 -0.81500

Int7 E= -564.569752 G= -564.609898

C	-2.68800	-0.26100	0.02300
C	-2.25300	0.87900	-0.09900
C	-1.70000	2.22100	-0.24500
C	-3.18600	-1.62500	0.16500
C	0.90700	-0.89000	-1.40200
C	0.97300	-0.22300	1.64300
C	3.60200	-0.04800	-0.04800
H	-0.58700	2.18700	-0.28900
H	-2.05500	2.71300	-1.17400
H	-1.97900	2.87500	0.60800
H	-3.62200	-1.79900	1.17100
H	-3.97500	-1.85300	-0.58200
H	-2.37100	-2.36600	0.02300
H	1.09900	-1.96700	-1.19800
H	-0.19100	-0.73100	-1.41200
H	1.30800	-0.65600	-2.40900
H	1.17600	-1.28500	1.90600
H	1.40400	0.41500	2.44100
H	-0.12700	-0.07800	1.62900
H	4.04300	0.19700	-1.03500
H	4.08400	0.59600	0.71600
H	3.85700	-1.10600	0.18800
Si	1.71500	0.18100	-0.05800

TS14-16Z E= -564.564049 G= -564.601841 imaginary eigenvalue=-222.76

C	-2.14600	-0.00700	-0.00000
C	-1.46400	1.02900	-0.00000
C	-1.14100	2.46500	-0.00000
C	-2.76500	-1.32500	-0.00000
C	0.87800	-1.15200	-1.55600

C	0.87700	-1.15200	1.55600
C	2.82000	0.69300	0.00000
H	-0.54200	2.74700	0.89000
H	-0.54200	2.74700	-0.89000
H	-2.07100	3.07400	-0.00000
H	-3.40600	-1.47600	0.89400
H	-3.40600	-1.47600	-0.89500
H	-2.00600	-2.13900	-0.00000
H	1.64800	-1.95500	-1.56800
H	-0.12100	-1.63200	-1.59700
H	1.00100	-0.54900	-2.47900
H	1.64800	-1.95500	1.56800
H	1.00100	-0.54900	2.47900
H	-0.12100	-1.63200	1.59700
H	2.98400	1.32500	-0.89700
H	2.98400	1.32500	0.89700
H	3.59600	-0.10600	0.00000
Si	1.07100	-0.07500	0.00000
16Z	E= -564.603113	G= -564.639612	
C	-2.02600	0.36900	-0.00200
C	-0.78700	0.84700	-0.00500
C	-0.49800	2.34500	-0.00300
C	-2.87600	-0.82600	-0.00200
C	1.72900	0.04200	1.61100
C	1.86700	0.22500	-1.47200
C	0.37900	-2.11900	-0.12800
H	0.14200	2.63200	0.86000
H	0.05600	2.64800	-0.91800
H	-1.43100	2.94000	0.04700
H	-3.54300	-0.84300	-0.89200

H	-2.29800	-1.78100	-0.00500
H	-3.53900	-0.84600	0.89000
H	1.11500	-0.22700	2.49500
H	2.65700	-0.56800	1.63900
H	2.02300	1.10700	1.71000
H	1.33100	0.08000	-2.43300
H	2.17700	1.28800	-1.40900
H	2.78800	-0.39500	-1.49800
H	1.33000	-2.68900	-0.16000
H	-0.19900	-2.48300	0.74500
H	-0.18900	-2.36100	-1.05000
Si	0.77500	-0.27100	-0.00000

15 E= -1717.762507 G= -1717.800055

C	0.26939	1.68618	0.73502
C	1.84240	-0.11279	-0.22107
C	-0.03981	-1.85832	-0.03343
C	-0.51215	0.38401	-1.56516
C	-1.61283	-0.05934	0.92266
H	0.52093	-0.39059	1.59200
Mn	0.04331	-0.03247	0.13236
O	0.42702	2.74966	1.16152
O	2.98446	-0.17516	-0.39292
O	-0.86318	0.64720	-2.63791
O	-2.63314	-0.08826	1.46659
O	-0.07569	-3.01308	-0.08785

TS16Z-17 E= -2282.375695 G= -2282.434096 imaginary eigenvalue=-72.35

C	-0.70900	-0.66500	-1.24400
C	-1.95100	-1.66700	0.80600
C	-2.85900	0.70200	1.36800
C	-3.51800	-0.44500	-1.11600

C	-1.74100	1.64800	-0.77100
C	1.21800	0.75900	1.21000
C	1.97100	-0.27800	0.88400
C	1.59000	-1.70400	1.25400
C	3.37400	1.46600	-1.30200
C	3.72200	-1.58800	-1.26500
C	5.05200	0.13900	0.93800
C	1.17100	2.23200	1.12400
H	1.31600	-2.28500	0.35600
H	2.43500	-2.23500	1.72500
H	0.74100	-1.73000	1.95200
H	3.39400	2.41000	-0.73600
H	4.20600	1.48900	-2.02500
H	2.43000	1.42800	-1.87000
H	2.82800	-1.72100	-1.89500
H	4.60000	-1.49700	-1.92600
H	3.84800	-2.49800	-0.65600
H	5.97700	0.23400	0.34300
H	4.96000	1.03500	1.57300
H	5.16300	-0.73600	1.60000
H	0.87800	2.57200	0.11600
H	0.43200	2.64900	1.83000
H	2.14800	2.68700	1.36600
H	-0.70400	0.26300	0.76700
Mn	-2.02500	-0.05300	-0.10200
O	0.17500	-1.00700	-1.88600
O	-1.85800	-2.64300	1.39500
O	-4.44100	-0.69100	-1.75000
O	-1.50800	2.70100	-1.15400
O	-3.30800	1.18200	2.30500

Si	3.54100	-0.04800	-0.18300
12	E= -1717.164107	G= -1717.202309	
C	0.00000	1.83200	0.41300
C	1.83200	0.00000	0.41300
C	0.00000	-1.83200	0.41300
C	0.00000	0.00000	-1.60900
C	-1.83200	0.00000	0.41300
Mn	0.00000	0.00000	0.19300
O	0.00000	2.98500	0.53400
O	0.00000	0.00000	-2.77100
O	2.98500	0.00000	0.53400
O	0.00000	-2.98500	0.53400
O	-2.98500	0.00000	0.53400
17(Z-Pro)	E= -565.257504	G= -565.293082	
C	-0.81000	0.84100	-0.00000
C	-2.06500	0.32000	-0.00000
C	2.28300	0.92800	-0.00000
C	0.87500	-1.31100	1.55700
C	0.87500	-1.31100	-1.55700
C	-0.62500	2.34400	0.00000
C	-2.47800	-1.12300	0.00000
H	-2.91500	1.03500	-0.00000
H	3.21800	0.33000	-0.00000
H	2.30100	1.58100	-0.89700
H	2.30100	1.58100	0.89700
H	0.04200	-2.04000	1.62000
H	1.82800	-1.88000	1.57000
H	0.84100	-0.68100	2.47000
H	0.84100	-0.68100	-2.47000
H	1.82800	-1.88000	-1.57000

H	0.04200	-2.04000	-1.61900
H	-0.04800	2.69000	0.88500
H	-0.04800	2.69000	-0.88500
H	-1.59700	2.88200	0.00000
H	-3.10700	-1.35600	-0.88700
H	-1.62400	-1.82600	0.00000
H	-3.10700	-1.35600	0.88700
Si	0.77700	-0.22700	0.00000

TS16Z-E E= -564.597962 G= -564.634505 imaginary eigenvalue=-228.06

C	-1.89000	0.00400	0.00700
C	-0.78400	0.72100	-0.00100
C	-0.72300	2.25000	-0.00300
C	-3.14100	-0.73000	-0.00400
C	1.85100	0.18800	1.57500
C	1.90500	0.27400	-1.51500
C	0.52300	-2.09400	-0.05900
H	-0.17700	2.62700	0.88900
H	-0.17100	2.62500	-0.89200
H	-1.73400	2.70500	-0.00600
H	-3.94200	-0.22100	-0.59300
H	-3.04400	-1.76000	-0.42900
H	-3.53600	-0.85200	1.02900
H	1.27400	-0.08600	2.48200
H	2.81700	-0.35900	1.60500
H	2.07400	1.27300	1.62700
H	1.35600	0.06200	-2.45500
H	2.14100	1.35800	-1.49400
H	2.86600	-0.28100	-1.54600
H	1.46600	-2.67800	-0.05500
H	-0.08100	-2.40900	0.81700

H	-0.04300	-2.36100	-0.97500
Si	0.87800	-0.23700	-0.00000
16E	E= -564.602759	G= -564.639450	
C	-1.80700	0.50400	0.00000
C	-0.85200	-0.41900	-0.00000
C	-1.12600	-1.92200	-0.00000
C	-3.26600	0.68200	0.00000
C	1.83000	-0.52400	-1.54300
C	1.82900	-0.52300	1.54400
C	1.03600	2.05400	-0.00100
H	-0.67200	-2.40800	-0.89000
H	-0.67200	-2.40900	0.89000
H	-2.21000	-2.15400	-0.00100
H	-3.80800	-0.29600	-0.00100
H	-3.60900	1.25000	0.89200
H	-3.60900	1.25000	-0.89100
H	1.34300	-0.15600	-2.47000
H	2.89500	-0.21400	-1.56800
H	1.80100	-1.63300	-1.56000
H	1.34300	-0.15500	2.47000
H	1.80000	-1.63300	1.56100
H	2.89500	-0.21300	1.56900
H	2.08700	2.40900	-0.00100
H	0.52900	2.46800	-0.89600
H	0.53000	2.46900	0.89600
Si	0.96400	0.16500	0.00000
16Z-large	E= -1139.145845	G= -1139.195626	
C	-0.40000	-1.76800	1.53300
C	-0.88500	-1.03200	0.53300
C	-2.35000	-0.97900	0.23600

C	-2.95900	0.20100	-0.25400
C	-3.17000	-2.11400	0.44100
C	-4.33600	0.24500	-0.52300
C	-4.54500	-2.07100	0.17000
C	-5.13600	-0.89100	-0.31500
C	0.30000	1.78100	-0.10900
C	0.39300	2.81900	-1.06500
C	0.22900	2.13900	1.25800
C	0.41800	4.16700	-0.67000
C	0.25900	3.48400	1.65800
C	0.35300	4.50200	0.69300
C	0.79000	-2.16800	2.28500
C	2.06300	-0.73600	-0.44400
C	2.34700	-2.05900	-0.85900
C	3.11900	0.03000	0.10000
C	3.63600	-2.60000	-0.73000
C	4.41100	-0.50700	0.23200
C	4.67200	-1.82400	-0.18100
C	-0.24000	-0.25100	-2.42200
H	-2.35100	1.10700	-0.40200
H	-2.70300	-3.03900	0.81300
H	-4.78800	1.17700	-0.89600
H	-5.16100	-2.96900	0.33300
H	-6.21500	-0.85800	-0.53200
H	0.44400	2.57600	-2.13800
H	0.13700	1.34900	2.02200
H	0.48800	4.96100	-1.43000
H	0.20200	3.74200	2.72700
H	0.37200	5.55800	1.00400
H	1.07200	-3.21900	2.05400

H	1.67700	-1.52900	2.06200
H	0.60400	-2.11900	3.38000
H	1.54500	-2.68700	-1.28300
H	2.92700	1.06400	0.43000
H	3.83500	-3.63200	-1.05800
H	5.22000	0.10700	0.65900
H	5.68300	-2.24700	-0.07700
H	0.48300	0.24300	-3.10300
H	-0.27300	-1.32800	-2.68600
H	-1.24700	0.17400	-2.59900
Si	0.30400	-0.04600	-0.62100

TS16Z-large-E E=-1139.140570 G=-1139.190223 imaginary eigenvalue=-176.37

C	0.11100	-2.04000	-0.98200
C	0.75100	-1.16400	-0.22300
C	-0.48200	-3.02500	-1.86100
C	-0.05000	-0.04100	2.60400
C	2.24200	-1.09400	-0.07900
C	2.88300	0.06900	0.40600
C	3.05200	-2.20200	-0.42900
C	4.28000	0.12500	0.53200
C	4.44600	-2.14700	-0.30200
C	5.06900	-0.98200	0.18000
C	-2.18600	-0.52500	0.41300
C	-2.61100	-1.81900	0.80000
C	-3.12700	0.31800	-0.22100
C	-3.92200	-2.25700	0.55600
C	-4.44200	-0.11400	-0.46500
C	-4.84200	-1.40300	-0.07900
C	-0.17900	1.80200	0.08600

C	-0.14300	2.92900	0.93900
C	-0.04500	2.01800	-1.30600
C	0.01700	4.22600	0.42100
C	0.11200	3.31100	-1.82900
C	0.14400	4.41900	-0.96400
H	-1.52700	-2.76700	-2.16000
H	0.10400	-3.17000	-2.80000
H	-0.53200	-4.01500	-1.35600
H	-0.20400	-1.07500	2.97300
H	0.99400	0.25200	2.83500
H	-0.73800	0.62500	3.16600
H	2.28300	0.95400	0.66900
H	2.56500	-3.11800	-0.79900
H	4.75500	1.04600	0.90500
H	5.05400	-3.02400	-0.57600
H	6.16400	-0.93900	0.28200
H	-1.90300	-2.50400	1.29500
H	-2.82500	1.33100	-0.53400
H	-4.23100	-3.26900	0.86400
H	-5.15800	0.56000	-0.96200
H	-5.87100	-1.74500	-0.27100
H	-0.24000	2.79900	2.02900
H	-0.05500	1.15600	-1.99300
H	0.04400	5.09000	1.10300
H	0.21500	3.45700	-2.91600
H	0.27100	5.43500	-1.37200
Si	-0.40200	0.03500	0.74500

16E-large E= -1139.142294 G= -1139.192340

C	-0.29400	-2.55300	-0.00700
C	0.39900	-1.43900	0.22400

C	1.88000	-1.33400	0.03600
C	2.67900	-0.56800	0.91800
C	2.52200	-1.98200	-1.04700
C	4.06600	-0.47300	0.73900
C	3.91000	-1.88500	-1.22700
C	4.69000	-1.13200	-0.33400
C	0.18300	1.65100	0.22300
C	0.33400	2.79200	1.04300
C	0.65200	1.72600	-1.11100
C	0.92800	3.96700	0.55200
C	1.24300	2.89800	-1.60800
C	1.38300	4.02200	-0.77600
C	-0.21600	-3.96500	-0.38400
C	-2.38500	-0.08300	0.15200
C	-3.24000	-1.13300	0.56800
C	-2.88000	0.83600	-0.80000
C	-4.53800	-1.26200	0.04600
C	-4.17900	0.71100	-1.32500
C	-5.01000	-0.34000	-0.90300
C	-0.71500	0.04900	2.74500
H	2.20700	-0.04000	1.76100
H	1.91600	-2.55000	-1.76900
H	4.66500	0.12600	1.44200
H	4.38500	-2.39400	-2.08100
H	5.77800	-1.05200	-0.47800
H	-0.01500	2.76800	2.08800
H	0.56200	0.84800	-1.77200
H	1.03700	4.84400	1.20900
H	1.60300	2.93400	-2.64900
H	1.85100	4.94100	-1.16200

H	-0.60200	-4.12700	-1.41300
H	0.83300	-4.34800	-0.35300
H	-0.82800	-4.60300	0.29000
H	-2.88900	-1.86700	1.31100
H	-2.24000	1.66600	-1.14100
H	-5.18500	-2.08700	0.38300
H	-4.54300	1.43900	-2.06700
H	-6.02700	-0.44000	-1.31300
H	-1.35500	0.87600	3.11600
H	-1.15600	-0.90600	3.09500
H	0.28800	0.14800	3.20800
Si	-0.62600	0.05700	0.85300

Face2-^{3}CO-7

Face-Int3 E= -7364.286722 G= -7364.350180

As	-0.72800	0.12000	-0.08500
Br	1.33600	-2.45600	0.82300
C	0.85600	-1.63800	-2.11100
C	1.65100	0.75000	-2.05000
C	3.17400	-1.16600	-1.19500
C	2.96300	1.65300	2.50300
C	4.35500	1.72100	-0.27300
C	-0.72500	0.98800	1.68100
C	-0.99300	2.35900	1.85300
C	-0.42500	0.18500	2.80200
C	-0.95600	2.92400	3.14000
C	-0.40100	0.75500	4.08500
C	-0.66300	2.12500	4.25600
C	-2.11000	-1.24000	0.20700
C	-2.07100	-2.47300	-0.47000

C	-3.18100	-0.95500	1.08000
C	-3.10100	-3.41000	-0.28100
C	-4.20600	-1.89600	1.26600
C	-4.16700	-3.12500	0.58700
C	-1.67800	1.41800	-1.21100
C	-1.03000	2.61700	-1.57400
C	-2.97500	1.15700	-1.69700
C	-1.67800	3.55100	-2.39800
C	-3.61600	2.09100	-2.52900
C	-2.97200	3.28900	-2.87800
H	2.05300	0.13800	0.60900
H	1.72900	2.61300	0.19500
H	1.99400	1.62400	3.03800
H	3.58400	0.80300	2.84800
H	3.48500	2.59900	2.75800
H	4.86600	2.64100	0.07700
H	5.00900	0.85500	-0.04600
H	4.22600	1.78800	-1.37000
H	-1.24100	2.99400	0.99000
H	-0.20000	-0.88500	2.66800
H	-1.16700	3.99700	3.26700
H	-0.16900	0.12200	4.95500
H	-0.64000	2.57000	5.26300
H	-1.24100	-2.71800	-1.14400
H	-3.21900	0.00400	1.61900
H	-3.06000	-4.37200	-0.81200
H	-5.03800	-1.66600	1.94900
H	-4.96900	-3.86400	0.73700
H	-0.01000	2.83200	-1.22100
H	-3.49000	0.22300	-1.42800

H	-1.16400	4.48500	-2.67100
H	-4.62700	1.87600	-2.90700
H	-3.47700	4.01900	-3.52900
Mn	1.51600	-0.55600	-0.85900
O	1.77100	1.56600	-2.88200
O	0.46700	-2.35000	-2.94800
O	4.23800	-1.57400	-1.42600
Si	2.71600	1.57100	0.63600

Face-TS2-3CO-4 E= -7364.24528 G= -7364.308523 imaginary eigenvalue=-553.97

As	-0.73700	0.13500	-0.04200
Br	1.76100	-2.45900	-0.11300
C	1.00600	-0.33000	-2.66100
C	1.48600	1.85400	-1.38900
C	3.26000	0.07700	-1.39000
C	2.79300	-0.19000	2.50900
C	3.94000	2.15700	0.91900
C	-0.91200	-0.11500	1.90800
C	-1.12500	0.95800	2.79300
C	-0.74800	-1.41800	2.42600
C	-1.15900	0.73200	4.18000
C	-0.78200	-1.63900	3.81200
C	-0.98200	-0.56200	4.69300
C	-1.99400	-1.26900	-0.61200
C	-1.71000	-2.07500	-1.72800
C	-3.19200	-1.47300	0.10600
C	-2.61600	-3.07200	-2.13000
C	-4.09700	-2.46700	-0.30000
C	-3.80900	-3.26800	-1.41800
C	-1.76300	1.77600	-0.36400

C	-1.21600	3.01300	0.03800
C	-3.00400	1.74900	-1.03200
C	-1.91600	4.20500	-0.20400
C	-3.69500	2.94700	-1.27900
C	-3.15700	4.17500	-0.86100
H	2.15100	-1.45200	0.88100
H	1.35200	2.00000	1.76900
H	1.91600	-0.77800	2.85100
H	3.61300	-0.88500	2.22700
H	3.15300	0.38600	3.38800
H	4.22300	2.62300	1.88500
H	4.79600	1.55300	0.55600
H	3.76000	2.96700	0.18200
H	-1.27700	1.97600	2.40900
H	-0.59900	-2.27200	1.74700
H	-1.32800	1.57900	4.86300
H	-0.65400	-2.65900	4.20400
H	-1.00600	-0.73500	5.78000
H	-0.78200	-1.92600	-2.29600
H	-3.42200	-0.85500	0.98800
H	-2.38300	-3.69700	-3.00600
H	-5.03000	-2.61600	0.26400
H	-4.51800	-4.05000	-1.73300
H	-0.23400	3.05400	0.53300
H	-3.43700	0.79500	-1.36500
H	-1.48100	5.16400	0.11700
H	-4.66200	2.91700	-1.80300
H	-3.70200	5.11200	-1.05500
Mn	1.52000	0.14900	-1.00000
O	1.49300	2.99600	-1.66300

O	0.77200	-0.54100	-3.78900
O	4.39800	0.02900	-1.65700
Si	2.37800	1.08600	1.12300

Face-Int4 E= -7364.247402 G= -7364.310919

As	-0.73600	0.12000	-0.04900
Br	1.76100	-2.44700	0.09600
C	1.10800	-0.69800	-2.60100
C	1.45300	1.66300	-1.63900
C	3.29200	-0.02900	-1.30700
C	2.89000	0.06600	2.43300
C	3.82600	2.40900	0.68400
C	-0.89400	0.01200	1.91400
C	-1.14400	1.14500	2.71200
C	-0.69100	-1.23900	2.53700
C	-1.17500	1.03100	4.11200
C	-0.72300	-1.34900	3.93600
C	-0.95900	-0.21200	4.72800
C	-2.03000	-1.28900	-0.53000
C	-1.87800	-2.00000	-1.73400
C	-3.13200	-1.57000	0.30700
C	-2.81300	-2.98400	-2.09900
C	-4.06300	-2.55500	-0.06000
C	-3.90400	-3.26500	-1.26200
C	-1.75500	1.74700	-0.46300
C	-1.17200	3.00600	-0.20700
C	-3.04000	1.68100	-1.03800
C	-1.87700	4.18300	-0.50400
C	-3.73600	2.86300	-1.34200
C	-3.15900	4.11400	-1.07300
H	2.28700	-2.10100	1.40100

H	1.28700	2.12100	1.60900
H	2.04900	-0.55500	2.80900
H	3.73000	-0.59200	2.12000
H	3.25300	0.66800	3.29300
H	4.09200	2.96000	1.61000
H	4.72100	1.85400	0.33800
H	3.56400	3.15100	-0.09700
H	-1.32700	2.12400	2.24600
H	-0.52300	-2.14100	1.93000
H	-1.37200	1.92400	4.72400
H	-0.56700	-2.33100	4.40900
H	-0.98200	-0.29700	5.82500
H	-1.03500	-1.78400	-2.40400
H	-3.26700	-1.02000	1.25000
H	-2.68200	-3.53300	-3.04400
H	-4.91900	-2.76600	0.59900
H	-4.63400	-4.03900	-1.54700
H	-0.16100	3.07500	0.22200
H	-3.50300	0.70700	-1.25400
H	-1.41300	5.16000	-0.29700
H	-4.73800	2.80100	-1.79400
H	-3.70700	5.03800	-1.31100
Mn	1.53500	0.02800	-1.00900
O	1.42700	2.75400	-2.07100
O	0.94300	-1.07100	-3.70100
O	4.44400	-0.07100	-1.51100
Si	2.36200	1.23300	1.00800
Face4	E= -4789.865303		G= -4789.926157
As	-0.50700	0.01500	0.06700
C	0.84400	-2.68600	-0.09900

C	2.05700	-0.81100	-1.53800
C	3.25900	-1.80800	0.43500
C	4.64200	0.93100	0.97300
C	2.74900	2.30700	-0.96800
C	-0.74100	1.91300	-0.36200
C	-1.10200	2.30000	-1.66800
C	-0.43900	2.89800	0.60100
C	-1.15500	3.66200	-2.00800
C	-0.49800	4.25800	0.25500
C	-0.85100	4.64200	-1.04900
C	-1.36700	-0.13500	1.82200
C	-0.94500	-1.17300	2.67600
C	-2.38500	0.74400	2.24200
C	-1.53700	-1.33300	3.93900
C	-2.97800	0.57800	3.50400
C	-2.55400	-0.45800	4.35400
C	-1.80500	-0.81300	-1.15200
C	-1.35300	-1.26900	-2.40700
C	-3.16100	-0.96000	-0.80100
C	-2.25700	-1.85300	-3.30900
C	-4.05800	-1.55400	-1.70400
C	-3.60900	-1.99900	-2.95900
H	2.08500	1.62900	1.65800
H	5.03700	1.94800	1.17900
H	4.77800	0.31500	1.88500
H	5.25800	0.48000	0.16800
H	3.37000	1.93800	-1.81000
H	1.72300	2.47300	-1.35000
H	3.16200	3.28100	-0.63300
H	-1.34300	1.54000	-2.42600

H	-0.15400	2.60900	1.62300
H	-1.43700	3.95700	-3.03000
H	-0.26200	5.02100	1.01200
H	-0.89100	5.70800	-1.31800
H	-0.15700	-1.87300	2.35100
H	-2.71800	1.56400	1.58600
H	-1.20100	-2.14600	4.60100
H	-3.77600	1.26500	3.82500
H	-3.01900	-0.58300	5.34400
H	-0.29400	-1.16800	-2.69100
H	-3.52300	-0.61900	0.18100
H	-1.89700	-2.20300	-4.28900
H	-5.11500	-1.67200	-1.42200
H	-4.31400	-2.46400	-3.66300
Mn	1.65500	-1.08400	0.13200
O	2.31300	-0.61500	-2.66900
O	0.40000	-3.73600	-0.35800
O	4.30600	-2.29600	0.61900
Si	2.81000	1.03400	0.45000
5	E= -155.736543		G= -155.763312
C	0.61300	-0.00100	-0.00000
C	-0.61300	-0.00000	-0.00000
C	-2.07200	0.00000	0.00000
C	2.07200	0.00000	0.00000
H	-2.48000	0.95700	-0.39000
H	-2.48100	-0.81600	-0.63300
H	-2.48000	-0.14000	1.02300
H	2.48000	1.02300	-0.14200
H	2.48000	-0.38800	0.95700
H	2.48100	-0.63400	-0.81500

Face-Int5 E= -4945.608559 G= -4945.674615

As	-0.24800	0.42200	-0.09400
C	0.24500	-2.17200	-1.85500
C	2.13200	-0.40500	-2.07800
C	2.71900	-2.48700	-0.97000
C	2.97900	-0.65300	2.48400
C	3.47500	1.60200	0.42000
C	-2.13200	-3.30700	0.95300
C	-0.93700	-3.13900	1.17300
C	0.47700	-2.87300	1.35300
C	-3.54800	-3.49200	0.67200
C	-2.14200	0.04800	-0.52600
C	-3.19600	0.19800	0.39500
C	-2.43300	-0.31300	-1.85600
C	-4.52300	-0.02800	-0.00800
C	-3.76000	-0.53700	-2.25600
C	-4.80900	-0.39900	-1.33100
C	-0.19300	2.24300	-0.84700
C	-1.25200	3.12500	-0.54200
C	0.85800	2.68300	-1.66900
C	-1.25000	4.43300	-1.04800
C	0.85400	3.99300	-2.18000
C	-0.19600	4.87000	-1.86900
C	-0.33800	0.85800	1.82500
C	-0.87600	-0.06900	2.74500
C	0.22700	2.05600	2.30700
C	-0.83600	0.19800	4.12300
C	0.27000	2.31500	3.68600
C	-0.25500	1.38600	4.59800
H	4.51200	-0.87500	0.25200

H	3.83800	-0.20500	3.02800
H	2.04700	-0.23200	2.91100
H	2.99000	-1.74600	2.67400
H	4.32000	1.90100	1.07600
H	3.75400	1.84300	-0.62500
H	2.59600	2.21800	0.69100
H	0.67700	-1.96800	1.95600
H	1.02700	-3.71200	1.82900
H	0.99600	-2.81600	0.33900
H	-4.18100	-2.96400	1.41500
H	-3.80500	-3.08000	-0.32600
H	-3.83200	-4.56500	0.68400
H	-2.99300	0.49800	1.43400
H	-1.62500	-0.41700	-2.59500
H	-5.33900	0.09000	0.72200
H	-3.97300	-0.81900	-3.29900
H	-5.84900	-0.57800	-1.64400
H	-2.08600	2.79200	0.09600
H	1.68500	2.01300	-1.92600
H	-2.08000	5.11300	-0.80200
H	1.68200	4.32500	-2.82500
H	-0.19700	5.89600	-2.26900
H	-1.34300	-1.00100	2.39100
H	0.62900	2.80200	1.60500
H	-1.26200	-0.53200	4.82900
H	0.71800	3.25300	4.04800
H	-0.21800	1.59000	5.67900
Mn	1.40100	-1.30400	-0.76800
O	2.66800	0.14000	-2.97000
O	3.57500	-3.26600	-1.13300

O	-0.39300	-2.76800	-2.63300
Si	3.16500	-0.27300	0.61600

Face-TS4-6 E= -4945.603312 G= -4945.670435 imaginary eigenvalue=-78.00

As	-0.66100	0.25400	-0.03700
C	1.07500	-1.25400	-2.13300
C	2.69800	-1.66500	-0.13000
C	3.07800	0.33900	-1.46800
C	2.44000	2.61400	1.13200
C	4.49000	0.39500	1.56000
C	0.41200	-3.78500	0.60600
C	0.24800	-3.18400	1.66400
C	0.09800	-2.49600	2.94000
C	0.65900	-4.51000	-0.63600
C	-0.70400	2.09700	-0.70700
C	0.07500	2.38600	-1.84900
C	-1.42300	3.12800	-0.07300
C	0.14000	3.69700	-2.34600
C	-1.36000	4.43700	-0.57900
C	-0.57700	4.72400	-1.71000
C	-2.10400	-0.58700	-1.06700
C	-3.00500	0.17600	-1.83400
C	-2.21000	-1.99200	-1.05100
C	-4.00400	-0.46700	-2.58300
C	-3.21700	-2.62800	-1.79400
C	-4.11200	-1.86800	-2.56500
C	-1.48100	0.41100	1.73600
C	-0.85400	1.20200	2.72200
C	-2.66300	-0.28700	2.04900
C	-1.40700	1.28800	4.00900

C	-3.20800	-0.20100	3.34100
C	-2.58100	0.58300	4.32300
H	1.95000	0.28000	2.56300
H	1.38800	2.94800	1.03500
H	2.89100	3.10700	2.02000
H	2.98100	2.96900	0.23000
H	4.85300	0.97200	2.43600
H	4.69100	-0.68000	1.74300
H	5.07800	0.70600	0.67200
H	0.63600	-1.52400	2.93300
H	-0.96500	-2.27900	3.17200
H	0.51100	-3.10300	3.77200
H	0.36900	-5.57800	-0.55000
H	0.09800	-4.07500	-1.48900
H	1.73700	-4.46900	-0.90100
H	0.63200	1.58100	-2.35900
H	-2.03300	2.91400	0.81800
H	0.75500	3.91400	-3.23200
H	-1.92700	5.23900	-0.08300
H	-0.52500	5.75300	-2.09700
H	-2.92800	1.27400	-1.85400
H	-1.51000	-2.58900	-0.44500
H	-4.70300	0.13300	-3.18600
H	-3.29600	-3.72600	-1.77400
H	-4.89600	-2.36800	-3.15400
H	0.06500	1.75700	2.48900
H	-3.16300	-0.90300	1.28700
H	-0.91200	1.91000	4.77100
H	-4.13100	-0.75200	3.57900
H	-3.00900	0.64800	5.33500

Mn	1.67600	-0.36200	-0.68000
O	0.79100	-1.90800	-3.06000
O	3.98700	0.86600	-1.99200
O	3.39600	-2.54100	0.22200
Si	2.63300	0.71100	1.27100
Face6	E= -4945.634661		G= -4945.699175
As	-0.68500	0.04400	0.01300
C	1.00000	-1.51100	-2.02700
C	3.35600	-0.78200	-1.13600
C	1.71700	0.95700	-1.86400
C	1.72600	3.25400	0.16100
C	4.34500	1.71400	0.46100
C	1.67300	-2.34300	0.25700
C	1.94000	-1.45600	1.13700
C	2.33400	-1.22200	2.54100
C	1.68800	-3.75500	-0.17900
C	-1.57300	1.71000	-0.53500
C	-1.37200	2.16700	-1.85300
C	-2.44700	2.41700	0.31600
C	-2.01700	3.32900	-2.30600
C	-3.08500	3.58300	-0.13900
C	-2.86800	4.04400	-1.44700
C	-2.06600	-1.24600	-0.56200
C	-3.30100	-0.82700	-1.09400
C	-1.79800	-2.62600	-0.44900
C	-4.25100	-1.77700	-1.50400
C	-2.75200	-3.57300	-0.85200
C	-3.98100	-3.15000	-1.38400
C	-0.95300	0.03900	1.96100
C	-0.57600	1.17200	2.71400

C	-1.40600	-1.11400	2.63200
C	-0.65600	1.15100	4.11500
C	-1.47300	-1.13500	4.03600
C	-1.09800	-0.00500	4.78000
H	2.12600	1.35800	2.03100
H	0.61700	3.26900	0.19100
H	2.10200	3.97800	0.91400
H	2.03400	3.60400	-0.84400
H	4.67600	2.58000	1.07100
H	4.86500	0.80700	0.82800
H	4.66600	1.88600	-0.58700
H	3.33800	-0.75200	2.60800
H	1.63000	-0.54500	3.06400
H	2.36400	-2.18800	3.08700
H	1.69500	-4.42700	0.70500
H	0.82900	-4.02900	-0.82300
H	2.60400	-3.96100	-0.77400
H	-0.71200	1.61900	-2.53900
H	-2.64000	2.05900	1.33800
H	-1.84700	3.67800	-3.33600
H	-3.76100	4.13000	0.53600
H	-3.36700	4.96000	-1.80000
H	-3.52800	0.24500	-1.19200
H	-0.83600	-2.96500	-0.04100
H	-5.21100	-1.43800	-1.92200
H	-2.52900	-4.64600	-0.75400
H	-4.72800	-3.89100	-1.70700
H	-0.21900	2.08200	2.21100
H	-1.71400	-2.00400	2.06600
H	-0.36400	2.04300	4.68900

H	-1.82600	-2.04300	4.54800
H	-1.15200	-0.02400	5.87900
Mn	1.64900	-0.43000	-0.75300
O	0.61500	-2.21000	-2.88100
O	1.83300	1.79700	-2.67700
O	4.46400	-1.04000	-1.39700
Si	2.45200	1.53200	0.56700

Face-TS6-7 E= -4945.628666 G= -4945.692095 imaginary eigenvalue=-86.02

As	0.81700	-0.09900	0.02200
C	-2.89300	0.71200	-1.84000
C	-1.14900	-1.16000	-1.89400
C	-0.55300	1.51700	-2.01300
C	-1.68600	1.80500	0.39500
C	-2.12600	0.79400	1.13600
C	-2.02500	0.65200	2.64200
C	-1.34900	3.22900	0.60800
C	-3.79500	-2.14800	-0.71900
C	-4.99200	0.26900	0.66700
C	1.72000	1.45300	0.80500
C	1.40400	1.89700	2.10500
C	2.57000	2.22900	-0.00900
C	1.94400	3.10000	2.58800
C	3.10400	3.43300	0.47800
C	2.79200	3.87100	1.77700
C	0.80800	-1.42300	1.46900
C	1.69600	-1.38000	2.56300
C	-0.13400	-2.46700	1.37500
C	1.63200	-2.37200	3.55600
C	-0.19100	-3.45700	2.36700
C	0.68800	-3.40900	3.46200

C	2.21100	-0.81800	-1.16300
C	2.15100	-0.56900	-2.54800
C	3.27900	-1.57400	-0.63900
C	3.15500	-1.06200	-3.39800
C	4.27900	-2.06700	-1.49200
C	4.21900	-1.81100	-2.87200
H	-3.16700	-1.53600	1.77600
H	-2.99200	0.39300	3.12000
H	-1.30800	-0.15000	2.91900
H	-1.66700	1.60600	3.08200
H	-0.33000	3.46500	0.24000
H	-2.04600	3.86400	0.01800
H	-1.43000	3.53700	1.67300
H	-2.97300	-2.88500	-0.81500
H	-4.67700	-2.67000	-0.28900
H	-4.06000	-1.78600	-1.73100
H	-4.98600	0.93300	1.55300
H	-5.14800	0.89500	-0.23400
H	-5.85200	-0.42800	0.75000
H	0.73000	1.31100	2.74600
H	2.81500	1.89700	-1.03000
H	1.69300	3.43900	3.60600
H	3.76900	4.03200	-0.16300
H	3.21100	4.81500	2.15600
H	2.44000	-0.57400	2.64800
H	-0.82700	-2.50500	0.52100
H	2.32600	-2.33300	4.40900
H	-0.93300	-4.26700	2.28600
H	0.63800	-4.18100	4.24400
H	1.32100	0.01200	-2.97600

H	3.33200	-1.78900	0.43900
H	3.09900	-0.86100	-4.47900
H	5.10700	-2.65900	-1.07400
H	5.00300	-2.20200	-3.54000
Mn	-1.37800	0.36700	-0.95200
O	-1.00100	-2.09900	-2.57900
O	-0.04500	2.33400	-2.68200
O	-3.80300	0.95500	-2.53700
Si	-3.38200	-0.73400	0.51000