Supporting Information

Tuning the Laplaza-Cummins Catalyst to Activate and Cleave CO_2

Nigel J. Brookes,[†] Alireza Ariafard,[†§] Robert Stranger,[‡] and Brian F. Yates[†,*]

†School of Chemistry, University of Tasmania, Private Bag 75, Hobart Tas7001, Australia

‡Department of Chemistry, The Australian National University, Canberra ACT 0200, Australia

§ Department of Chemistry, Faculty of Science, Central Tehran Branch, Islamic Azad University, Shahrak Gharb, Tehran, Iran

Table of Contents

1. General Basis Sets

These basis sets are LANL2TZ+(3f) for tantalum, niobium, vanadium and rhenium.
They was obtained in the same way as described in Yates, B.F. J. Mol. Struct. (Theochem), 2000, 506, 223-232 for platinum.
a) The triple-zeta split was obtained by uncontracting the LANL2DZ basis set of Hay and Wadt to give: [341/321/31] -> [3311/3111/211]
b) The f-function exponent was taken from Frenking and co-workers (Chem. Phys. Lett., 1993, 208, 111-114) and then split according to the even scaling rule to give three exponents.
c) Diffuse s, p and d functions were added using an even tempered extension of the two outermost exponents.

1.1 Tantalum GBS

```
-C -H -N -O -Si 0
6-311+G(2d,p)
****
-Ta 0
 S   3 1.00       0.000000000000
      0.2044000000D+01 -0.1310478632D+01
      0.1267000000D+01  0.1657992800D+01
      0.4157000000D+00  0.4848339339D+00
 S   3 1.00       0.000000000000
      0.2044000000D+01  0.1189732273D+01
      0.1267000000D+01 -0.1665046381D+01
      0.4157000000D+00 -0.1056334242D+01
 S   1 1.00       0.000000000000
      0.1671000000D+00  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.4820000000D-01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.1390000000D-01  0.1000000000D+01
 P   3 1.00       0.000000000000
      0.2565000000D+01 -0.2917238002D+00
      0.1229000000D+01  0.7570649005D+00
      0.4244000000D+00  0.5240081003D+00
 P   1 1.00       0.000000000000
      0.4360000000D+00  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.8400000000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.2800000000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.0933000000D-01  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.8948000000D+00  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.2989000000D+00  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.9350000000D-01  0.1000000000D+01
```

```
D   1 1.00       0.000000000000
     0.2925000000D-01  0.1000000000D+01
F   1 1.00       0.000000000000
     3.1600000000D+00  0.1000000000D+01
F   1 1.00       0.000000000000
     0.7900000000D+00  0.1000000000D+01
F   1 1.00       0.000000000000
     0.1975000000D+00  0.1000000000D+01
****

Ta 0
lanl2dz
```

1.2 Rhenium GBS

```
-C -H -N -O -Si 0
6-311G(d,p)
****
-Re 0
S 3 1.00 0.000000000000
          0.2185000000D+01 -0.1622372663D+01
          0.1451000000D+01 0.1993864586D+01
          0.4585000000D+00 0.4531165060D+00
S 3 1.00 0.000000000000
          0.2185000000D+01 0.1545973736D+01
          0.1451000000D+01 -0.2075891303D+01
          0.4585000000D+00 -0.1192239025D+01
S 1 1.00 0.000000000000
          0.2314000000D+00 0.1000000000D+01
S 1 1.00 0.000000000000
          0.5660000000D-01 0.1000000000D+01
S 1 1.00 0.000000000000
          0.1384000000D-01 0.1000000000D+01
P 3 1.00 0.000000000000
          0.3358000000D+01 -0.2318666976D+00
          0.1271000000D+01 0.7458682922D+00
          0.4644000000D+00 0.4632685952D+00
P 1 1.00 0.000000000000
          0.4960000000D+00 0.10000000000D+01
P 1 1.00 0.000000000000
          0.8900000000D-01 0.10000000000D+01
P 1 1.00 0.000000000000
          0.2800000000D-01 0.1000000000D+01
P 1 1.00 0.000000000000
          0.0881000000D-01 0.1000000000D+01
D 1 1.00 0.000000000000
          0.1116000000D+01 0.1000000000D+01
D 1 1.00 0.000000000000
          0.4267000000D+00 0.1000000000D+01
D 1 1.00 0.000000000000
          0.1378000000D+00 0.1000000000D+01
D 1 1.00 0.000000000000
          0.4399000000D-01 0.1000000000D+01
F 1 1.00 0.000000000000
          3.476000000D+00 0.1000000000D+01
F 1 1.00 0.000000000000
```

```
          0.869000000D+00 0.1000000000D+01
F 1 1.00 0.000000000000
          0.217200000D+00 0.1000000000D+01
****

Re 0
lanl2dz
```

1.3 Vanadium GBS

```
-C -H -N -O -Si 0
6-311+G(2d,p)
****
-V 0
 S   3 1.00       0.000000000000
      0.4590000000D+01 -0.4277302118D+00
      0.1493000000D+01  0.7069691196D+00
      0.5570000000D+00  0.5895813163D+00
 S   3 1.00       0.000000000000
      0.4590000000D+01  0.2501080876D+00
      0.1493000000D+01 -0.4697776766D+00
      0.5570000000D+00 -0.7129414645D+00
 S   1 1.00       0.000000000000
      0.9750000000D-01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.3420000000D-01  0.1000000000D+01
 S   1 1.00       0.000000000000
      0.1120000000D-01  0.1000000000D+01
 P   2 1.00       0.000000000000
      0.1376000000D+02 -0.4823120145D-01
      0.1712000000D+01  0.6141161185D+00
 P   1 1.00       0.000000000000
      0.5587000000D+00  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.5900000000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.1800000000D-01  0.1000000000D+01
 P   1 1.00       0.000000000000
      0.5490000000D-02  0.1000000000D+01
 D   3 1.00       0.000000000000
      0.2570000000D+02  0.3310329953D-01
      0.6530000000D+01  0.1795752975D+00
      0.2078000000D+01  0.4373061938D+00
 D   1 1.00       0.000000000000
      0.6243000000D+00  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.1542000000D+00  0.1000000000D+01
 D   1 1.00       0.000000000000
      0.3809000000D-01  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.7004000000D+01  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.1751000000D+01  0.1000000000D+01
 F   1 1.00       0.000000000000
      0.4377500000D+00  0.1000000000D+01
****
```

V 0
lanl2dz

1.4 Niobium GBS

-C -H -N -O -Si 0
6-311+G(2d,p)
****
-Nb 0
S 3 1.00 0.000000000000
0.2182000000D+01 -0.8846140757D+00
0.1209000000D+01 0.1103377596D+01
0.4165000000D+00 0.6298773691D+00
S 3 1.00 0.000000000000
0.2182000000D+01 0.7790287762D+00
0.1209000000D+01 -0.1075279105D+01
0.4165000000D+00 -0.1150601113D+01
S 1 1.00 0.000000000000
0.1454000000D+00 0.1000000000D+01
S 1 1.00 0.000000000000
0.3920000000D-01 0.1000000000D+01
S 1 1.00 0.000000000000
0.1056800000D-01 0.1000000000D+01
P 3 1.00 0.000000000000
0.4519000000D+01 -0.8173030017D-01
0.9406000000D+00 0.6995115015D+00
0.3492000000D+00 0.3980996008D+00
P 1 1.00 0.000000000000
0.4106000000D+00 -0.1212175669D+00
P 1 1.00 0.000000000000
0.7520000000D-01 0.1000000000D+01
P 1 1.00 0.000000000000
0.2470000000D-01 0.1000000000D+01
P 1 1.00 0.000000000000
0.8113000000D-02 0.1000000000D+01
D 2 1.00 0.000000000000
0.3466000000D+01 0.3159829928D-01
0.9938000000D+00 0.4834305890D+00
D 1 1.00 0.000000000000
0.3350000000D+00 0.1000000000D+01
D 1 1.00 0.000000000000
0.1024000000D+00 0.1000000000D+01
D 1 1.00 0.000000000000
0.3130000000D-01 0.1000000000D+01
F 1 1.00 0.000000000000
3.80800000000D+00 0.1000000000D+01
F 1 1.00 0.000000000000
0.9520000000D+00 0.1000000000D+01
F 1 1.00 0.000000000000
0.238000000D+00 0.1000000000D+01
****

Nb 0
lanl2dz

2 Geometric and Energetic details of Tantalum structures

2.1 Model-opt level of theory (Ta)

CO_2
B3LYP/GBS(1) = -188.577570 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -188.650304 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -188.562181 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -188.675365 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -188.658053 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -188.562101 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -188.563813 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -188.563228 a.u.

Enthalpy Correction = 0.015204
Gibbs Free Energy Correction = -0.009752

Atomic No	x-coord	y-coord	z-coord
8	0.000000	0.000000	1.169591
6	0.000000	0.000000	0.000000
8	0.000000	0.000000	-1.169591

CO
B3LYP/GBS(1) = -113.306914 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -113.351691 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -113.298430 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -113.364144 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -113.348950 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -113.288405 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -113.288882 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -113.288715 a.u.
Enthalpy Correction = 0.008341
Gibbs Free Energy Correction = -0.014102

Atomic No	x-coord	y-coord	z-coord
6	0.000000	0.000000	-0.650147
8	0.000000	0.000000	0.487611

Structure 1Ta_T
B3LYP/GBS(1) = -225.708774 a.u.

B3LYP/GBS(2)//B3LYP/GBS(1) = -225.808896 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -225.357747 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -225.797179 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -225.870092 a.u.
Enthalpy Correction = 0.08288
Gibbs Free Energy Correction = 0.040502

Atomic No	x-coord	y-coord	z-coord
73	-0.005987	-0.001075	-0.001464
7	1.221845	-1.584875	0.003802
7	-1.974011	-0.267798	0.003073
7	0.751498	1.854185	0.003573
1	-2.665588	0.477879	0.005406
1	1.088561	2.342689	0.832560
1	1.679910	-1.963090	0.832413
1	-2.445608	-1.168824	0.005495
1	1.685812	-1.963952	-0.821160
1	1.098643	2.343177	-0.821003

Structure 1Ta_T to 1Ta_S MECP
B3LYP/GBS(1) = -225.708709a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -225.808344 a.u.

GBS2 coordinates

Atomic No	x-coord	y-coord	z-coord
73	-0.0487998	-0.0055547	-0.0887017
7	1.2385191	-1.5554675	-0.0087650
7	-2.0224747	-0.2747629	-0.0021807
7	0.7786376	1.8318096	-0.0062460
1	-2.7157235	0.4638854	0.0278745
1	1.0847519	2.3014611	0.8411775
1	1.6595124	-1.9267941	0.8383698
1	-2.4953597	-1.1706201	0.0267272
1	1.7666688	-1.9252669	-0.7943127
1	1.1893426	2.3296258	-0.7912473

Structure 1Ta_S
B3LYP/GBS(1) = -225.714351 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -225.816289 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -225.374290 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -225.802065 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -225.876058 a.u.
Enthalpy Correction = 0.081946
Gibbs Free Energy Correction = 0.039708

Atomic No	x-coord	y-coord	z-coord
73	-0.152391	-0.079066	2.521992

7	-1.839224	-0.653209	1.703466
7	0.113335	1.866331	2.600645
7	1.036333	-1.125305	3.678026
1	0.865400	2.333614	3.100475
1	0.850278	-1.774532	4.434437
1	-2.611890	-1.206103	2.057971
1	-0.493877	2.556561	2.166238
1	-1.910506	-0.532800	0.688503
1	2.016239	-1.178563	3.383435

Structure 2Ta_T
B3LYP/GBS(1) = -414.303612 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -414.476987 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -413.948166 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -414.500046 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -414.551133 a.u.
Enthalpy Correction = 0.098635
Gibbs Free Energy Correction = 0.098635

Atomic No	x-coord	y-coord	z-coord
73	0.284947	0.000278	-0.014248
7	1.747043	-0.012877	1.311565
7	0.658492	1.670991	-1.024945
7	0.670561	-1.643832	-1.063360
1	1.591544	2.055867	-1.163944
1	1.606717	-2.017765	-1.211236
1	2.115825	0.813177	1.782251
1	0.020509	2.100758	-1.691861
1	2.118998	-0.848904	1.761779
1	0.036017	-2.062967	-1.740210
8	-1.422753	-0.016913	1.227410
6	-2.092618	-0.004233	0.123099
8	-3.235712	0.000031	-0.227169

Structure 2Ta_S
B3LYP/GBS(1) = -414.358248 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -414.535299 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -414.007668 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -414.560989 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -414.612033 a.u.
Enthalpy Correction = 0.09892
Gibbs Free Energy Correction = 0.051827

Atomic No	x-coord	y-coord	z-coord
73	-0.263505	0.026836	0.009547
7	-1.480956	-0.607400	1.443415
7	-0.394683	-1.518773	-1.212706
7	-0.943255	1.546172	-1.050068
1	-1.259890	-2.041038	-1.335621
1	-0.772725	2.512740	-0.781278
1	-2.254922	-0.061042	1.812804

1	0.378852	-1.975922	-1.682826
1	-1.349615	-1.442842	2.010398
1	-1.302049	1.494683	-1.998182
8	1.282553	0.803280	0.967209
6	1.854106	-0.065349	0.046432
8	3.017931	-0.302465	-0.125371

Structure 2Ta_TS_S
B3LYP/GBS(1) = -414.354311 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -414.533223 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -414.004507 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -414.561453 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -414.610906 a.u.
Enthalpy Correction = 0.097524
Gibbs Free Energy Correction = 0.051315

Atomic No	x-coord	y-coord	z-coord
73	0.239362	-0.037486	0.006986
7	1.739189	0.409224	1.241028
7	0.425134	1.704582	-0.939198
7	0.808731	-1.501774	-1.185968
1	1.324505	2.163106	-1.071328
1	0.443261	-2.446249	-1.101190
1	2.254632	-0.302436	1.753692
1	-0.328666	2.279819	-1.298122
1	1.924415	1.324079	1.641945
1	1.422577	-1.420800	-1.990702
8	-1.143879	-0.823332	1.005192
6	-1.916190	0.186408	-0.034288
8	-3.084669	0.290372	-0.011393

Structure 3Ta_T
B3LYP/GBS(1) = -640.136525 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -640.407819 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -639.447539 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -640.423563 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -640.542917 a.u.
Enthalpy Correction = 0.183941
Gibbs Free Energy Correction = 0.114044

Atomic No	x-coord	y-coord	z-coord
73	2.340856	0.000004	0.024649
7	3.643980	-0.000361	1.514867
7	2.568358	1.687102	-1.001755
7	2.568640	-1.686646	-1.002434
1	3.461467	2.062865	-1.314503
1	1.813314	-2.112047	-1.537612
1	3.970344	-0.831894	2.003607
1	1.812863	2.112495	-1.536704
1	3.970518	0.830818	2.004084
1	3.461876	-2.062005	-1.315318

8	-0.007641	0.000314	-0.714991
6	0.316537	-0.000007	0.555834
8	-0.660611	-0.000204	1.402309
73	-2.261195	-0.000019	0.008335
7	-3.830212	-0.000274	1.225537
7	-2.587484	-1.722337	-0.934428
7	-2.587692	1.722536	-0.933935
1	-2.200838	-1.966114	-1.841737
1	-3.158874	2.483081	-0.575339
1	-4.819244	-0.000304	0.972507
1	-3.158588	-2.483044	-0.576060
1	-3.749350	-0.000369	2.241849
1	-2.201067	1.966636	-1.841167

Structure 3Ta_S
B3LYP/GBS(1) = -640.148093 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -640.424827 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -639.451865 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -640.449371 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -640.569616 a.u.
Enthalpy Correction = 0.183629
Gibbs Free Energy Correction = 0.114099

Atomic No	x-coord	y-coord	z-coord
73	-2.278432	0.005505	0.022480
7	-2.588195	1.678894	-1.022042
7	-3.451903	-0.070900	1.614815
7	-2.550432	-1.670516	-1.029406
1	-3.792172	0.740176	2.125947
1	-1.824460	-2.242312	-1.452475
1	-3.509749	1.961170	-1.352538
1	-3.729865	-0.927078	2.088011
1	-1.876233	2.183479	-1.544738
1	-3.448581	-1.910291	-1.448099
8	0.283969	0.133394	-0.781215
6	-0.340202	-0.040530	0.452002
8	0.658743	-0.157761	1.351626
73	2.152006	0.006520	0.001361
7	2.625845	-1.511825	-1.187562
7	3.642922	-0.294393	1.296534
7	2.708384	1.824985	-0.563534
1	3.997215	0.424881	1.925000
1	3.674522	2.096656	-0.725793
1	3.579372	-1.813975	-1.367384
1	3.902883	-1.206967	1.667227
1	1.974168	-1.988710	-1.803130
1	2.075199	2.549546	-0.889358

Structure 4Ta_S
B3LYP/GBS(1) = -301.077335 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -301.216384 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -300.740397 a.u.

TPSS/GBS(2)//B3LYP/GBS(1) = -301.219039 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -301.284828 a.u.
Enthalpy Correction = 0.087979
Gibbs Free Energy Correction = 0.045451

Atomic No	x-coord	y-coord	z-coord
73	0.000014	-0.000058	0.039592
7	1.585973	-1.027063	-0.599337
7	0.097443	1.888227	-0.595452
7	-1.683602	-0.858127	-0.598828
1	0.320545	2.678829	0.001414
1	-2.479379	-1.063629	-0.002506
1	2.044636	-0.894943	-1.495877
1	-0.243865	2.220549	-1.492508
1	2.158810	-1.617745	-0.004346
1	-1.801166	-1.315268	-1.498199
8	0.000091	-0.003104	1.769644

Structure 5Ta_T
B3LYP/GBS(1) = -339.075310 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -339.220664 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -338.719206 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -339.232558 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -339.289822 a.u.
Enthalpy Correction = 0.093229
Gibbs Free Energy Correction = 0.045649

Atomic No	x-coord	y-coord	z-coord
73	-0.177054	0.000029	-0.012863
7	-1.347653	-0.001318	1.609865
7	-0.516131	-1.719172	-0.965086
7	-0.517080	1.720024	-0.963320
1	-1.437182	-1.991959	-1.304199
1	0.180524	2.350180	-1.349562
1	-1.580708	0.828192	2.150354
1	0.181620	-2.347393	-1.354189
1	-1.577283	-0.830904	2.151711
1	-1.437611	1.991165	-1.305166
6	1.863525	0.000400	0.145777
8	3.010058	-0.000070	0.413149

Structure 5Ta_T to 5Ta_S MECP
B3LYP/GBS(2)//B3LYP/GBS(1) = -339.211740 a.u.

Atomic No	x-coord	y-coord	z-coord
73	-0.1559242	-0.0040839	0.0100143

7	-0.9835903	1.6662750	-0.6647815
7	-0.2634798	0.0148598	1.9929721
7	-1.0102789	-1.6931900	-0.6086187
1	-1.1396153	-0.1212611	2.4894528
1	-0.8178608	-2.6323877	-0.2805423
1	-1.1098762	1.8812224	-1.6488684
1	0.4964765	0.0492357	2.6594058
1	-1.1994625	2.4862746	-0.1111874
1	-1.7419604	-1.7347664	-1.3096528
6	1.8787254	0.0349732	-0.1120879
8	3.0396986	0.0549919	-0.2507207

Structure 5Ta-S
B3LYP/GBS(1) = -339.070794 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -339.213043 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -338.710807 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -339.225015 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -339.282803 a.u.
Enthalpy Correction = 0.093933
Gibbs Free Energy Correction = 0.048103

Atomic No	x-coord	y-coord	z-coord
73	-0.193936	0.000088	-0.051967
7	-0.977498	1.741614	-0.612732
7	-0.268507	-0.001302	1.935149
7	-0.981707	-1.738812	-0.615194
1	-1.155589	-0.001374	2.439983
1	-1.007153	-2.571996	-0.032932
1	-1.387803	1.952240	-1.520426
1	0.500587	-0.002607	2.596985
1	-1.002178	2.573475	-0.028550
1	-1.394869	-1.946219	-1.522324
6	1.846868	-0.001627	-0.145574
8	3.014637	-0.001336	-0.277033

2.2 Gen-opt level of theory (Ta)

Gen-opt Structure 1Ta_T
B3LYP/GBS(1) = -1384.234118 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.978629 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1389.893031 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -1389.900878 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -1389.897888 a.u.
Enthalpy Correction = 0.700207
Gibbs Free Energy Correction = 0.590026

Atomic No	x-coord	y-coord	z-coord
73	0.054352	-0.279520	-0.330990
7	-1.857522	-0.795263	-0.693401
7	0.453036	1.668717	-0.766735
7	1.442907	-1.675713	0.094818
6	-2.700437	-0.920009	-1.917256
6	-1.769820	-0.961690	-3.149446
6	-3.541580	-2.221996	-1.892421
6	-3.651186	0.297893	-2.041661
1	-1.178843	-0.042140	-3.218483
1	-1.087400	-1.816098	-3.084736

1	-2.370180	-1.057850	-4.061398
1	-4.218883	-2.231287	-1.033761
1	-4.138408	-2.292029	-2.808934
1	-2.882178	-3.094696	-1.835043
1	-4.247116	0.224208	-2.958660
1	-4.329678	0.340824	-1.183946
1	-3.063022	1.221069	-2.072456
6	1.446593	-3.170912	0.160939
6	0.304237	-3.702208	-0.730726
6	2.779790	-3.768213	-0.352299
6	1.211553	-3.619271	1.625994
1	0.473578	-3.411631	-1.773288
1	0.267782	-4.795445	-0.668511
1	-0.658652	-3.295569	-0.412109
1	3.624648	-3.442078	0.260133
1	2.719918	-4.861199	-0.311471
1	2.955787	-3.467518	-1.390683
1	1.206090	-4.713419	1.691740
1	2.007346	-3.235717	2.272485
1	0.249570	-3.233306	1.979501
6	1.281075	2.316560	-1.831818
6	1.774276	1.230930	-2.813558
6	0.466769	3.361277	-2.639769
6	2.512359	3.016933	-1.199203
1	2.371902	0.480421	-2.288499
1	0.926498	0.736560	-3.299220
1	2.397059	1.695902	-3.586745
1	0.124040	4.175590	-1.995935
1	1.097974	3.785708	-3.428870
1	-0.403174	2.883017	-3.103693
1	3.118872	3.489629	-1.980510
1	2.191179	3.788849	-0.492752
1	3.125251	2.283876	-0.665868
6	-0.123953	2.554846	0.201374
6	0.480981	2.726111	1.463653
6	-1.334271	3.236984	-0.049260
6	-0.106084	3.534781	2.438223
1	1.412881	2.209102	1.661773
6	-1.914501	4.051249	0.924743
1	-1.819259	3.100548	-1.008296
6	-1.305417	4.201246	2.173826
1	-1.760518	4.828989	2.931239
6	-2.525271	-0.823864	0.579233
6	-2.790624	-2.049502	1.233060
6	-2.886246	0.368502	1.242102
6	-3.374272	-2.075825	2.497617
1	-2.519842	-2.973544	0.737804
6	-3.456538	0.336214	2.516486
1	-2.686530	1.317481	0.761984
6	-3.705653	-0.882556	3.149308
1	-4.150274	-0.906231	4.137478
6	2.603298	-1.002495	0.606878
6	3.737161	-0.774400	-0.197900
6	2.606860	-0.503474	1.924773
6	4.830710	-0.064583	0.296088
1	3.737542	-1.149403	-1.213707
6	3.703822	0.211586	2.415403
1	1.740381	-0.685386	2.550483
6	4.816991	0.433514	1.603667
1	5.666464	0.989741	1.982501
1	3.686723	0.591722	3.430855

1	5.692170	0.107199	-0.339546
1	-3.701313	1.268951	3.012313
1	-3.564946	-3.027811	2.981523
1	-2.847475	4.562164	0.711891
1	0.373648	3.645781	3.404615

Gen-opt Structure 1Ta_T to 1Ta_S MECP (GBS1 only)
B3LYP/GBS(1) = -1384.225671 a.u.

Atomic No	x-coord	y-coord	z-coord
73	-0.0282312	-0.1681973	-0.2823480
7	-1.9068768	-0.7241836	-0.6167225
7	0.6229447	1.5629448	-0.9916581
7	1.3230173	-1.5578998	0.2252116
6	-2.8646042	-0.7043604	-1.7669581
6	-2.0812208	-0.4092870	-3.0633827
6	-3.5547386	-2.0840729	-1.9147939
6	-3.9444277	0.3886752	-1.5708381
1	-1.6008682	0.5718425	-3.0104960
1	-1.3033737	-1.1622935	-3.2156790
1	-2.7738321	-0.4211493	-3.9129709
1	-4.1420932	-2.3279922	-1.0252032
1	-4.2247808	-2.0643708	-2.7811843
1	-2.8011000	-2.8626296	-2.0709371
1	-4.6156465	0.4036968	-2.4362685
1	-4.5356518	0.1965197	-0.6711402
1	-3.4692730	1.3707956	-1.4773519
6	1.4229950	-3.0486737	0.1386521
6	0.4492639	-3.5517229	-0.9507373
6	2.8490051	-3.5130043	-0.2501904
6	1.0408045	-3.6747096	1.5045317
1	0.7405637	-3.1573617	-1.9287302
1	0.4731714	-4.6472215	-0.9803792
1	-0.5721039	-3.2258946	-0.7416587
1	3.5875423	-3.2064156	0.4952580
1	2.8575768	-4.6062244	-0.3207370
1	3.1314264	-3.0987963	-1.2238598
1	1.0913202	-4.7684760	1.4462707
1	1.7291622	-3.3348592	2.2851285
1	0.0238978	-3.3759341	1.7766593
6	1.3752549	2.1385084	-2.1472799
6	1.8720737	0.9805405	-3.0412320
6	0.4491426	3.0539941	-2.9872052
6	2.6036214	2.9507414	-1.6644059
1	2.5393315	0.3247945	-2.4749958
1	1.0296994	0.3855022	-3.4023754
1	2.4200722	1.3964705	-3.8953372
1	0.0827618	3.8924323	-2.3870646
1	0.9992199	3.4537656	-3.8464360
1	-0.4053922	2.4754010	-3.3526588
1	3.1626114	3.3168172	-2.5329994
1	2.2944845	3.8102200	-1.0626589
1	3.2580117	2.3123714	-1.0626987
6	0.1530907	2.5062065	0.0122161
6	0.9694126	2.9060387	1.0908414

6	-1.1192115	3.1024784	-0.1216791
6	0.5220324	3.8557849	2.0065781
1	1.9392261	2.4392481	1.2109069
6	-1.5663277	4.0500115	0.8023724
1	-1.7473658	2.8038508	-0.9523694
6	-0.7481223	4.4281174	1.8688818
1	-1.0954564	5.1606314	2.5887190
6	-2.4900809	-0.9980430	0.6853814
6	-2.6144562	-2.3216145	1.1474312
6	-2.9714355	0.0430708	1.5046621
6	-3.1922762	-2.5952385	2.3900356
1	-2.2480443	-3.1285864	0.5272549
6	-3.5506262	-0.2326461	2.7429874
1	-2.8668446	1.0658324	1.1656951
6	-3.6603725	-1.5529366	3.1908293
1	-4.1014345	-1.7648035	4.1582548
6	2.3890796	-0.8742368	0.9070573
6	3.5734675	-0.5165716	0.2308625
6	2.2525872	-0.5007442	2.2588500
6	4.5844077	0.1904309	0.8818427
1	3.6761772	-0.7836743	-0.8128930
6	3.2669839	0.2105574	2.9073829
1	1.3375386	-0.7610071	2.7748479
6	4.4338537	0.5575861	2.2234247
1	5.2175528	1.1140978	2.7250423
1	3.1395282	0.4972127	3.9450700
1	5.4849263	0.4625712	0.3422591
1	-3.9021714	0.5825401	3.3652069
1	-3.2752268	-3.6216344	2.7300360
1	-2.5489756	4.4945739	0.6864975
1	1.1568120	4.1414177	2.8383138

Gen-opt Structure 1Ta_S
B3LYP/GBS(1) = -1384.226041 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1390.972955 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1389.884494 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -1389.890342 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -1389.888021 a.u.
Enthalpy Correction = 0.700358
Gibbs Free Energy Correction = 0.591571

Atomic No	x-coord	y-coord	z-coord
73	0.110469	0.053884	-0.402095
7	2.038387	-0.454778	-0.549235
7	-1.280661	-1.337246	-0.701227
7	-0.450793	1.978601	-0.391266
6	2.875604	-1.315883	-1.439965
6	2.032628	-1.726267	-2.666396
6	4.121701	-0.540742	-1.938856
6	3.336494	-2.592129	-0.691435
1	1.149096	-2.292355	-2.356030
1	1.697765	-0.837772	-3.209558
1	2.639809	-2.351562	-3.331332
1	4.767670	-0.257664	-1.102888
1	4.696621	-1.175370	-2.622540
1	3.808954	0.362113	-2.473976
1	3.942525	-3.215278	-1.358538

1	3.935717	-2.332185	0.186346
1	2.465689	-3.168921	-0.363396
6	0.143749	3.272261	-0.848963
6	1.228453	2.965559	-1.905790
6	-0.918139	4.188604	-1.507161
6	0.778394	4.011571	0.356280
1	0.774736	2.505347	-2.788724
1	1.726435	3.896844	-2.199339
1	1.977307	2.276046	-1.508203
1	-1.703152	4.461719	-0.796862
1	-0.430276	5.104824	-1.857924
1	-1.373486	3.683528	-2.365528
1	1.225657	4.956521	0.026427
1	0.015588	4.232143	1.110005
1	1.553364	3.386155	0.809846
6	-2.261614	-1.742493	-1.752711
6	-2.111597	-0.790018	-2.959432
6	-1.977735	-3.191848	-2.222359
6	-3.714356	-1.652675	-1.220854
1	-2.307666	0.242594	-2.655502
1	-1.097147	-0.842951	-3.363261
1	-2.829376	-1.074782	-3.737972
1	-2.075406	-3.895559	-1.390284
1	-2.691068	-3.473915	-3.005013
1	-0.963009	-3.258361	-2.628476
1	-4.414269	-1.916137	-2.021965
1	-3.866477	-2.341585	-0.384665
1	-3.926140	-0.633897	-0.881838
6	-1.306599	-2.084906	0.538534
6	-2.170329	-1.733492	1.598126
6	-0.482592	-3.219397	0.697429
6	-2.194552	-2.481953	2.772838
1	-2.795706	-0.855931	1.494127
6	-0.505929	-3.962396	1.879728
1	0.176317	-3.499144	-0.115479
6	-1.360747	-3.596402	2.921154
1	-1.378921	-4.171974	3.839441
6	2.660850	0.002834	0.673746
6	3.454582	1.166457	0.690726
6	2.471912	-0.693499	1.886321
6	4.036745	1.619638	1.877126
1	3.597529	1.717293	-0.229355
6	3.051355	-0.235381	3.070444
1	1.859758	-1.586971	1.884364
6	3.835137	0.922111	3.069505
1	4.281807	1.278250	3.990742
6	-1.668065	2.058877	0.370968
6	-2.924138	2.115724	-0.265735
6	-1.632681	2.033504	1.779614
6	-4.102948	2.143404	0.480106
1	-2.959157	2.116881	-1.347797
6	-2.815633	2.058576	2.523666
1	-0.669017	1.977502	2.269726
6	-4.052568	2.113294	1.877733
1	-4.969643	2.130074	2.455483
1	-5.060464	2.181714	-0.027539
1	-2.768620	2.030207	3.606536
1	-2.855002	-2.189197	3.581503
1	0.139514	-4.827707	1.984692
1	2.883225	-0.777154	3.994283
1	4.641876	2.519434	1.869138

Gen-opt Structure 2Ta_T
B3LYP/GBS(1) = -1572.814507 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1579.625271 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1578.461732 a.u.
Enthalpy Correction = 0.717106
Gibbs Free Energy Correction = 0.604832

Atomic No	x-coord	y-coord	z-coord
73	-0.008610	-0.099714	-0.754272
8	-0.468385	0.391090	-2.808794
6	0.131972	-0.708749	-3.058850
8	0.432407	-1.380018	-4.005899
7	-0.954039	1.628584	-0.254527
7	1.987289	-0.326654	-0.481908
7	-0.846315	-1.573194	0.333197
6	-0.471778	3.061392	-0.346246
6	0.623303	3.142461	-1.435471
6	-1.617687	4.014991	-0.774362
6	0.108195	3.531069	1.009964
6	-1.833281	-2.653377	-0.028581
6	-2.140565	-2.594751	-1.540329
6	-1.272057	-4.062209	0.296452
6	-3.157463	-2.448491	0.751964
6	2.938425	-1.408729	-0.963616
6	2.161583	-2.706824	-1.293560
6	3.689175	-0.963613	-2.246692
6	3.974174	-1.746285	0.141582
6	2.609577	0.682589	0.328203
6	2.394867	0.695804	1.719661
6	3.451801	1.670331	-0.223772
6	2.987788	1.668882	2.526458
6	4.047260	2.635849	0.588231
6	3.817850	2.641982	1.966675
6	-2.356670	1.472097	-0.028023
6	-3.189420	0.999014	-1.060481
6	-2.952510	1.795324	1.209853
6	-4.558285	0.809619	-0.848704
6	-4.320887	1.621385	1.410432
6	-5.129829	1.116293	0.386423
6	-0.475687	-1.541143	1.725874
6	0.578592	-2.332799	2.223231
6	-1.150268	-0.695646	2.623819
6	0.946608	-2.273247	3.567310
6	-0.775527	-0.631336	3.967988
6	0.273636	-1.418623	4.445886
1	1.764325	-2.887551	3.927665
1	1.470612	2.505751	-1.176796
1	0.218662	2.844919	-2.407193
1	0.994046	4.171725	-1.502535
1	-2.403091	4.072668	-0.017228
1	-1.197311	5.016239	-0.918861
1	-2.062592	3.680964	-1.716947
1	0.509371	4.546665	0.909859
1	-0.672474	3.545472	1.777276

1	0.909554	2.865538	1.334886
1	-1.240919	-2.776464	-2.136050
1	-2.872336	-3.373461	-1.782671
1	-2.571631	-1.627421	-1.815348
1	-1.078281	-4.170733	1.366918
1	-2.006737	-4.819284	0.000264
1	-0.345005	-4.240947	-0.257256
1	-3.872049	-3.229478	0.467516
1	-2.984258	-2.513704	1.829978
1	-3.587815	-1.471413	0.517711
1	1.550759	-3.017269	-0.444974
1	1.523337	-2.583703	-2.170038
1	2.884774	-3.499576	-1.516450
1	4.353907	-0.120079	-2.045635
1	4.299019	-1.795779	-2.618093
1	2.971486	-0.687367	-3.024939
1	4.607598	-2.570103	-0.205162
1	4.612001	-0.888167	0.367246
1	3.465052	-2.053817	1.060369
1	1.780686	-0.077323	2.159963
1	3.624156	1.683389	-1.292127
1	4.280478	3.394973	2.593899
1	-2.755572	0.813362	-2.036343
1	-2.329232	2.184385	2.005415
1	-6.191910	0.976002	0.548903
1	1.115988	-2.979234	1.543897
1	-1.965800	-0.094264	2.248093
1	0.564008	-1.369951	5.488926
1	4.687875	3.388762	0.142444
1	2.805123	1.657177	3.595175
1	-4.759576	1.877095	2.368787
1	-5.178710	0.439899	-1.657823
1	-1.307063	0.031939	4.641445

Gen-opt Structure 2Ta_S
B3LYP/GBS(1) = -1572.875232 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1579.689588 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1578.524298 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -1578.534097 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -1578.530478 a.u.
Enthalpy Correction = 0.717344
Gibbs Free Energy Correction = 0.606854

Atomic No	x-coord	y-coord	z-coord
73	0.427097	-0.487180	-0.696370
8	0.608952	-1.317506	-2.548285
6	1.732398	-1.648447	-1.880279
8	2.693399	-2.273190	-2.268643
7	0.082196	1.378733	-1.315973
7	1.615468	-0.358174	0.934436
7	-1.171373	-1.572037	-0.151158
6	0.937740	2.224138	-2.227953
6	2.340014	1.580777	-2.355504
6	0.299576	2.299622	-3.636849
6	1.098621	3.653083	-1.653504

6	-1.889204	-2.681575	-0.923807
6	-0.934541	-3.882268	-1.135896
6	-3.130744	-3.186851	-0.143648
6	-2.380624	-2.137814	-2.286867
6	2.733817	-1.256570	1.428471
6	2.375547	-2.737255	1.157230
6	4.063260	-0.928580	0.702656
6	2.925600	-1.090204	2.958572
6	1.467830	0.872852	1.669847
6	0.453217	1.006384	2.632895
6	2.342516	1.959803	1.468062
6	0.304566	2.194213	3.354418
6	2.196987	3.140361	2.195580
6	1.171679	3.265903	3.139862
6	-1.213307	1.920449	-1.015095
6	-2.323491	1.611771	-1.822112
6	-1.395328	2.759473	0.097906
6	-3.585652	2.125500	-1.519752
6	-2.658531	3.276587	0.391847
6	-3.756782	2.962047	-0.412535
6	-1.704611	-1.282353	1.151462
6	-1.315098	-2.035452	2.274588
6	-2.649787	-0.258037	1.321805
6	-1.848185	-1.764095	3.533744
6	-3.177997	0.015644	2.586654
6	-2.780645	-0.732839	3.695466
1	-3.899716	0.816391	2.699173
1	-1.535485	-2.352460	4.389252
1	2.784854	1.409192	-1.370189
1	2.302068	0.639089	-2.908730
1	2.994686	2.263490	-2.907930
1	-0.679327	2.785860	-3.594641
1	0.949179	2.882906	-4.299430
1	0.186255	1.292341	-4.050556
1	1.755649	4.229855	-2.313850
1	0.133245	4.162336	-1.592216
1	1.540801	3.612949	-0.654324
1	-0.571824	-4.248980	-0.170027
1	-1.472182	-4.693856	-1.639946
1	-0.080739	-3.600294	-1.754644
1	-3.845182	-2.378492	0.033776
1	-3.616214	-3.957725	-0.751542
1	-2.853447	-3.624625	0.818444
1	-2.918188	-2.928907	-2.822307
1	-3.062564	-1.297087	-2.124010
1	-1.538581	-1.813964	-2.901028
1	1.419380	-2.986769	1.624586
1	2.327731	-2.942058	0.087135
1	3.154098	-3.376104	1.589410
1	4.367970	0.104649	0.893922
1	4.854549	-1.591250	1.072811
1	3.949458	-1.092873	-0.372138
1	3.682368	-1.807262	3.293903
1	3.262571	-0.082809	3.215921
1	1.988733	-1.292924	3.487255
1	-0.207349	0.172202	2.817635
1	3.130623	1.873483	0.732216
1	1.058663	4.185124	3.702874
1	-2.183875	0.957515	-2.673472
1	-0.549306	2.984948	0.732916
1	-4.736519	3.363051	-0.179974

1	-0.585396	-2.824373	2.145931
1	-2.963244	0.319674	0.462558
1	-3.192127	-0.520120	4.675351
1	2.882539	3.963506	2.026276
1	-0.490474	2.273145	4.087145
1	-2.784338	3.919678	1.255486
1	-4.433328	1.874023	-2.147289

Gen-opt Structure 2Ta_TS_S
B3LYP/GBS(1) = -1572.861224 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1579.677735 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1578.510318 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -1578.518642 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -1578.515558 a.u.
Enthalpy Correction = 0.71553
Gibbs Free Energy Correction = 0.60698

Atomic No	x-coord	y-coord	z-coord
73	0.513962	-0.643164	-0.787449
8	1.187242	-1.315784	-2.410419
6	1.520598	-2.508084	-1.306792
8	2.002793	-3.507113	-1.707489
7	0.123829	1.233228	-1.470485
7	1.704601	-0.327094	0.828594
7	-1.238670	-1.492935	-0.380896
6	0.935836	2.072645	-2.428605
6	2.408267	1.593097	-2.426224
6	0.379167	1.925972	-3.868516
6	0.908088	3.566917	-2.018831
6	-2.125018	-2.358325	-1.265321
6	-1.904297	-3.854499	-0.930250
6	-3.614267	-1.992867	-1.039302
6	-1.796873	-2.130947	-2.758576
6	2.974781	-1.034339	1.298433
6	2.637598	-2.478919	1.746366
6	4.029149	-1.045126	0.165100
6	3.615247	-0.318996	2.519564
6	1.333891	0.807543	1.633755
6	0.435318	0.659594	2.701555
6	1.898800	2.077002	1.404653
6	0.101369	1.751804	3.508323
6	1.569651	3.163257	2.213436
6	0.664346	3.005234	3.269436
6	-1.160128	1.786262	-1.132046
6	-2.279906	1.588105	-1.963071
6	-1.328636	2.531568	0.048262
6	-3.527421	2.111505	-1.621188
6	-2.579600	3.052160	0.388805
6	-3.683718	2.844809	-0.440328
6	-1.628819	-1.483827	1.006124
6	-1.130356	-2.451074	1.896582
6	-2.521143	-0.510685	1.485592
6	-1.523186	-2.448433	3.236090
6	-2.915281	-0.517268	2.824895
6	-2.421831	-1.484700	3.703522
1	-3.603871	0.240218	3.181296
1	-1.127644	-3.197285	3.913031
1	2.829283	1.643854	-1.417607

1	2.488112	0.569623	-2.799304
1	2.995653	2.248738	-3.078565
1	-0.638165	2.322029	-3.935311
1	1.011884	2.487252	-4.565959
1	0.382000	0.870512	-4.157499
1	1.543370	4.135240	-2.707257
1	-0.106012	3.972493	-2.064470
1	1.288800	3.692325	-1.000683
1	-2.176072	-4.066839	0.107217
1	-2.534192	-4.466502	-1.585318
1	-0.857576	-4.128122	-1.094884
1	-3.782475	-0.933827	-1.255254
1	-4.226552	-2.595295	-1.718833
1	-3.926612	-2.201466	-0.013379
1	-2.500412	-2.719261	-3.357316
1	-1.915008	-1.077188	-3.024006
1	-0.782062	-2.442108	-3.008446
1	1.886671	-2.449225	2.542371
1	2.256074	-3.069575	0.913292
1	3.541680	-2.964328	2.132104
1	4.288117	-0.018790	-0.115579
1	4.936211	-1.554066	0.510798
1	3.662203	-1.569984	-0.718629
1	4.508926	-0.883652	2.805717
1	3.912333	0.704485	2.279384
1	2.930549	-0.291460	3.371170
1	0.002614	-0.312089	2.893625
1	2.591080	2.199912	0.582159
1	0.406301	3.850649	3.896777
1	-2.162918	1.006945	-2.867744
1	-0.475309	2.696741	0.689809
1	-4.653173	3.250127	-0.174394
1	-0.423790	-3.185078	1.531495
1	-2.889923	0.249728	0.810886
1	-2.730109	-1.486700	4.742596
1	2.015906	4.132884	2.021253
1	-0.600672	1.615554	4.322780
1	-2.686598	3.620073	1.306194
1	-4.376940	1.946475	-2.274886

Gen-opt Structure 3Ta_T
B3LYP/GBS(1) = -2957.142394 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2970.686837 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2968.479605 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -2968.488640 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -2968.485171 a.u.
Enthalpy Correction = 1.420845
Gibbs Free Energy Correction = 1.229475

Atomic No	x-coord	y-coord	z-coord
73	-2.262633	-0.069042	-0.003935
73	2.501209	-0.048645	0.050281
6	0.345985	-0.071934	0.122059
8	-0.499714	0.772330	0.725550
8	-0.460642	-0.932229	-0.541261
7	2.982178	-2.020553	-0.132931
7	3.311699	0.624264	1.792501
7	2.938845	1.211231	-1.508693

7	-3.092469	0.320318	1.782134
7	-2.886999	1.337628	-1.307324
7	-3.175894	-1.797803	-0.597654
6	-2.573046	-0.146921	3.126691
6	-2.234790	2.588283	-1.886615
6	-2.792559	-2.863300	-1.620349
6	2.637757	1.029658	-2.974788
6	2.525803	-3.276367	0.559447
6	3.761597	2.351615	-1.231492
6	3.186201	3.584112	-0.870060
6	5.163878	2.277915	-1.337194
6	3.984882	4.698031	-0.605741
6	5.960343	3.397233	-1.083762
6	5.375368	4.610219	-0.713171
6	4.036198	-2.226613	-1.089198
6	3.789566	-2.771578	-2.367339
6	5.364622	-1.881750	-0.767051
6	4.826691	-2.954033	-3.282792
6	6.396157	-2.048121	-1.693370
6	6.134675	-2.588241	-2.954485
6	-4.364675	-2.170803	0.133072
6	-4.312547	-3.057785	1.224932
6	-5.621920	-1.689561	-0.271294
6	-5.475946	-3.440877	1.894762
6	-6.783904	-2.069627	0.404001
6	-6.718614	-2.945337	1.489828
6	-4.204831	1.122584	-1.869157
6	-4.385996	0.405768	-3.065222
6	-5.336260	1.679098	-1.249600
6	-5.658445	0.230541	-3.610627
6	-6.609524	1.503208	-1.796602
6	-6.778600	0.776030	-2.975617
6	2.727039	1.479401	2.898682
6	-4.117475	1.321352	1.887082
6	-3.782224	2.687102	1.893520
6	-5.468016	0.955880	2.010867
6	-4.773884	3.662159	2.013780
6	-6.456380	1.934495	2.138631
6	-6.115898	3.289093	2.138250
6	4.631347	0.134929	2.088868
6	4.835103	-0.990718	2.911418
6	5.763657	0.788387	1.572767
6	6.122337	-1.448926	3.195285
6	7.051534	0.324332	1.850874
6	7.238296	-0.796268	2.662505
6	-1.883794	1.021807	3.872468
6	1.984038	0.598526	3.933490
6	-4.054106	-3.386531	-2.361935
6	3.900042	0.603946	-3.767996
6	-3.196648	3.804255	-1.795949
6	3.735609	-4.055522	1.137789
6	-3.729814	-0.699582	3.997726
6	3.835976	2.285599	3.626067
6	-2.098115	-4.057411	-0.919085
6	2.089086	2.339616	-3.598027
6	-1.870033	2.349302	-3.373524
6	1.747840	-4.207993	-0.406719
6	-1.539988	-1.274791	2.908763
6	1.741081	2.500438	2.290057
6	1.557005	-0.062934	-3.118123
6	-1.830414	-2.303483	-2.697057

```
6    -0.953469    2.958472   -1.116676
6     1.581552   -2.889961    1.715658
1     1.279923   -3.794073    2.256946
1     2.107095    3.650988   -0.804527
1     5.616168    1.327264   -1.593883
1     3.521447    5.636817   -0.322078
1     7.039060    3.318918   -1.168764
1     5.994531    5.476790   -0.511786
1     2.776531   -3.032532   -2.642821
1     5.580525   -1.497783    0.220003
1     4.609952   -3.370204   -4.260790
1     7.407955   -1.769970   -1.417949
1     6.936832   -2.724496   -3.670593
1    -3.354382   -3.438948    1.550535
1    -5.681077   -1.026092   -1.121195
1    -5.411075   -4.126239    2.732965
1    -7.741260   -1.682136    0.072944
1    -7.621506   -3.243204    2.010289
1    -3.524791   -0.023273   -3.556153
1    -5.213506    2.250001   -0.342168
1    -5.774440   -0.331269   -4.530920
1    -7.466551    1.937520   -1.294330
1    -7.766903    0.638399   -3.398818
1    -2.741119    2.969148    1.795106
1    -5.735596   -0.091152    1.983633
1    -4.499012    4.711167    2.013784
1    -7.494653    1.635447    2.230534
1    -6.885129    4.046533    2.234675
1     3.974967   -1.510583    3.311567
1     5.617578    1.658336    0.948358
1     6.254884   -2.320598    3.827172
1     7.908749    0.844931    1.437118
1     8.237149   -1.156508    2.880130
1    -2.601942    1.815012    4.098114
1    -1.466812    0.651428    4.815843
1    -1.072960    1.425448    3.261368
1     2.675750   -0.093354    4.424039
1     1.524011    1.228892    4.704114
1     1.199090    0.026819    3.432011
1    -3.730687   -4.095505   -3.131937
1    -4.740394   -3.900427   -1.685147
1    -4.585735   -2.560397   -2.842783
1     3.631343    0.446768   -4.819786
1     4.662223    1.386988   -3.725028
1     4.309370   -0.325585   -3.369167
1    -2.670866    4.690153   -2.168319
1    -4.094613    3.654704   -2.398917
1    -3.491890    3.978444   -0.757368
1     3.373937   -4.927677    1.694772
1     4.394386   -4.402611    0.336691
1     4.313523   -3.414693    1.808325
1    -3.309277   -1.085433    4.933294
1    -4.450228    0.085344    4.240990
1    -4.247484   -1.509226    3.477662
1     3.360250    2.948944    4.357113
1     4.536432    1.631764    4.152080
1     4.392995    2.895660    2.908141
1    -2.790124   -4.574489   -0.249054
1    -1.755043   -4.774953   -1.673598
1    -1.234233   -3.701481   -0.353266
1     2.841284    3.132820   -3.574850
```

1	1.814388	2.149271	-4.641923
1	1.201380	2.676210	-3.057065
1	-2.767292	2.182237	-3.975172
1	-1.350445	3.230292	-3.766678
1	-1.207208	1.483631	-3.464519
1	2.411758	-4.630262	-1.165725
1	1.306161	-5.037354	0.158909
1	0.947174	-3.644607	-0.893474
1	-1.955455	-2.070823	2.284166
1	-0.627796	-0.886820	2.454774
1	-1.273991	-1.709219	3.878636
1	2.270951	3.138916	1.577811
1	0.910823	2.003014	1.784892
1	1.333865	3.128424	3.092310
1	1.878162	-0.994484	-2.643263
1	0.617156	0.256396	-2.662937
1	1.383389	-0.267812	-4.180872
1	-2.267796	-1.432331	-3.189251
1	-0.871934	-2.024843	-2.265986
1	-1.671636	-3.079597	-3.454474
1	-1.159836	3.107115	-0.054523
1	-0.183428	2.192869	-1.210565
1	-0.564396	3.893794	-1.535522
1	2.082954	-2.214614	2.415000
1	0.687557	-2.399723	1.324990

Gen-opt Structure 3Ta_S

B3LYP/GBS(1) = -2957.166473 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2970.710208 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2968.498717 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -2968.507448 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -2968.504047 a.u.
Enthalpy Correction = 1.421389
Gibbs Free Energy Correction = 1.234086

Atomic No	x-coord	y-coord	z-coord
73	-2.169986	-0.097133	0.070718
73	2.446603	0.200112	-0.205518
6	0.423233	0.092157	-0.045226
8	-0.405247	0.495643	0.960691
8	-0.460293	-0.380806	-0.987970
7	3.059503	-1.736338	-0.369572
7	2.992005	0.910755	1.596514
7	3.009490	1.169442	-1.911356
7	-2.916123	0.093782	1.944746
7	-3.034464	1.338173	-1.038916
7	-2.991237	-1.876146	-0.528916
6	-2.351965	-0.438517	3.250935
6	-2.427594	2.612359	-1.600234
6	-2.686567	-2.845525	-1.670706
6	2.498642	1.196522	-3.324610
6	2.413743	-3.087205	-0.139055
6	4.164769	1.993827	-1.672928
6	4.071813	3.397494	-1.557221
6	5.439041	1.406174	-1.544250

6	5.204138	4.173958	-1.309766
6	6.566841	2.185583	-1.277269
6	6.456902	3.572205	-1.160300
6	4.384645	-1.862433	-0.927738
6	4.590181	-2.034138	-2.311154
6	5.515503	-1.831389	-0.093592
6	5.876567	-2.161229	-2.836773
6	6.803533	-1.951947	-0.620698
6	6.991529	-2.118027	-1.994175
6	-4.102717	-2.353615	0.264483
6	-3.937290	-3.344577	1.250051
6	-5.401357	-1.873584	0.021709
6	-5.028493	-3.825402	1.976210
6	-6.491349	-2.353453	0.750968
6	-6.312382	-3.330048	1.732895
6	-4.369395	1.101861	-1.535325
6	-4.586662	0.407113	-2.738415
6	-5.483737	1.605897	-0.844616
6	-5.878997	0.205328	-3.225694
6	-6.776254	1.398633	-1.331354
6	-6.981443	0.696437	-2.520482
6	2.783472	2.315599	2.111406
6	-3.944880	1.076342	2.158809
6	-3.622474	2.443334	2.241599
6	-5.286333	0.692384	2.324700
6	-4.613653	3.399167	2.469295
6	-6.274066	1.650134	2.566905
6	-5.945392	3.005636	2.635693
6	3.688399	0.052183	2.510135
6	2.977220	-0.798085	3.375006
6	5.093156	0.056074	2.574901
6	3.653271	-1.632604	4.266394
6	5.766265	-0.771296	3.476964
6	5.049894	-1.621236	4.322714
6	-1.648618	0.691528	4.042033
6	2.138159	2.280769	3.519051
6	-4.003439	-3.286669	-2.371214
6	3.666907	1.026614	-4.330933
6	-3.415514	3.801926	-1.476892
6	3.414241	-4.055597	0.551564
6	-3.483985	-1.038790	4.126837
6	4.115819	3.100955	2.182004
6	-1.966619	-4.113522	-1.144970
6	1.756252	2.521261	-3.641237
6	-2.064497	2.402793	-3.091225
6	1.941094	-3.716883	-1.473617
6	-1.318410	-1.553684	2.972664
6	1.802970	3.038763	1.164455
6	1.510648	0.025625	-3.506895
6	-1.788836	-2.200603	-2.751142
6	-1.152563	2.978782	-0.819102
6	1.205858	-2.944391	0.805939
1	0.811489	-3.943391	1.028044
1	3.104526	3.872918	-1.648811
1	5.538274	0.339510	-1.679719
1	5.106223	5.250658	-1.222419
1	7.533799	1.703842	-1.179868
1	7.333479	4.177750	-0.960803
1	3.733691	-2.043794	-2.970809
1	5.370391	-1.701511	0.968565
1	6.009607	-2.286243	-3.906016

1	7.659122	-1.920925	0.045554
1	7.990269	-2.213121	-2.404483
1	-2.947499	-3.729902	1.451962
1	-5.550249	-1.129557	-0.746674
1	-4.874439	-4.587271	2.732755
1	-7.481969	-1.963499	0.543172
1	-7.159120	-3.704416	2.296526
1	-3.736625	0.012667	-3.276721
1	-5.333243	2.155765	0.071805
1	-6.023797	-0.338115	-4.152928
1	-7.621320	1.789003	-0.775439
1	-7.985324	0.536127	-2.896388
1	-2.588457	2.741702	2.120215
1	-5.547089	-0.353203	2.239748
1	-4.345909	4.448741	2.524787
1	-7.304164	1.334391	2.691103
1	-6.714552	3.747298	2.817969
1	1.895016	-0.790176	3.335384
1	5.643698	0.689203	1.889422
1	3.089744	-2.287671	4.921803
1	6.850295	-0.758245	3.511709
1	5.572919	-2.266847	5.018661
1	-2.355113	1.482927	4.306987
1	-1.229317	0.277295	4.966421
1	-0.839211	1.109547	3.439564
1	2.800659	1.813675	4.252569
1	1.930901	3.308426	3.839044
1	1.196259	1.727586	3.481630
1	-3.743346	-3.914641	-3.230469
1	-4.645037	-3.864493	-1.702462
1	-4.559871	-2.415071	-2.725413
1	3.262487	0.965339	-5.347696
1	4.356488	1.874393	-4.280679
1	4.225116	0.112109	-4.112884
1	-2.913891	4.707482	-1.835525
1	-4.315492	3.642840	-2.074963
1	-3.705112	3.948065	-0.432159
1	2.897529	-4.996567	0.771219
1	4.275245	-4.272785	-0.084882
1	3.767287	-3.619348	1.491478
1	-3.033498	-1.473423	5.026514
1	-4.197450	-0.271106	4.435524
1	-4.014902	-1.822734	3.581297
1	3.912243	4.119668	2.532836
1	4.806172	2.629542	2.886865
1	4.582153	3.156992	1.195682
1	-2.622967	-4.699306	-0.496559
1	-1.676740	-4.743804	-1.994029
1	-1.066513	-3.831494	-0.594951
1	2.450560	3.365926	-3.657246
1	1.283426	2.450454	-4.628050
1	0.981436	2.700603	-2.891076
1	-2.962224	2.217853	-3.687697
1	-1.572375	3.302137	-3.478356
1	-1.379258	1.556066	-3.191916
1	2.790341	-3.917644	-2.132677
1	1.429402	-4.665965	-1.275685
1	1.242696	-3.040918	-1.975681
1	-1.748149	-2.331748	2.338310
1	-0.430363	-1.143842	2.493594
1	-1.030263	-2.011646	3.925737

1	2.176407	3.030843	0.136337
1	0.822082	2.560694	1.202194
1	1.705785	4.085992	1.473654
1	2.009243	-0.927733	-3.309184
1	0.657372	0.117266	-2.830601
1	1.141539	0.016141	-4.538924
1	-2.226950	-1.269385	-3.119053
1	-0.795035	-1.982674	-2.368722
1	-1.707837	-2.900069	-3.590481
1	-1.375083	3.102815	0.243869
1	-0.373198	2.223699	-0.933977
1	-0.765236	3.928375	-1.205976
1	1.519771	-2.472467	1.739782
1	0.417663	-2.345878	0.352081

Gen-opt Structure 3Ta_TS_T
B3LYP/GBS(1) = -2957.122862 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2970.669097 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2968.460855 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -2968.468971 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -2968.465844 a.u.
Enthalpy Correction = 1.418988
Gibbs Free Energy Correction = 1.229845

Atomic No	x-coord	y-coord	z-coord
73	-2.276013	-0.098978	-0.056164
73	2.501972	-0.010217	0.066134
6	0.461077	0.187894	0.438821
8	-0.415993	0.812000	1.087564
8	-0.609214	-0.742151	-0.576781
7	2.915256	-1.949414	-0.437841
7	3.359352	0.460409	1.847497
7	3.035880	1.352303	-1.366592
7	-3.058414	-0.112998	1.810100
7	-2.900460	1.565227	-1.049436
7	-3.352947	-1.582717	-0.898738
6	-2.558635	-0.818013	3.050433
6	-2.201405	2.840650	-1.493849
6	-2.971514	-2.444547	-2.103625
6	2.597368	1.439384	-2.805439
6	2.365518	-3.288100	-0.022817
6	4.039222	2.313736	-1.011712
6	3.678610	3.571431	-0.492594
6	5.406586	2.033136	-1.189262
6	4.652088	4.508407	-0.143841
6	6.379107	2.977107	-0.848989
6	6.007327	4.215585	-0.321438
6	4.035564	-2.050298	-1.338714
6	3.859860	-2.309163	-2.713875
6	5.352430	-1.912387	-0.859230
6	4.955546	-2.418731	-3.571125
6	6.446254	-2.000773	-1.723730

6	6.254825	-2.257474	-3.082693
6	-4.570792	-2.037539	-0.274106
6	-4.559887	-3.096355	0.651322
6	-5.805245	-1.461431	-0.615191
6	-5.746398	-3.560271	1.222392
6	-6.990271	-1.924613	-0.039029
6	-6.968675	-2.973926	0.881714
6	-4.256959	1.517869	-1.551183
6	-4.543380	1.025014	-2.837660
6	-5.317087	2.030461	-0.786734
6	-5.846124	1.034261	-3.337372
6	-6.621765	2.036092	-1.286260
6	-6.894245	1.538705	-2.561032
6	2.848615	1.251663	3.039205
6	-4.055162	0.880466	2.104400
6	-3.676392	2.213972	2.348494
6	-5.415004	0.538336	2.190729
6	-4.633865	3.179963	2.661372
6	-6.368634	1.506359	2.514879
6	-5.985038	2.828473	2.748822
6	4.615503	-0.191242	2.106742
6	4.671376	-1.436387	2.762746
6	5.825643	0.415846	1.728880
6	5.895433	-2.053712	3.024541
6	7.049399	-0.205726	1.987376
6	7.091157	-1.442164	2.635533
6	-1.867492	0.181576	4.012635
6	1.989537	0.342799	3.951246
6	-4.223656	-2.769784	-2.962127
6	3.766712	1.098712	-3.765121
6	-3.092067	4.082761	-1.212564
6	3.497245	-4.217487	0.487961
6	-3.724090	-1.509556	3.803705
6	4.020165	1.837357	3.871814
6	-2.335607	-3.771775	-1.619314
6	2.083064	2.860429	-3.153409
6	-1.884060	2.789087	-3.009909
6	1.630939	-3.987631	-1.196239
6	-1.535286	-1.892236	2.633191
6	2.001977	2.445417	2.543908
6	1.450198	0.431309	-3.028968
6	-1.951162	-1.727839	-3.024102
6	-0.888367	3.048576	-0.717700
6	1.349231	-3.071288	1.111814
1	0.981487	-4.041953	1.464334
1	2.626334	3.795358	-0.367627
1	5.694015	1.062125	-1.573959
1	4.353560	5.468907	0.262082
1	7.428294	2.740498	-0.990885
1	6.762945	4.945078	-0.053488
1	2.857077	-2.408766	-3.106783
1	5.511302	-1.755336	0.197427
1	4.792906	-2.616773	-4.625157
1	7.448426	-1.885905	-1.324910
1	7.103992	-2.335317	-3.751856
1	-3.615133	-3.543933	0.928627
1	-5.831959	-0.660723	-1.338001
1	-5.715193	-4.378573	1.933602
1	-7.930686	-1.461649	-0.316729
1	-7.889689	-3.334485	1.325081
1	-3.739049	0.623641	-3.436610

```
1   -5.112573    2.429575    0.194502
1   -6.042552    0.646565   -4.331089
1   -7.421964    2.431762   -0.671274
1   -7.906639    1.544753   -2.948292
1   -2.627223    2.476409    2.283953
1   -5.718284   -0.478903    1.986849
1   -4.325803    4.203952    2.842293
1   -7.414201    1.225234    2.575431
1   -6.727882    3.577925    2.996774
1    3.745837   -1.918808    3.050068
1    5.792708    1.369726    1.221319
 1    5.916426   -3.014950    3.526651
 1    7.970598    0.279973    1.683732
 1    8.040940   -1.924232    2.836555
 1   -2.584420    0.913808    4.395112
 1   -1.448738   -0.369309    4.862611
 1   -1.061362    0.701873    3.491725
 1    2.595920   -0.465469    4.372351
 1    1.570726    0.927475    4.779112
 1    1.168307   -0.085944    3.372607
 1   -3.898494   -3.332482   -3.844006
 1   -4.947130   -3.374681   -2.411522
 1   -4.712489   -1.848672   -3.291437
 1    3.406071    1.129463   -4.800356
 1    4.574653    1.828396   -3.660681
 1    4.153440    0.100353   -3.554155
 1   -2.521326    4.981272   -1.471345
 1   -4.008356    4.071124   -1.806032
 1   -3.356624    4.126591   -0.151833
 1    3.058734   -5.152996    0.854106
 1    4.205044   -4.454640   -0.311199
 1    4.042285   -3.734867    1.303551
 1   -3.309500   -2.069966    4.649291
 1   -4.432554   -0.773237    4.191204
 1   -4.253868   -2.196903    3.141005
 1    3.597311    2.449208    4.676512
 1    4.636682    1.053238    4.317773
 1    4.653717    2.472212    3.244575
 1   -3.059625   -4.373423   -1.063400
 1   -2.001805   -4.353552   -2.486460
 1   -1.470273   -3.558661   -0.986112
 1    2.883962    3.599002   -3.059471
 1    1.721441    2.868359   -4.188224
 1    1.260868    3.141261   -2.491880
 1   -2.802760    2.736898   -3.599603
 1   -1.340696    3.695417   -3.300045
 1   -1.258178    1.920693   -3.235153
 1    2.331185   -4.263926   -1.988861
 1    1.147718   -4.902392   -0.832430
 1    0.864665   -3.318668   -1.599318
 1   -1.967200   -2.580323    1.899841
 1   -0.639337   -1.432178    2.217198
 1   -1.238049   -2.472870    3.513375
 1    2.610652    3.076643    1.891432
 1    1.114599    2.107486    2.008669
 1    1.677322    3.037801    3.408216
 1    1.754683   -0.577666   -2.735841
 1    0.567196    0.703658   -2.448324
 1    1.181076    0.413953   -4.091495
 1   -2.334323   -0.757280   -3.349869
 1   -0.997344   -1.580990   -2.519965
```

1	-1.797835	-2.350628	-3.912566
1	-1.070512	3.088197	0.358117
1	-0.166351	2.257534	-0.918400
1	-0.447646	3.999619	-1.036891
1	1.814079	-2.546085	1.953095
1	0.506511	-2.486400	0.741405

Gen-opt Structure 3Ta_TS_S
B3LYP/GBS(1) = -2957.136596 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2970.681024 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2968.466223 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -2968.474286 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -2968.471143 a.u.
Enthalpy Correction = 1.419927
Gibbs Free Energy Correction = 1.232594

Atomic No	x-coord	y-coord	z-coord
73	-2.201495	-0.102573	0.184341
73	2.571885	-0.029783	-0.006600
6	0.584992	0.314906	-0.342891
8	-0.286736	0.704522	-1.143976
8	-0.544762	-0.412452	0.923235
7	3.329546	1.055909	1.542176
7	3.139276	0.880417	-1.726759
7	2.874460	-1.975588	0.543808
7	-2.977440	1.617118	-0.566952
7	-2.843189	-1.687576	-0.907369
7	-3.277453	-0.194891	1.885794
6	-2.529353	3.030380	-0.287082
6	-2.089576	-2.724104	-1.721262
6	-2.857352	-0.942822	3.154150
6	2.373580	-2.822628	1.682377
6	2.896174	2.104293	2.533326
6	3.776980	-2.637115	-0.350007
6	3.321526	-3.558577	-1.319126
6	5.161266	-2.377895	-0.281591
6	4.216361	-4.190057	-2.182275
6	6.050849	-3.004073	-1.157726
6	5.584948	-3.914711	-2.108127
6	4.726121	0.708335	1.676388
6	5.175760	-0.237214	2.621901
6	5.689678	1.308295	0.845833
6	6.524447	-0.580326	2.713491
6	7.039855	0.957403	0.929823
6	7.464414	0.009582	1.861771
6	-4.478692	0.583469	2.051674
6	-4.488792	1.769572	2.810620
6	-5.689997	0.143480	1.495068
6	-5.666556	2.496309	2.988752
6	-6.865706	0.878399	1.666896
6	-6.861618	2.058874	2.411277
6	-4.251862	-2.009690	-0.826986

6	-4.745944	-2.890529	0.153125
6	-5.154005	-1.499284	-1.773606
6	-6.096423	-3.237441	0.194210
6	-6.507785	-1.841240	-1.727112
6	-6.986617	-2.709479	-0.745499
6	3.290516	0.287087	-3.110018
6	-3.825005	1.520411	-1.720867
6	-3.269388	1.237088	-2.983106
6	-5.210231	1.737645	-1.625915
6	-4.080326	1.167151	-4.117263
6	-6.014648	1.684751	-2.766259
6	-5.456264	1.396867	-4.013876
6	3.339999	2.299172	-1.657592
6	2.244864	3.146307	-1.412377
6	4.602394	2.889265	-1.873759
6	2.413130	4.531256	-1.335749
6	4.763822	4.273216	-1.807541
6	3.672343	5.101382	-1.528055
6	-1.751128	3.624328	-1.488952
6	2.912985	1.318265	-4.204089
6	-4.099475	-1.301468	4.011937
6	3.541524	-3.602548	2.340288
6	-2.755860	-2.909898	-3.111191
6	3.731421	3.399526	2.343087
6	-3.742390	3.945561	0.021300
6	4.733691	-0.221295	-3.346696
6	-1.881243	-0.076199	3.990224
6	1.300832	-3.840873	1.217840
6	-2.055464	-4.089721	-0.989998
6	3.057533	1.626582	4.002382
6	-1.601645	3.003337	0.941109
6	2.301809	-0.890045	-3.227232
6	1.729635	-1.896113	2.734786
6	-2.147907	-2.274720	2.803788
6	-0.648134	-2.255164	-1.962959
6	1.419258	2.448398	2.299079
1	1.096803	3.179620	3.049652
1	2.259809	-3.755973	-1.395052
1	5.528757	-1.705269	0.481741
1	3.844951	-4.892942	-2.920358
1	7.110792	-2.786278	-1.085560
1	6.277501	-4.404847	-2.782640
1	4.454967	-0.712982	3.270702
1	5.360143	2.059008	0.142616
1	6.842162	-1.315799	3.444908
1	7.759538	1.434434	0.272689
1	8.511401	-0.262447	1.931174
1	-3.569512	2.127647	3.252652
1	-5.706605	-0.784491	0.945511
1	-5.648543	3.408247	3.575663
1	-7.786262	0.514790	1.223581
1	-7.774867	2.626267	2.547967
1	-4.066598	-3.288527	0.891417
1	-4.789940	-0.838879	-2.545841
1	-6.453453	-3.913843	0.963044
1	-7.183833	-1.423533	-2.464191
1	-8.037053	-2.974920	-0.712550
1	-2.200250	1.075097	-3.052463
1	-5.646500	1.923324	-0.653968
1	-3.637957	0.943694	-5.082020
1	-7.081652	1.857006	-2.676463

```
1   -6.083947    1.351897   -4.896556
1    1.263119    2.704318   -1.309361
1    5.452542    2.255376   -2.090718
1    1.552356    5.162184   -1.142032
1    5.744047    4.706937   -1.973234
1    3.802498    6.175910   -1.473261
1   -2.395980    3.712333   -2.368010
1   -1.390451    4.625339   -1.223312
1   -0.900225    2.985217   -1.732153
1    3.613972    2.155537   -4.234245
1    2.928987    0.812323   -5.175820
1    1.906106    1.708472   -4.025300
1   -3.768100   -1.915980    4.855927
1   -4.597608   -0.411595    4.402309
1   -4.819191   -1.873972    3.418520
1    3.163344   -4.149811    3.211205
1    3.979107   -4.319691    1.639668
1    4.324596   -2.913105    2.666208
1   -2.141611   -3.596556   -3.703997
1   -3.761500   -3.327400   -3.026257
1   -2.812774   -1.948275   -3.630746
1    3.372946    4.168375    3.037509
1    4.791131    3.218330    2.544655
1    3.622324    3.768244    1.319371
1   -3.370689    4.938192    0.301550
1   -4.383338    4.053775   -0.857487
1   -4.328627    3.536783    0.846797
1    4.790843   -0.725916   -4.318410
1    5.445294    0.609400   -3.352431
1    5.019311   -0.929173   -2.565603
1   -2.367141    0.839011    4.338373
1   -1.551294   -0.642144    4.869470
1   -1.007589    0.182284    3.386884
1    1.725397   -4.584139    0.537401
1    0.897667   -4.368874    2.090459
1    0.485683   -3.312572    0.719265
1   -3.060596   -4.503272   -0.876120
1   -1.456207   -4.796274   -1.575585
1   -1.596370   -3.976573   -0.003486
1    4.105279    1.429164    4.243592
1    2.692980    2.410507    4.675960
1    2.469339    0.719930    4.173613
1   -2.114210    2.573203    1.805015
1   -0.700739    2.427287    0.730501
1   -1.296520    4.024223    1.195087
1    2.516045   -1.655397   -2.478232
1    1.279849   -0.527975   -3.102513
1    2.402399   -1.360839   -4.212147
1    2.465610   -1.196363    3.131582
1    0.903829   -1.332268    2.292237
1    1.335811   -2.501016    3.559565
1   -2.824269   -2.937045    2.260987
1   -1.251990   -2.102220    2.209789
1   -1.856743   -2.769928    3.737187
1   -0.641372   -1.298550   -2.487285
1   -0.092542   -2.141482   -1.030135
1   -0.133497   -2.999750   -2.580518
1    1.293433    2.882574    1.306682
1    0.792630    1.556373    2.373000
```

Gen-opt Structure 4Ta_S
B3LYP/GBS(1) = -1459.602659 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1466.383258 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1465.269042 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -1465.276408 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -1465.273529 a.u.
Enthalpy Correction = 0.706249
Gibbs Free Energy Correction = 0.598736

Atomic No	x-coord	y-coord	z-coord
73	0.004088	0.012744	-1.066934
7	1.582414	-1.091017	-0.471197
7	-1.740283	-0.812115	-0.482599
7	0.157512	1.925226	-0.446251
6	2.352181	-2.134833	-1.239975
6	1.414868	-2.803384	-2.273559
6	3.547342	-1.493311	-1.988599
6	2.873098	-3.233267	-0.279007
1	0.558748	-3.259586	-1.764296
1	1.051534	-2.074832	-3.001784
1	1.965056	-3.589501	-2.802338
1	4.257489	-1.055041	-1.281046
1	4.072593	-2.255295	-2.576043
1	3.182755	-0.714382	-2.666353
1	3.369994	-4.012641	-0.867034
1	3.589240	-2.828232	0.440810
1	2.038818	-3.682136	0.269838
6	0.705989	3.123899	-1.176689
6	1.736083	2.656145	-2.232215
6	-0.431061	3.894593	-1.892509
6	1.428816	4.071149	-0.185581
1	2.550219	2.106163	-1.746407
1	1.269352	2.013118	-2.981821
1	2.160554	3.533770	-2.732024
1	-1.151233	4.282784	-1.166283
1	-0.014734	4.740496	-2.451680
1	-0.945627	3.227603	-2.592099
1	1.868604	4.903747	-0.745272
1	0.736331	4.476538	0.556928
1	2.228378	3.534062	0.335025
6	-3.040676	-0.919177	-1.237143
6	-3.130105	0.228579	-2.270871
6	-3.130285	-2.273698	-1.983950
6	-4.237666	-0.785311	-0.262359
1	-3.060311	1.197445	-1.763859
1	-2.330913	0.155355	-3.011767
1	-4.096353	0.174458	-2.784557
1	-3.119963	-3.107524	-1.275780
1	-4.061787	-2.321700	-2.559716
1	-2.284336	-2.372309	-2.672279
1	-5.169178	-0.805788	-0.838361
1	-4.254702	-1.603687	0.462051
1	-4.177577	0.163740	0.280133
6	-1.675129	-1.545162	0.751861

6	-1.929066	-0.903136	1.976073
6	-1.329884	-2.910644	0.767822
6	-1.843431	-1.608507	3.178813
1	-2.185561	0.147704	1.974754
6	-1.248944	-3.612814	1.970698
1	-1.102973	-3.403448	-0.169032
6	-1.507195	-2.963634	3.182604
1	-1.442486	-3.508812	4.117237
6	2.154783	-0.693389	0.785997
6	3.165007	0.286027	0.847276
6	1.693426	-1.257665	1.987853
6	3.702617	0.681670	2.072440
1	3.500808	0.748120	-0.072122
6	2.229902	-0.854653	3.213075
1	0.910582	-2.003279	1.951489
6	3.236794	0.111388	3.261865
1	3.652487	0.421067	4.213841
6	-0.494012	2.202330	0.805061
6	-1.845850	2.596827	0.851172
6	0.202566	2.053672	2.016875
6	-2.475991	2.842945	2.071413
1	-2.398436	2.682943	-0.075797
6	-0.433537	2.295443	3.236729
1	1.237756	1.741565	1.991908
6	-1.770998	2.693731	3.270538
1	-2.262301	2.882612	4.218136
8	0.015491	0.025989	-2.804393
1	4.477984	1.439413	2.100402
1	1.853999	-1.296409	4.128862
1	-2.036195	-1.092697	4.112570
1	-0.978648	-4.663080	1.963725
1	-3.517906	3.143519	2.087817
1	0.120254	2.166389	4.159605

Gen-opt Structure 5Ta_T
B3LYP/GBS(1) = -1497.599578a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1504.384407 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1503.251552 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (diethylether) = -1503.258220 a.u.
M06/GBS(2)//B3LYP/GBS(1) Solvent (benzene) = -1503.255663 a.u.
Enthalpy Correction = 0.711019
Gibbs Free Energy Correction = 0.59983

Atomic No	x-coord	y-coord	z-coord
73	0.019998	0.002841	-0.916152
7	-1.147162	-1.587530	-0.443773
7	-0.784784	1.804738	-0.440938
7	1.966474	-0.214427	-0.388536
6	0.056163	0.003030	-2.923430
8	0.079337	0.004763	-4.104869
6	-2.293948	-2.286779	-1.118895
6	-2.809812	-1.426722	-2.294134
6	-1.845806	-3.663826	-1.672073
6	-3.466877	-2.493888	-0.125015
6	3.145363	-0.916013	-1.002062

6	2.664917	-1.828403	-2.152877
6	4.157881	0.109853	-1.572587
6	3.859356	-1.803993	0.050730
6	-0.750271	3.166279	-1.075777
6	0.316773	3.193312	-2.192891
6	-2.126961	3.515956	-1.696721
6	-0.374636	4.245108	-0.026409
6	-1.584031	1.710926	0.750843
6	-0.996969	1.864645	2.020757
6	-2.963078	1.427400	0.681116
6	-1.764636	1.735423	3.181005
6	-3.726559	1.299942	1.841602
6	-3.129474	1.453817	3.097805
6	-0.723347	-2.180165	0.796694
6	0.231732	-3.216707	0.819303
6	-1.233202	-1.714666	2.023233
6	0.665460	-3.763297	2.027280
6	-0.795574	-2.263903	3.231020
6	0.153488	-3.287599	3.239563
6	2.244797	0.488919	0.834524
6	2.708978	1.819777	0.820175
6	2.025889	-0.129919	2.079690
6	2.945769	2.506919	2.010821
6	2.261373	0.562680	3.270038
6	2.722404	1.880026	3.241870
1	2.080621	0.068949	4.218203
1	-3.079257	-0.423882	-1.945844
1	-2.060804	-1.339235	-3.084014
1	-3.702737	-1.899866	-2.718104
1	-1.526380	-4.323068	-0.859565
1	-2.679329	-4.142661	-2.198741
1	-1.015584	-3.528969	-2.373792
1	-4.305374	-2.966066	-0.648682
1	-3.169712	-3.136126	0.708329
1	-3.795296	-1.529507	0.274665
1	1.903925	-2.530334	-1.795092
1	2.249187	-1.243706	-2.976466
1	3.516912	-2.402871	-2.533200
1	4.564474	0.737218	-0.774008
1	4.988889	-0.416695	-2.055840
1	3.662986	0.745527	-2.314643
1	4.686367	-2.339119	-0.429139
1	4.262210	-1.200200	0.868442
1	3.157842	-2.533678	0.466711
1	1.294363	2.898781	-1.796460
1	0.050317	2.525635	-3.015117
1	0.394065	4.212437	-2.588291
1	-2.900934	3.557422	-0.924745
1	-2.075590	4.494216	-2.188378
1	-2.400642	2.760039	-2.440767
1	-0.310100	5.221607	-0.519040
1	-1.125435	4.302867	0.766169
1	0.594190	4.008684	0.424320
1	0.061623	2.077587	2.087725
1	-3.416911	1.287533	-0.292129
1	-3.723520	1.353399	3.998894
1	0.640757	-3.568793	-0.119473
1	-1.967012	-0.919803	2.019918
1	0.492982	-3.711627	4.177584
1	2.859237	2.307667	-0.134723
1	1.668163	-1.150644	2.102538

1	2.905675	2.415690	4.166223
1	-1.196349	-1.884988	4.164426
1	1.405178	-4.556369	2.024538
1	-4.785190	1.076389	1.767868
1	-1.290454	1.851161	4.149134
1	3.299455	3.531656	1.980185

Gen-opt Structure 5Ta_S
B3LYP/GBS(1) = -1497.593270 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1504.376316 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1503.235895 a.u.
Enthalpy Correction = 0.711451
Gibbs Free Energy Correction = 0.60057

Atomic No	x-coord	y-coord	z-coord
73	0.102179	0.054780	-0.632413
7	-0.918509	1.719741	-0.159248
7	2.120639	-0.291697	-0.530981
7	-0.869641	-1.667820	-0.180503
6	-0.299109	0.287601	-2.581872
8	-0.536545	0.469289	-3.723797
6	-0.438075	3.149029	-0.158639
6	0.893666	3.223777	-0.938708
6	-1.469555	4.058324	-0.871431
6	-0.210042	3.653623	1.287926
6	-1.795707	-2.648459	-0.852575
6	-2.063927	-2.237331	-2.313674
6	-1.193001	-4.079677	-0.863956
6	-3.155377	-2.684114	-0.103429
6	3.045106	-0.984399	-1.478673
6	2.237829	-2.113959	-2.164599
6	3.577891	-0.047207	-2.598433
6	4.224198	-1.626979	-0.707756
6	2.641034	0.462892	0.548688
6	2.090012	0.262449	1.838306
6	3.626856	1.473510	0.416009
6	2.459772	1.066874	2.919233
6	4.015699	2.244400	1.508671
6	3.425885	2.061394	2.764459
6	-2.301428	1.531614	0.183315
6	-3.256217	1.337499	-0.829927
6	-2.728229	1.533791	1.523634
6	-4.600544	1.140417	-0.509379
6	-4.075423	1.344382	1.838458
6	-5.015827	1.145401	0.824619
6	-0.545667	-2.023375	1.178482
6	0.542878	-2.868919	1.479565
6	-1.280301	-1.484397	2.252198
6	0.883237	-3.157718	2.800474
6	-0.933398	-1.769398	3.575450
6	0.147548	-2.608065	3.855672
1	1.730766	-3.801243	3.009036
1	1.671122	2.623269	-0.458954
1	0.755525	2.889813	-1.971700
1	1.242508	4.262552	-0.949073
1	-2.419469	4.084525	-0.331427
1	-1.065971	5.075372	-0.922038
1	-1.649842	3.701506	-1.890711

```
1       0.200304    4.669296    1.255824
1      -1.152225    3.683050    1.842049
1       0.500001    3.002474    1.806626
1      -1.139683   -2.226272   -2.897107
1      -2.747991   -2.968395   -2.759647
1      -2.521186   -1.247738   -2.365384
1      -1.036358   -4.453292    0.151535
1      -1.881187   -4.758858   -1.379658
1      -0.236451   -4.080825   -1.397593
1      -3.837909   -3.373767   -0.613357
1      -3.023700   -3.026560    0.927181
1      -3.600670   -1.684795   -0.093146
1       1.824973   -2.796737   -1.417742
1       1.413283   -1.699809   -2.757050
1       2.890033   -2.674567   -2.843059
1       4.282244    0.692013   -2.209480
1       4.098119   -0.641354   -3.358842
1       2.737802    0.473651   -3.068426
1       4.861029   -2.184718   -1.403103
1       4.830315   -0.865194   -0.209547
1       3.838217   -2.314714    0.052307
1       1.423025   -0.574527    1.995973
1       4.070593    1.662499   -0.550821
1       3.727988    2.672737    3.606433
1      -2.928866    1.339278   -1.862234
1      -1.993934    1.659206    2.309268
1      -6.059984    0.994096    1.071606
1       1.132548   -3.267083    0.664044
1      -2.113688   -0.831980    2.027776
1       0.417573   -2.829012    4.881786
1       4.775034    3.007791    1.376181
1       2.015302    0.882122    3.891080
1      -4.388925    1.344986    2.876511
1      -5.323132    0.986442   -1.302794
1      -1.509911   -1.337954    4.386648
```

2.3 Solvent Calculations in diethyl ether and benzene

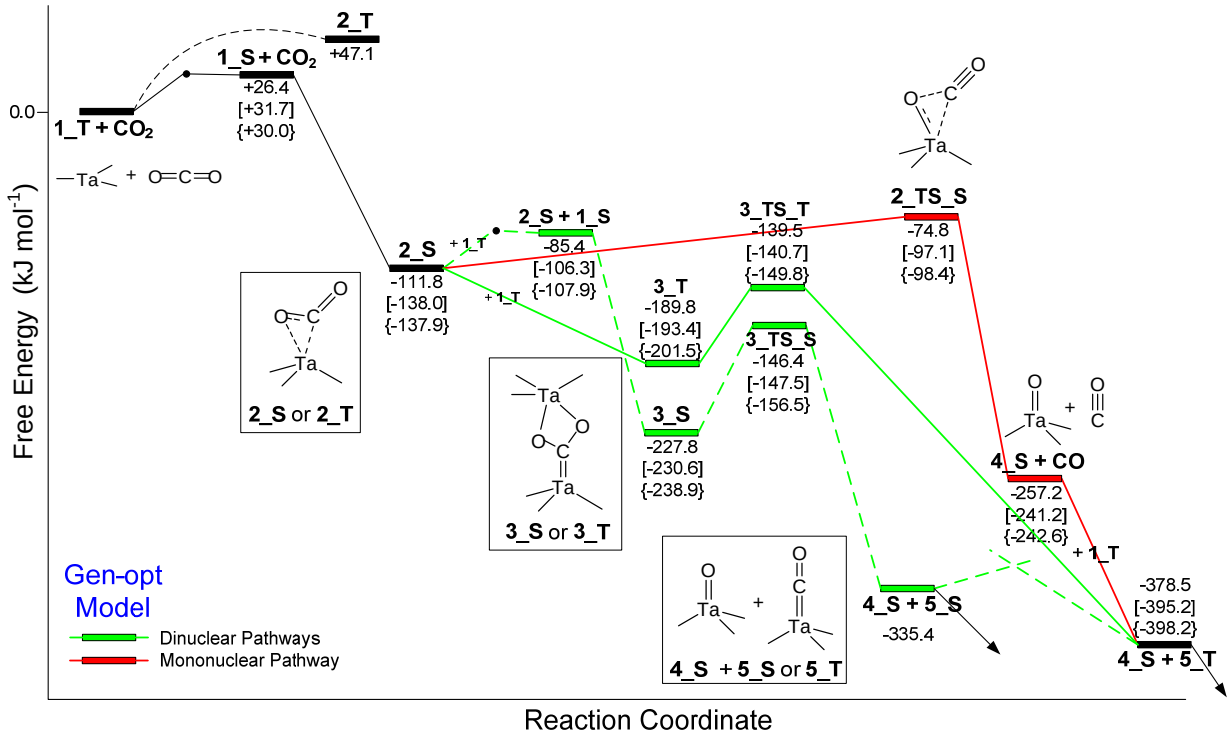

Figure S1. Relative energy surface of the reaction Ta[N(^{t}Bu)Ph]$_3$ + CO_2 at the Gen-opt level of theory. Values in normal type are solvent free Gibbs free energies, those in square brackets are diethylether solvent Gibbs free energies and those in brackets are benzene solvent Gibbs free energies. All values in kJ mol^{-1}.

.

3 Geometric and Energetic details of Niobium structures

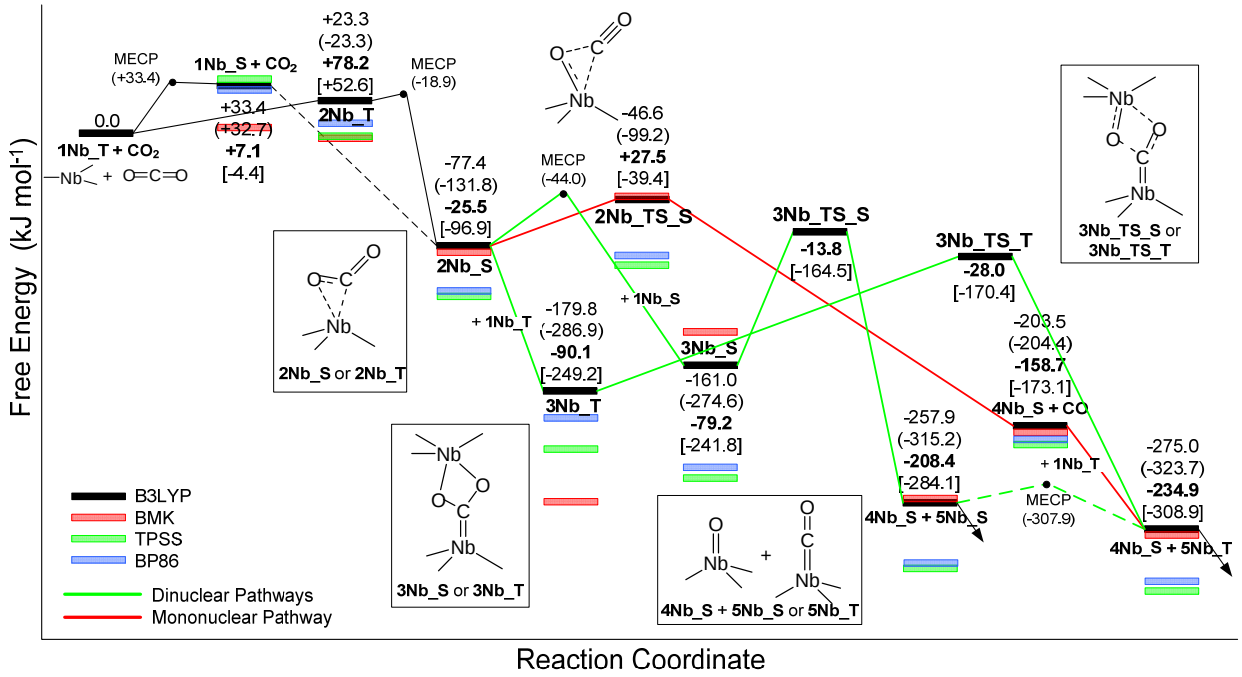

Figure S2. Potential energy surface displaying the reaction $Nb(NRR')_3 + CO_2$. Normal script = Model-opt Gibbs corrected; (Parentheses) = Model-opt uncorrected electronic energies; **Bold** = Gen-opt Gibbs corrected; [Square brackets] = Gen-opt uncorrected electronic energies. All values in kJ mol^{-1}. The figure includes alternate density functionals displayed at the Model-opt Gibbs corrected level of theory and an alternate dinuclear pathway.

3.1 Model-opt level of theory (Nb)

Structure 1Nb_T
B3LYP/GBS(1) = -224.200241 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -224.301991 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -223.870833 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -224.293502 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -224.363457 a.u.
Enthalpy Correction = 0.08259
Gibbs Free Energy Correction = 0.040978

Atomic No	x-coord	y-coord	z-coord
41	0.000375	-0.049530	-0.130759
7	-0.005808	1.929610	0.196528
7	1.814575	-0.871532	0.155773
7	-1.809787	-0.880730	0.155845
1	2.030604	-1.743986	0.631229
1	-2.678667	-0.376802	-0.012429
1	-0.011120	2.396043	1.101535
1	2.680176	-0.359724	-0.005490
1	-0.008916	2.625019	-0.547902
1	-2.020321	-1.751247	0.637170

Structure 1Nb_T to 1Nb_S MECP

B3LYP/GBS(1) = -224.186624 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -224.289255 a.u.

Atomic No	x-coord	y-coord	z-coord
41	-0.0083316	0.0194798	-0.0167297
7	-1.7337585	-0.9051399	0.1995574
7	-0.0335865	1.9857166	0.1924187
7	1.7348099	-0.9086025	0.1307977
1	0.7746995	2.5870824	0.0750483
1	1.9569785	-1.8106370	0.5316238
1	-2.1394794	-1.4182878	0.9688714
1	-0.8426572	2.5485081	0.4252234
1	-2.2968331	-1.0053809	-0.6468937
1	2.5799114	-0.4864919	-0.2441769

Structure 1Nb_S
B3LYP/GBS(1) = -224.187125 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -224.289526 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -223.869575 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -224.279377 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -224.351297 a.u.
Enthalpy Correction = 0.082085
Gibbs Free Energy Correction = 0.04125

Atomic No	x-coord	y-coord	z-coord
41	0.000585	-0.039164	-0.121872
7	-1.754641	-0.889895	0.182673
7	-0.012959	1.921721	0.177369
7	1.765071	-0.871775	0.183147
1	0.814063	2.499946	0.302241
1	2.132015	-1.548666	0.842433
1	-2.120481	-1.562230	0.847109
1	-0.848562	2.485110	0.312134
1	-2.440106	-0.712919	-0.560481
1	2.456768	-0.675881	-0.549012

Structure 2Nb_T
B3LYP/GBS(1) = -412.786237 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -412.961162 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -412.451995 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -412.987546 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -413.036520 a.u.
Enthalpy Correction = 0.098434
Gibbs Free Energy Correction = 0.048967

Atomic No	x-coord	y-coord	z-coord
41	-0.407717	0.000810	-0.018634
7	-1.864008	-0.068089	1.332687
7	-0.747526	-1.609407	-1.155746
7	-0.756999	1.715525	-0.987850

1	-0.089161	-1.971043	-1.843189
1	-1.689195	2.092636	-1.150169
1	-2.209904	-0.922334	1.768881
1	-1.676588	-1.977687	-1.352415
1	-2.210193	0.740336	1.848790
1	-0.100131	2.152367	-1.631663
8	1.342196	-0.063747	1.212774
6	2.026540	-0.004383	0.132218
8	3.171810	0.015324	-0.211924

Structure 2Nb_T to 2Nb_S MECP
B3LYP/GBS(1) = -412.783016 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -412.959506 a.u.

GBS2 geometry

Atomic No	x-coord	y-coord	z-coord
41	-0.4016182	-0.0611653	-0.0715759
7	-1.8235989	-0.0508540	1.3264696
7	-0.7809147	-1.6526662	-1.2083238
7	-0.6938077	1.6754071	-1.0049091
1	-0.1783634	-2.0003135	-1.9470969
1	-1.6071458	2.0497653	-1.2415301
1	-2.1466865	-0.8796799	1.8178659
1	-1.7039769	-2.0638563	-1.3035523
1	-2.0887034	0.7723710	1.8593673
1	0.0222479	2.1774658	-1.5184065
8	1.2761789	-0.2168065	1.2520796
6	1.9014969	0.0700441	0.1760483
8	3.0140149	0.2805962	-0.1926769

Structure 2Nb_S
B3LYP/GBS(1) = -412.825597 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -413.002489 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -412.485446 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -413.033260 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -413.085106 a.u.
Enthalpy Correction = 0.09921
Gibbs Free Energy Correction = 0.051923

Atomic No	x-coord	y-coord	z-coord
41	0.375725	-0.081118	0.000222
7	1.234054	1.687916	-0.005277
7	0.918330	-1.011415	-1.672247
7	0.893920	-0.994214	1.690776
1	0.751242	-2.002381	-1.841400
1	1.151006	-0.532736	2.559365
1	2.240791	1.832568	0.017832
1	1.238830	-0.565039	-2.527358
1	0.710343	2.561381	-0.009028

1	0.803635	-1.996952	1.846272
8	-1.298155	1.248677	-0.010166
6	-1.756736	0.039215	-0.004682
8	-2.837379	-0.496463	-0.004767

Structure 2Nb_TS_S
B3LYP/GBS(1) = -412.808506 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -412.990077 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -412.469588 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -413.024967 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -413.074158 a.u.
Enthalpy Correction = 0.097202
Gibbs Free Energy Correction = 0.051267

Atomic No	x-coord	y-coord	z-coord
41	0.327507	-0.059310	0.013986
7	1.849593	0.473297	1.210281
7	0.488417	1.659386	-0.999019
7	0.898939	-1.575657	-1.136609
1	1.386410	2.117918	-1.142407
1	0.536161	-2.517185	-1.013370
1	2.345522	-0.208862	1.780087
1	-0.273501	2.232733	-1.344304
1	2.040463	1.412593	1.547107
1	1.492415	-1.516939	-1.958871
8	-1.049455	-0.793997	1.059495
6	-1.850256	0.183418	-0.053057
8	-3.014593	0.282969	-0.015231

Structure 3Nb_T
B3LYP/GBS(1) = -637.086958 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -637.363568 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -636.442505 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -637.387387 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -637.501594 a.u.
Enthalpy Correction = 0.183042
Gibbs Free Energy Correction = 0.112974

Atomic No	x-coord	y-coord	z-coord
41	2.206780	0.026876	-0.000146
41	-2.347295	0.038090	-0.000005
6	-0.337040	-0.740695	-0.000477
8	0.119328	0.525740	-0.001254
8	0.516615	-1.654050	0.000335
7	-2.483159	1.107001	-1.688164
7	-2.480854	1.106092	1.688928
7	-3.777444	-1.351166	0.000165
7	3.060571	1.829461	-0.001298

7	2.955118	-0.779124	1.669916
7	2.956569	-0.782685	-1.667864
1	3.233840	2.397264	0.828092
1	3.234157	2.395602	-0.831768
1	3.858878	-0.555047	2.081267
1	2.637050	-1.686566	2.006175
1	2.638531	-1.690782	-2.002398
1	3.860730	-0.559797	-2.078995
1	-1.694423	1.641420	-2.049830
1	-3.349256	1.463331	-2.087942
1	-4.151162	-1.803728	-0.832182
1	-4.150314	-1.804324	0.832571
1	-3.346345	1.462374	2.090056
1	-1.691484	1.640256	2.049599

Structure 3Nb_S
B3LYP/GBS(1) = -637.079884 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -637.358893 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -636.400289 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -637.398047 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -637.517577 a.u.
Enthalpy Correction = 0.183226
Gibbs Free Energy Correction = 0.115479

Atomic No	x-coord	y-coord	z-coord
41	0.676370	-0.306526	-0.331589
7	1.270159	0.951086	-1.780606
7	1.307437	-2.162855	-0.704189
7	1.326366	0.180791	1.504866
1	1.425320	-2.888044	-0.000104
1	0.804870	0.720388	2.191752
1	2.235337	1.003668	-2.102771
1	1.469730	-2.547844	-1.632401
1	0.786480	1.815441	-2.014663
1	2.316271	0.195408	1.747442
8	-1.322805	1.241536	-0.063601
6	-1.326470	-0.111409	-0.139878
8	-2.556545	-0.556103	-0.026680
41	-3.415645	1.332312	0.197914
7	-3.700604	2.412868	-1.455849
7	-3.169612	2.386465	1.878399
7	-5.283104	0.677182	0.501022
1	-3.917779	2.931070	2.302359
1	-5.892806	0.344589	-0.246134
1	-4.520133	2.997848	-1.605354
1	-2.268920	2.664594	2.257866
1	-2.971972	2.647824	-2.124807
1	-5.610362	0.288188	1.385368

Structure 4Nb_S
B3LYP/GBS(1) = -299.536084 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -299.678442 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -299.213213 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -299.687639 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -299.752802 a.u.
Enthalpy Correction = 0.087708
Gibbs Free Energy Correction = 0.045641

Atomic No	x-coord	y-coord	z-coord
41	0.000032	-0.000079	0.062440
7	-1.244126	-1.437697	-0.588409
7	1.865668	-0.362032	-0.590594
7	-0.621121	1.793455	-0.597369
1	2.685403	-0.364261	0.009556
1	-1.023360	2.507508	0.003033
1	-1.702291	-1.445394	-1.495387
1	2.099622	-0.762537	-1.494678
1	-1.662489	-2.140080	0.014781
1	-0.395851	2.192817	-1.504138
8	-0.000662	0.007388	1.792674

Structure 5Nb_T
B3LYP/GBS(1) = -337.552570 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -337.699130 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -337.214504 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -337.714845 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -337.770120 a.u.
Enthalpy Correction = 0.092787
Gibbs Free Energy Correction = 0.04512

Atomic No	x-coord	y-coord	z-coord
41	-0.271883	0.000173	-0.019644
7	-0.532054	1.740659	-0.998695
7	-1.445193	-0.005881	1.627291
7	-0.527719	-1.736337	-1.006873
1	-1.669096	-0.836281	2.171396
1	-1.431346	-2.028681	-1.376238
1	-1.434195	2.027208	-1.376173
1	-1.679722	0.822528	2.169935
1	0.196966	2.319457	-1.407788
1	0.201960	-2.306158	-1.427219
6	1.818238	0.001090	0.171168
8	2.948499	-0.000099	0.459052

Structure 5Nb_T to 5Nb_S MECP
B3LYP/GBS(2)//B3LYP/GBS(1) = -337.692788 a.u.

Atomic No	x-coord	y-coord	z-coord
41	-0.2399388	0.1040378	0.0040356
7	-0.6395419	1.7128551	-1.1167053
7	-1.1953114	-0.0311816	1.7674588
7	-0.5941959	-1.5079524	-1.1320129
1	-1.1035457	-0.7419261	2.4845194
1	-1.5309179	-1.8023850	-1.3933899
1	-0.6592315	1.7294474	-2.1297145
1	-1.9573755	0.5912134	2.0166554
1	-0.7085387	2.6605530	-0.7597870
1	0.0678583	-2.2251791	-1.4001187
6	1.7948665	-0.1841371	0.2533526
8	2.9403272	-0.3076674	0.3919187

Structure 5Nb_S
B3LYP/GBS(1) = -337.552351 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -337.695900 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -337.210102 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -337.712202 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -337.768384 a.u.
Enthalpy Correction = 0.093683
Gibbs Free Energy Correction = 0.048381

Atomic No	x-coord	y-coord	z-coord
41	0.054682	-0.243304	2.102191
7	-1.345949	-0.508217	3.506911
7	-0.155372	1.669318	1.524922
7	1.715731	-1.066059	2.876281
1	0.577449	2.270933	1.153388
1	1.714692	-1.815278	3.564412
1	-1.307397	-0.035781	4.410550
1	-1.027036	2.190418	1.584213
1	-2.172382	-1.096188	3.462266
1	2.674985	-0.795422	2.667566
6	-0.822724	-1.523274	0.726517
8	-1.284994	-2.237326	-0.073260

3.2 Gen-opt level of theory (Nb)

Gen-opt Structure 1Nb_T
B3LYP/GBS(1) = -1382.733391 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.478135 a.u.

M06/GBS(2)//B3LYP/GBS(1) = -1388.402733 a.u.
Enthalpy Correction = 0.699688
Gibbs Free Energy Correction = 0.590197

Atomic No	x-coord	y-coord	z-coord
41	-0.188292	-0.295911	-0.258267
7	-2.193762	-0.553698	-0.475053
7	0.538632	1.471488	-1.001760
7	1.167472	-1.823758	-0.131956
6	-3.296690	-0.577762	-1.457343
6	-2.668354	-0.691371	-2.861966
6	-4.243784	-1.783926	-1.226471
6	-4.113605	0.737476	-1.365606
1	-2.010090	0.163599	-3.046962
1	-2.079838	-1.611959	-2.939431
1	-3.454676	-0.705570	-3.624654
1	-4.725958	-1.715853	-0.246245
1	-5.024134	-1.795167	-1.995835
1	-3.678911	-2.720712	-1.283945
1	-4.926712	0.736385	-2.100620
1	-4.544757	0.847957	-0.364865
1	-3.457615	1.592494	-1.561472
6	1.054787	-3.300649	-0.303236
6	-0.237028	-3.602652	-1.094433
6	2.255613	-3.880543	-1.093408
6	0.975326	-3.990114	1.084549
1	-0.182127	-3.156852	-2.093945
1	-0.359868	-4.686579	-1.197638
1	-1.114009	-3.194084	-0.582835
1	3.194939	-3.719417	-0.557216
1	2.113177	-4.958058	-1.231699
1	2.321345	-3.406046	-2.078484
1	0.890578	-5.075970	0.962697
1	1.873824	-3.772616	1.670434
1	0.099776	-3.622954	1.631181
6	1.171149	1.823836	-2.305936
6	1.249867	0.550653	-3.178086
6	0.351670	2.892183	-3.077561
6	2.609096	2.359807	-2.072832
1	1.805957	-0.236218	-2.659869
1	0.245897	0.179054	-3.408169
1	1.759551	0.782793	-4.120322
1	0.299502	3.826349	-2.511326
1	0.827518	3.097584	-4.043521
1	-0.665765	2.526237	-3.256291
1	3.084718	2.593134	-3.032572
1	2.584912	3.269311	-1.464435
1	3.204596	1.605116	-1.549832
6	0.394795	2.528669	-0.053527
6	1.311463	2.672237	1.009565
6	-0.705693	3.414272	-0.100765
6	1.125450	3.647626	1.990677
1	2.158926	1.998202	1.055291
6	-0.884411	4.391553	0.878972
1	-1.425063	3.304424	-0.903905
6	0.028730	4.511801	1.931168
1	-0.113062	5.269484	2.693258
6	-2.453280	-0.485819	0.925183
6	-2.764259	-1.640398	1.693094
6	-2.230359	0.730771	1.620392

6	-2.836052	-1.575741	3.078453
1	-2.923098	-2.578889	1.176002
6	-2.267341	0.773399	3.021208
1	-2.051301	1.640290	1.058259
6	-2.574799	-0.370551	3.751377
1	-2.615596	-0.334463	4.833827
6	2.379176	-1.328920	0.447763
6	3.524328	-1.072433	-0.335272
6	2.431993	-1.016664	1.821758
6	4.672011	-0.523142	0.234318
1	3.489641	-1.290497	-1.395059
6	3.581979	-0.459710	2.388232
1	1.558033	-1.215080	2.432203
6	4.705403	-0.211429	1.598007
1	5.597204	0.221429	2.036105
1	5.539537	-0.328396	-0.386640
1	3.597845	-0.222346	3.446253
1	1.839322	3.733571	2.802882
1	-1.740239	5.056176	0.825846
1	-2.067671	1.711365	3.527112
1	-3.075820	-2.467862	3.647126

Gen-opt Structure 1Nb_S
B3LYP/GBS(1) = -1382.730400 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1389.471748 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1388.404422 a.u.
Enthalpy Correction = 0.698778
Gibbs Free Energy Correction = 0.594599

Atomic No	x-coord	y-coord	z-coord
41	0.147178	0.034260	-0.020001
7	1.383199	1.569074	-0.356563
7	1.144847	-1.725609	-0.393537
7	-1.612958	0.053627	-1.007842
6	2.707923	2.045216	-0.809867
6	3.280648	1.010859	-1.794253
6	2.596311	3.417338	-1.520297
6	3.641523	2.178693	0.421039
1	3.332197	0.030152	-1.316340
1	2.633451	0.930762	-2.673499
1	4.284168	1.313973	-2.111816
1	2.232292	4.183143	-0.829145
1	3.584274	3.720483	-1.884597
1	1.913165	3.344823	-2.373348
1	4.632356	2.531566	0.112537
1	3.218855	2.893164	1.135546
1	3.743635	1.206992	0.915063
6	-2.158866	0.570988	-2.293095
6	-1.005424	1.230311	-3.080108
6	-2.745715	-0.586758	-3.141411
6	-3.262515	1.626906	-2.029264
1	-0.227866	0.493917	-3.304509

1	-1.391473	1.638337	-4.021015
1	-0.560104	2.039573	-2.495781
1	-3.574626	-1.073525	-2.618758
1	-3.116000	-0.193974	-4.095002
1	-1.967999	-1.330419	-3.345357
1	-3.632674	2.019391	-2.983312
1	-4.101447	1.180754	-1.486134
1	-2.853047	2.449804	-1.435283
6	1.624243	-2.721406	-1.373554
6	1.267584	-2.201721	-2.781506
6	3.148725	-3.004400	-1.307091
6	0.865376	-4.050812	-1.109997
1	0.197417	-1.980720	-2.836996
1	1.821876	-1.284024	-2.999455
1	1.516740	-2.958964	-3.533019
1	3.419391	-3.474175	-0.356965
1	3.423140	-3.689826	-2.116941
1	3.716427	-2.077295	-1.429511
1	1.176340	-4.820559	-1.825922
1	1.074682	-4.404420	-0.094475
1	-0.212155	-3.885833	-1.208408
6	1.433950	-1.770173	0.982016
6	0.311286	-1.644380	1.875329
6	2.743289	-1.605935	1.551874
6	0.512431	-1.355207	3.247689
1	-0.659176	-2.005599	1.543207
6	2.905018	-1.340462	2.894293
1	3.607940	-1.669292	0.905122
6	1.784030	-1.190121	3.754868
1	1.936778	-0.970485	4.805004
6	0.532208	2.334058	0.485863
6	-0.278581	3.425694	0.044105
6	0.257738	1.756343	1.779839
6	-1.283719	3.927959	0.841254
1	-0.088710	3.854451	-0.932615
6	-0.804955	2.291320	2.567682
1	1.030255	1.173175	2.280915
6	-1.562257	3.344842	2.111734
1	-2.356999	3.755401	2.724909
6	-2.520903	-0.617108	-0.121642
6	-2.703579	-2.013815	-0.196162
6	-3.210963	0.098182	0.879236
6	-3.547614	-2.671381	0.701395
1	-2.162372	-2.568191	-0.952912
6	-4.057094	-0.562645	1.769037
1	-3.041493	1.164857	0.963199
6	-4.229501	-1.948290	1.683344
1	-4.883522	-2.459802	2.380141
1	-3.669912	-3.746923	0.636108
1	-4.572876	0.000976	2.538784
1	-0.353516	-1.283518	3.897632
1	3.904108	-1.220821	3.300320
1	-0.985255	1.869502	3.551240
1	-1.871780	4.774305	0.502942

Gen-opt Structure 2Nb_T
B3LYP/GBS(1) = -1571.304622 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1578.116667 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1576.959756 a.u.
Enthalpy Correction = 0.717066
Gibbs Free Energy Correction = 0.605143

Atomic No	x-coord	y-coord	z-coord
41	0.017319	-0.110801	-0.813905
8	-0.547691	0.331528	-2.912417
6	0.118873	-0.715701	-3.151188
8	0.475431	-1.401955	-4.068413
7	-0.939290	1.638386	-0.342076
7	2.030460	-0.320763	-0.520372
7	-0.864508	-1.627155	0.207290
6	-0.459346	3.058798	-0.529779
6	0.650564	3.068466	-1.607505
6	-1.603568	3.978335	-1.030501
6	0.103584	3.620145	0.799831
6	-1.824830	-2.708425	-0.200478
6	-2.126409	-2.592882	-1.709562
6	-1.241749	-4.119365	0.072655
6	-3.156765	-2.552091	0.580121
6	3.006729	-1.363193	-1.017893
6	2.258976	-2.672850	-1.367321
6	3.741887	-0.880986	-2.297380
6	4.049187	-1.690692	0.083584
6	2.594364	0.684367	0.329686
6	2.300566	0.681459	1.707346
6	3.451136	1.692431	-0.163459
6	2.826172	1.659701	2.554576
6	3.982799	2.658708	0.689351
6	3.670652	2.650565	2.052147
6	-2.334177	1.493788	-0.075380
6	-3.202717	1.019643	-1.077615
6	-2.886267	1.828947	1.179022
6	-4.565992	0.848743	-0.822674
6	-4.250371	1.672478	1.422927
6	-5.095979	1.172196	0.427378
6	-0.516089	-1.612331	1.601638
6	0.532160	-2.409174	2.106325
6	-1.199929	-0.771888	2.498498
6	0.882562	-2.361916	3.455201
6	-0.842146	-0.720261	3.847806
6	0.198873	-1.514127	4.332595
1	1.695510	-2.979458	3.820805
1	1.492333	2.446001	-1.298711
1	0.257589	2.715122	-2.565074
1	1.027052	4.090215	-1.731738
1	-2.399824	4.072264	-0.287928
1	-1.188225	4.973164	-1.225979
1	-2.032882	3.587670	-1.958352
1	0.506405	4.626791	0.635866
1	-0.688964	3.687382	1.551635
1	0.899713	2.978053	1.180675
1	-1.224102	-2.751880	-2.307427
1	-2.856312	-3.361708	-1.985809
1	-2.554921	-1.614861	-1.948039
1	-1.058518	-4.267933	1.140293
1	-1.957642	-4.877735	-0.263633

1	-0.304829	-4.255326	-0.476771
1	-3.858733	-3.331548	0.262223
1	-2.988793	-2.654235	1.656126
1	-3.598640	-1.572012	0.380156
1	1.685854	-3.028907	-0.510122
1	1.588839	-2.536615	-2.217710
1	2.996497	-3.436349	-1.639922
1	4.378619	-0.017608	-2.089687
1	4.378537	-1.688512	-2.677910
1	3.013462	-0.621092	-3.071305
1	4.701002	-2.496954	-0.270160
1	4.666881	-0.820171	0.318581
1	3.544260	-2.017858	0.998169
1	1.684276	-0.111400	2.108078
1	3.685856	1.718676	-1.219432
1	4.082594	3.406036	2.710943
1	-2.797814	0.811694	-2.061085
1	-2.232336	2.206540	1.955365
1	-6.154292	1.046023	0.622914
1	1.078588	-3.048000	1.427052
1	-2.005151	-0.159530	2.117964
1	0.475684	-1.475037	5.379735
1	4.637149	3.424865	0.288322
1	2.581694	1.635089	3.610619
1	-4.655877	1.937125	2.393418
1	-5.215185	0.478519	-1.608673
1	-1.380518	-0.060841	4.519688

Gen-opt Structure 2Nb_S
B3LYP/GBS(1) = -1571.344851 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1578.158625 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1577.001747 a.u.
Enthalpy Correction = 0.717318
Gibbs Free Energy Correction = 0.607642

Atomic No	x-coord	y-coord	z-coord
41	0.363747	-0.401362	-0.848676
8	0.223715	-1.134429	-2.809761
6	1.487662	-1.218755	-2.460799
8	2.474344	-1.583072	-3.061599
7	-0.178454	1.503164	-1.147780
7	1.854079	-0.502857	0.547058
7	-1.117322	-1.634833	-0.216705
6	0.565354	2.543825	-1.948238
6	1.944129	1.984677	-2.372198
6	-0.230968	2.897867	-3.228858
6	0.785080	3.821024	-1.100204
6	-1.829609	-2.772596	-0.941884
6	-0.816156	-3.841958	-1.420138
6	-2.853031	-3.475706	-0.010851
6	-2.609440	-2.196160	-2.149906
6	2.994685	-1.471893	0.728812
6	2.535637	-2.877269	0.274472
6	4.229828	-1.071700	-0.120849
6	3.389291	-1.554785	2.226142

6	1.874242	0.658433	1.392383
6	0.929088	0.787318	2.426900
6	2.822429	1.691682	1.228683
6	0.911453	1.919719	3.245935
6	2.810931	2.811790	2.058522
6	1.849802	2.936881	3.067497
6	-1.486791	1.891300	-0.708884
6	-2.620339	1.586492	-1.483807
6	-1.659351	2.573726	0.507840
6	-3.894736	1.957462	-1.051928
6	-2.935040	2.954091	0.928698
6	-4.055980	2.648073	0.153442
6	-1.502322	-1.438142	1.151022
6	-0.887235	-2.169703	2.185940
6	-2.523891	-0.534301	1.485022
6	-1.277664	-1.997191	3.512808
6	-2.908260	-0.357583	2.817112
6	-2.289457	-1.085438	3.834514
1	-3.693176	0.351339	3.054010
1	-0.791852	-2.568349	4.296207
1	2.515021	1.637864	-1.506312
1	1.846075	1.170755	-3.095189
1	2.515917	2.786003	-2.852976
1	-1.201259	3.335489	-2.978971
1	0.339604	3.625020	-3.817301
1	-0.387254	1.999559	-3.835342
1	1.354568	4.547725	-1.690589
1	-0.170732	4.273483	-0.822849
1	1.345263	3.580285	-0.192774
1	-0.253263	-4.236857	-0.568155
1	-1.357517	-4.668956	-1.894247
1	-0.122778	-3.423640	-2.151123
1	-3.612506	-2.775984	0.347797
1	-3.346814	-4.263110	-0.590226
1	-2.363404	-3.931921	0.853278
1	-3.157403	-3.002168	-2.652191
1	-3.326838	-1.445876	-1.801574
1	-1.923657	-1.740457	-2.865636
1	1.647711	-3.187783	0.831255
1	2.319900	-2.890195	-0.796240
1	3.339844	-3.596825	0.464271
1	4.643759	-0.114835	0.208015
1	5.010120	-1.833623	-0.005537
1	3.949299	-1.017289	-1.176408
1	4.155492	-2.327522	2.349472
1	3.792064	-0.603969	2.584983
1	2.518135	-1.818395	2.834996
1	0.226694	-0.016169	2.593718
1	3.559826	1.616260	0.441540
1	1.841388	3.811080	3.707964
1	-2.488188	1.049312	-2.414805
1	-0.793559	2.777671	1.123970
1	-5.045539	2.941082	0.484505
1	-0.093995	-2.861588	1.933524
1	-3.009054	0.025703	0.697423
1	-2.590803	-0.948323	4.866583
1	3.550271	3.592187	1.914610
1	0.169492	1.992507	4.033341
1	-3.053144	3.479954	1.869462
1	-4.759962	1.711003	-1.657079

Gen-opt Structure 2Nb_TS_S
B3LYP/GBS(1) = -1571.321359 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1578.139557 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1576.979856 a.u.
Enthalpy Correction = 0.715037
Gibbs Free Energy Correction = 0.605929

Atomic No	x-coord	y-coord	z-coord
41	-0.242652	0.155287	-1.075208
8	-0.243618	0.155782	-2.963460
6	-1.247620	1.439430	-2.551733
8	-1.668067	2.097085	-3.433606
7	0.788476	-1.610823	-0.861442
7	-1.964353	-0.146675	-0.008569
7	0.927186	1.623461	-0.369956
6	0.683965	-2.880469	-1.663850
6	-0.676273	-2.914211	-2.401970
6	1.816271	-2.943372	-2.722560
6	0.776672	-4.125903	-0.745183
6	1.928909	2.494342	-1.106561
6	1.317431	3.890497	-1.386097
6	3.211226	2.653641	-0.248730
6	2.327621	1.850370	-2.454021
6	-3.415570	0.168164	-0.348077
6	-3.629065	1.703601	-0.345823
6	-3.788360	-0.431801	-1.725869
6	-4.395505	-0.429129	0.699148
6	-1.778192	-0.865401	1.220773
6	-1.512139	-0.179317	2.416147
6	-1.908350	-2.267635	1.267757
6	-1.364596	-0.876111	3.619625
6	-1.767765	-2.959349	2.469033
6	-1.490256	-2.264720	3.652676
6	1.861555	-1.584138	0.090969
6	3.169137	-1.225123	-0.293332
6	1.626773	-1.899979	1.441635
6	4.203089	-1.177881	0.642256
6	2.664557	-1.849724	2.375533
6	3.954997	-1.487941	1.983546
6	0.618103	2.078896	0.958577
6	-0.423461	2.998420	1.176835
6	1.356005	1.609480	2.058050
6	-0.712221	3.445812	2.466847
6	1.067217	2.067579	3.345002
6	0.036608	2.986787	3.554921
1	1.644602	1.697274	4.184401
1	-1.520958	4.151130	2.621714
1	-1.501310	-2.818228	-1.689247
1	-0.741945	-2.109193	-3.137277
1	-0.777022	-3.874254	-2.920204
1	2.796384	-3.002699	-2.240783
1	1.685366	-3.836095	-3.345191
1	1.773695	-2.056106	-3.361853
1	0.653298	-5.027882	-1.354940
1	1.745071	-4.174569	-0.240292
1	-0.011636	-4.100122	0.012824
1	1.076803	4.405820	-0.452412

1	2.044341	4.495344	-1.939277
1	0.410872	3.791634	-1.991240
1	3.643379	1.673240	-0.029044
1	3.938304	3.244524	-0.815990
1	3.000402	3.169595	0.690864
1	3.102288	2.472734	-2.914831
1	2.737139	0.848300	-2.300531
1	1.482976	1.781226	-3.140637
1	-3.361916	2.108418	0.635661
1	-3.018722	2.183662	-1.111262
1	-4.682950	1.929029	-0.546449
1	-3.677790	-1.521155	-1.703047
1	-4.830630	-0.189285	-1.962567
1	-3.157929	-0.030977	-2.521559
1	-5.412451	-0.152101	0.401734
1	-4.328678	-1.518832	0.739334
1	-4.201652	-0.031218	1.698676
1	-1.422927	0.897614	2.395439
1	-2.116574	-2.803260	0.350626
1	-1.378645	-2.803306	4.586650
1	3.358679	-0.969010	-1.327276
1	0.629624	-2.181365	1.747823
1	4.758706	-1.450561	2.709809
1	-1.008635	3.338317	0.332281
1	2.138640	0.880201	1.898852
1	-0.185366	3.339274	4.555512
1	-1.872853	-4.038695	2.484789
1	-1.151955	-0.325854	4.528902
1	2.458392	-2.094071	3.411665
1	5.202020	-0.898798	0.325036

Gen-opt Structure 3Nb_T
B3LYP/GBS(1) = -2954.122040a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2967.663212 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2965.462487 a.u.
Enthalpy Correction = 1.42193
Gibbs Free Energy Correction = 1.231231

Atomic No	x-coord	y-coord	z-coord
41	-2.397614	-0.011015	0.050608
41	2.583857	0.015055	-0.050823
6	0.338855	-0.074984	0.090868
8	-0.417680	-0.223214	-0.956191
8	-0.310694	0.076573	1.176543
7	2.758296	1.931114	-0.728812
7	3.558323	-1.182654	-1.379242
7	3.020633	-0.606912	1.832377
7	-3.122478	-0.603356	-1.783544
7	-3.444791	-1.168020	1.379930
7	-2.763317	1.897360	0.695856
6	-3.222864	0.114054	-3.113512
6	-3.061362	-2.333524	2.248608
6	-2.305878	2.642403	1.942371
6	3.175837	0.150194	3.130295
6	2.226708	2.544470	-1.998911

```
6     3.175003   -2.026587    1.914624
6     2.062796   -2.859658    1.694423
6     4.407622   -2.635615    2.235420
6     2.185732   -4.251512    1.743036
6     4.521968   -4.023047    2.298638
6     3.414650   -4.839634    2.041731
6     3.584719    2.788013    0.064726
6     3.043074    3.821056    0.858176
6     4.981567    2.605251    0.071740
6     3.872426    4.641811    1.622310
6     5.805202    3.421929    0.849935
6     5.256390    4.445885    1.624296
6    -3.632196    2.678665   -0.136286
6    -3.138218    3.722580   -0.946987
6    -5.020043    2.445916   -0.131293
6    -4.001583    4.503088   -1.715713
6    -5.879645    3.223712   -0.910326
6    -5.377433    4.257811   -1.702371
6    -4.837923   -0.815172    1.464135
6    -5.326367    0.058213    2.456600
6    -5.761722   -1.341895    0.544407
6    -6.679055    0.395120    2.518391
6    -7.113900   -0.999231    0.600654
6    -7.580555   -0.128167    1.587080
6     3.145668   -2.347973   -2.232860
6    -3.244380   -2.023995   -1.874857
6    -2.129543   -2.855126   -1.647594
6    -4.466657   -2.645408   -2.216860
6    -2.244493   -4.247771   -1.701558
6    -4.572348   -4.033199   -2.286139
6    -3.465054   -4.844984   -2.015919
6     4.950249   -0.833991   -1.460156
6     5.424555    0.072907   -2.429520
6     5.878945   -1.375756   -0.552781
6     6.772185    0.430066   -2.480671
6     7.227011   -1.013391   -0.600730
6     7.679502   -0.108191   -1.562772
6    -2.817768   -0.809327   -4.294627
6     3.430292   -2.082091   -3.734662
6    -3.419529    3.602121    2.445940
6     4.631615    0.646187    3.318488
6    -3.894767   -3.588804    1.875582
6     3.325365    3.376256   -2.709680
6    -4.664441    0.636142   -3.338630
6     3.908461   -3.628682   -1.801680
6    -1.027970    3.470259    1.643846
6     2.762265   -0.735998    4.333748
6    -3.280572   -2.017319    3.752384
6     1.006426    3.458404   -1.713840
6    -2.244088    1.307798   -3.119281
6     1.633878   -2.595792   -2.056554
6     2.220762    1.362593    3.093585
6    -1.980766    1.668767    3.100523
6    -1.569507   -2.663300    2.041472
6     1.767199    1.414829   -2.946413
1     1.373148    1.855609   -3.868971
1     1.097876   -2.400084    1.524344
1     5.268917   -2.010989    2.432993
1     1.312548   -4.870418    1.567452
1     5.477779   -4.471466    2.547269
1     3.509900   -5.918110    2.088320
```

1	1.969608	3.956491	0.887611
1	5.409838	1.836922	-0.558919
1	3.435905	5.429252	2.227022
1	6.877773	3.261886	0.838829
1	5.896883	5.083200	2.222828
1	-2.071864	3.905952	-0.978196
1	-5.416769	1.672717	0.511537
1	-3.598876	5.300206	-2.331436
1	-6.945312	3.023644	-0.886312
1	-6.046504	4.864600	-2.301516
1	-4.633832	0.485094	3.166201
1	-5.395540	-2.021292	-0.210293
1	-7.027675	1.073121	3.290022
1	-7.803569	-1.418582	-0.124420
1	-8.630526	0.137295	1.633308
1	-1.167403	-2.391594	-1.469323
1	-5.327569	-2.025017	-2.430790
1	-1.368953	-4.862441	-1.519431
1	-5.522200	-4.485547	-2.550830
1	-3.552983	-5.924033	-2.065941
1	4.720907	0.502107	-3.129505
1	5.520571	-2.082401	0.182353
1	7.113802	1.132771	-3.232954
1	7.924296	-1.442485	0.111073
1	8.725798	0.172216	-1.601466
1	-3.507777	-1.647499	-4.415069
1	-2.824827	-0.216607	-5.216195
1	-1.809418	-1.205648	-4.137646
1	4.498205	-1.922606	-3.908779
1	3.108688	-2.948986	-4.322557
1	2.875212	-1.204065	-4.078383
1	-3.087878	4.061900	3.383467
1	-3.626959	4.393921	1.722490
1	-4.344309	3.047373	2.631321
1	4.695568	1.257092	4.226570
1	5.324218	-0.194226	3.423294
1	4.936358	1.255898	2.464080
1	-3.571801	-4.433158	2.495713
1	-4.960330	-3.416901	2.051323
1	-3.742987	-3.843336	0.823170
1	2.932975	3.747358	-3.662876
1	3.630343	4.230889	-2.099486
1	4.206190	2.757855	-2.905930
1	-4.708366	1.211876	-4.271211
1	-5.372014	-0.194976	-3.416414
1	-4.964816	1.280756	-2.510624
1	3.574538	-4.473230	-2.415580
1	4.986582	-3.505168	-1.940720
1	3.706262	-3.853298	-0.751037
1	-1.230965	4.257795	0.913337
1	-0.675812	3.943583	2.568830
1	-0.243904	2.810805	1.263234
1	3.430659	-1.591236	4.458420
1	2.800152	-0.126357	5.242989
1	1.740190	-1.103581	4.198069
1	-4.335563	-1.819935	3.961227
1	-2.964120	-2.877438	4.353330
1	-2.686038	-1.146545	4.045235
1	1.292824	4.325679	-1.113375
1	0.596561	3.820138	-2.664366
1	0.231502	2.892217	-1.189915

1	-2.502084	2.021033	-2.338009
1	-1.221862	0.955176	-2.973570
1	-2.314799	1.827836	-4.082063
1	1.410247	-2.859806	-1.018360
1	1.048632	-1.715327	-2.332336
1	1.331556	-3.431309	-2.698038
1	2.506132	2.056991	2.302113
1	1.194463	1.025458	2.931442
1	2.281918	1.903621	4.045024
1	-2.846487	1.052365	3.339757
1	-1.142988	1.022740	2.848248
1	-1.717106	2.259328	3.985647
1	-1.383216	-2.944699	0.999701
1	-0.944947	-1.807270	2.301969
1	-1.300167	-3.511041	2.681661
1	2.603517	0.760977	-3.198984
1	0.968684	0.821452	-2.490075

Gen-opt Structure 3Nb_S
B3LYP/GBS(1) = -2954.112138 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2967.657420 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2965.459681 a.u.
Enthalpy Correction = 1.420998
Gibbs Free Energy Correction = 1.232605

Atomic No	x-coord	y-coord	z-coord
41	2.163221	-0.042497	-0.093641
41	-2.530316	-0.147172	0.006082
6	-0.458455	-0.068918	-0.014499
8	0.367857	0.518563	0.865118
8	0.352969	-0.676232	-0.903091
7	-3.123430	0.992315	-1.594600
7	-2.927187	0.889003	1.714321
7	-3.156101	-2.079305	-0.347194
7	2.994989	1.254555	1.248984
7	2.902414	-1.874995	0.350891
7	2.993951	0.515899	-1.894571
6	2.532889	2.643899	1.643024
6	2.225628	-3.022393	1.074043
6	2.674801	0.213100	-3.353957
6	-2.769386	-3.132371	-1.344370
6	-2.476372	1.944403	-2.565039
6	-4.223025	-2.436594	0.537136
6	-4.041886	-3.341027	1.607901
6	-5.501451	-1.866341	0.366580
6	-5.093797	-3.654519	2.467705
6	-6.546670	-2.170585	1.241819
6	-6.350813	-3.067810	2.293200
6	-4.521719	0.779150	-1.861030
6	-4.964289	-0.138362	-2.836712
6	-5.497390	1.481177	-1.130785
6	-6.324646	-0.347985	-3.062812
6	-6.859794	1.264743	-1.351811
6	-7.281308	0.349853	-2.318491
6	4.157606	1.362306	-1.776865

6	4.084902	2.754361	-1.976392
6	5.416630	0.798466	-1.506550
6	5.224537	3.554263	-1.879834
6	6.556228	1.600496	-1.410788
6	6.466974	2.982085	-1.592340
6	4.180334	-2.247359	-0.199072
6	4.280667	-2.832882	-1.474015
6	5.355799	-2.078413	0.552411
6	5.518462	-3.224634	-1.986295
6	6.593830	-2.467273	0.035393
6	6.682370	-3.039735	-1.234980
6	-2.869154	0.339488	3.116481
6	3.962201	0.719207	2.166868
6	3.563650	-0.006254	3.304655
6	5.334747	0.946826	1.964099
6	4.508817	-0.493245	4.209209
6	6.276991	0.467726	2.876980
6	5.870885	-0.255212	4.001011
6	-3.252089	2.278918	1.627976
6	-2.236552	3.218692	1.379218
6	-4.567607	2.749361	1.808270
6	-2.527940	4.580425	1.282656
6	-4.854033	4.113391	1.722522
6	-3.838225	5.034436	1.452769
6	1.724635	2.603611	2.964664
6	-2.183563	1.353110	4.067616
6	3.957297	-0.273180	-4.086387
6	-4.029973	-3.725162	-2.026239
6	3.175049	-3.635179	2.136569
6	-3.299833	3.259610	-2.648127
6	3.753577	3.587509	1.822795
6	-4.279610	-0.001004	3.660214
6	2.141693	1.468207	-4.093500
6	-1.969679	-4.286184	-0.683266
6	1.818122	-4.121410	0.060478
6	-2.360955	1.333308	-3.987553
6	1.643939	3.246318	0.532396
6	-2.001242	-0.937244	3.091396
6	-1.874660	-2.484175	-2.423261
6	1.610823	-0.897820	-3.479069
6	0.960445	-2.520600	1.796748
6	-1.063289	2.312126	-2.077674
1	-0.634336	3.051318	-2.764521
1	-3.066141	-3.781312	1.766754
1	-5.669273	-1.202747	-0.470030
1	-4.930113	-4.350947	3.283154
1	-7.518302	-1.713918	1.087412
1	-7.164528	-3.309656	2.967183
1	-4.230968	-0.701228	-3.396823
1	-5.167453	2.192674	-0.387633
1	-6.639454	-1.064645	-3.813861
1	-7.590760	1.818133	-0.771550
1	-8.337939	0.182022	-2.492599
1	3.128443	3.205504	-2.201148
1	5.494537	-0.270633	-1.373599
1	5.142110	4.624928	-2.032614
1	7.514717	1.138215	-1.199815
1	7.351657	3.604114	-1.519987
1	3.383091	-2.967421	-2.061590
1	5.295779	-1.637328	1.535778
1	5.573098	-3.671849	-2.972746

1	7.487979	-2.321279	0.631354
1	7.643538	-3.341845	-1.634438
1	2.508560	-0.188126	3.464670
1	5.649806	1.481942	1.079015
1	4.181374	-1.052052	5.079186
1	7.331221	0.654577	2.703483
1	6.604014	-0.628058	4.706902
1	-1.221859	2.856964	1.279236
1	-5.360667	2.036115	1.994693
1	-1.729005	5.286894	1.084162
1	-5.873680	4.457019	1.860068
1	-4.064985	6.091903	1.381730
1	2.342275	2.238028	3.789978
1	1.386791	3.617178	3.210154
1	0.853089	1.956260	2.843109
1	-2.771198	2.269544	4.166691
1	-2.080678	0.893098	5.057145
1	-1.188872	1.608031	3.690930
1	3.687835	-0.559607	-5.109043
1	4.712911	0.514344	-4.134042
1	4.384906	-1.138213	-3.574410
1	-3.722778	-4.437312	-2.800583
1	-4.658456	-4.247547	-1.298940
1	-4.620177	-2.928083	-2.485879
1	2.634311	-4.419984	2.677149
1	4.059715	-4.077785	1.673172
1	3.493787	-2.867867	2.847205
1	-2.787179	3.962510	-3.314728
1	-4.303576	3.076791	-3.040588
1	-3.383800	3.709845	-1.654148
1	3.380695	4.593931	2.044488
1	4.393350	3.266059	2.647771
1	4.344194	3.624916	0.902911
1	-4.185762	-0.479639	4.642330
1	-4.877040	0.906998	3.783405
1	-4.797319	-0.685140	2.983770
1	2.914703	2.236085	-4.175003
1	1.837064	1.181793	-5.106808
1	1.274034	1.875999	-3.569650
1	-2.603984	-4.874074	-0.014380
1	-1.582466	-4.956368	-1.460109
1	-1.127810	-3.875882	-0.119779
1	2.699713	-4.577244	-0.398107
1	1.255608	-4.904361	0.581345
1	1.182647	-3.692184	-0.719636
1	-3.349035	1.139513	-4.413864
1	-1.836497	2.035556	-4.646071
1	-1.793411	0.397708	-3.949275
1	2.187153	3.277506	-0.412183
1	0.729128	2.669019	0.413378
1	1.379561	4.272729	0.811892
1	-2.435220	-1.689970	2.428098
1	-0.988844	-0.691284	2.763402
1	-1.959433	-1.372152	4.096740
1	-2.411366	-1.680179	-2.934066
1	-0.962307	-2.073465	-1.982022
1	-1.594803	-3.241143	-3.165207
1	1.911128	-1.792497	-2.927791
1	0.645590	-0.572227	-3.096759
1	1.508618	-1.158591	-4.538253
1	1.201833	-1.703114	2.481311

1	0.198759	-2.185936	1.090650
1	0.540541	-3.346222	2.382687
1	-1.111402	2.745711	-1.076978
1	-0.415901	1.434916	-2.052920

Gen-opt Structure 4Nb_S
B3LYP/GBS(1) = -1458.066020 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1464.848956 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1463.742359 a.u.
Enthalpy Correction = 0.706167
Gibbs Free Energy Correction = 0.600044

Atomic No	x-coord	y-coord	z-coord
41	0.069614	-0.003079	-1.188725
7	-1.779093	-0.691840	-0.688809
7	0.344892	1.907397	-0.544513
7	1.545366	-1.219184	-0.496612
6	-3.032968	-0.710694	-1.519068
6	-2.955868	0.402814	-2.590647
6	-3.204989	-2.078488	-2.227605
6	-4.270461	-0.434691	-0.625888
1	-2.814609	1.377997	-2.110572
1	-2.132003	0.225927	-3.285618
1	-3.895414	0.425327	-3.153567
1	-3.313399	-2.882340	-1.493504
1	-4.102132	-2.062060	-2.857093
1	-2.333736	-2.280654	-2.859560
1	-5.164388	-0.394252	-1.257812
1	-4.405183	-1.220391	0.122051
1	-4.157146	0.524882	-0.111231
6	2.320540	-2.255946	-1.267071
6	1.360510	-2.978097	-2.244124
6	3.463988	-1.598367	-2.081325
6	2.914664	-3.312934	-0.302311
1	0.538583	-3.439544	-1.686767
1	0.951833	-2.277105	-2.976469
1	1.907743	-3.762799	-2.778404
1	4.186276	-1.117553	-1.414426
1	3.991133	-2.359947	-2.667860
1	3.048460	-0.851052	-2.764602
1	3.406995	-4.093475	-0.892344
1	3.650048	-2.867660	0.372873
1	2.119985	-3.770423	0.295805
6	1.026560	3.053559	-1.238055
6	2.049224	2.502108	-2.259335
6	-0.003188	3.936440	-1.988799
6	1.794775	3.921073	-0.207474
1	2.782836	1.865426	-1.751808
1	1.554029	1.920648	-3.040463
1	2.578947	3.340714	-2.724192
1	-0.711035	4.388203	-1.287651
1	0.515005	4.741506	-2.522411
1	-0.551791	3.327780	-2.715576
1	2.326294	4.719148	-0.737265
1	1.113625	4.374614	0.517238

1	2.523614	3.307117	0.331464
6	-0.362873	2.235784	0.659255
6	0.242374	2.044633	1.914131
6	-1.684148	2.724110	0.617844
6	-0.451783	2.339507	3.089832
1	1.251639	1.657899	1.955650
6	-2.371951	3.022193	1.794372
1	-2.167159	2.842069	-0.343820
6	-1.756889	2.832383	3.036613
1	-2.292783	3.062846	3.950249
6	-1.842607	-1.406834	0.552781
6	-1.598527	-2.793471	0.609102
6	-2.122616	-0.726145	1.750755
6	-1.644941	-3.477323	1.824290
1	-1.348812	-3.316967	-0.305109
6	-2.163711	-1.413563	2.965551
1	-2.298062	0.340489	1.718282
6	-1.930116	-2.789467	3.008524
1	-1.964566	-3.321374	3.952398
6	2.053787	-0.871949	0.797401
6	3.130691	0.024925	0.946578
6	1.461209	-1.405686	1.954738
6	3.603477	0.367521	2.213195
1	3.571784	0.465621	0.061580
6	1.933032	-1.054265	3.221855
1	0.628888	-2.088416	1.849264
6	3.005808	-0.171599	3.357939
1	3.372192	0.097985	4.341826
8	0.189766	-0.007925	-2.923636
1	-1.451968	-4.544293	1.849101
1	-2.374550	-0.868058	3.878311
1	0.030997	2.177760	4.046860
1	-3.388864	3.395849	1.743432
1	4.432517	1.060302	2.308804
1	1.455703	-1.471946	4.100950

Gen-opt Structure 5Nb_T
B3LYP/GBS(1) = -1496.084314 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1502.869497 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1501.742847 a.u.
Enthalpy Correction = 0.710563
Gibbs Free Energy Correction = 0.598754

Atomic No	x-coord	y-coord	z-coord
41	0.035521	-0.010803	-0.927538
7	-1.355390	-1.474740	-0.552347
7	-0.557434	1.924460	-0.562689
7	1.983818	-0.473892	-0.466739
6	0.102633	-0.025905	-2.982300
8	0.144457	-0.030463	-4.150045
6	-2.556994	-2.026442	-1.250848
6	-2.920805	-1.115059	-2.443780
6	-2.281395	-3.456724	-1.784538
6	-3.774691	-2.069085	-0.288823
6	3.058780	-1.323717	-1.064141

6	2.467230	-2.162239	-2.218920
6	4.212101	-0.451837	-1.626755
6	3.632122	-2.299113	-0.001493
6	-0.328288	3.255542	-1.205060
6	0.750156	3.119097	-2.302244
6	-1.632099	3.789368	-1.854308
6	0.176788	4.284452	-0.158094
6	-1.397948	1.931789	0.597645
6	-0.836554	2.008251	1.887844
6	-2.799613	1.813062	0.486942
6	-1.648615	1.964073	3.023832
6	-3.606936	1.769984	1.623283
6	-3.033984	1.845253	2.898082
6	-1.018460	-2.100451	0.692887
6	-0.187155	-3.239831	0.738600
6	-1.472620	-1.558330	1.911692
6	0.179086	-3.810880	1.957122
6	-1.102023	-2.132494	3.130231
6	-0.276417	-3.257915	3.159482
6	2.328528	0.213978	0.742015
6	2.964117	1.473885	0.715684
6	1.990348	-0.335201	1.995069
6	3.247532	2.157118	1.897802
6	2.271999	0.355052	3.176795
6	2.901035	1.600445	3.134596
1	1.996975	-0.084598	4.129035
1	-3.053772	-0.081523	-2.106399
1	-2.145555	-1.142087	-3.213074
1	-3.858981	-1.462216	-2.890778
1	-2.069846	-4.143741	-0.959739
1	-3.157486	-3.827899	-2.328925
1	-1.423595	-3.439112	-2.465775
1	-4.652839	-2.440850	-0.828436
1	-3.580927	-2.730178	0.560538
1	-3.988607	-1.064853	0.090312
1	1.614996	-2.753312	-1.866584
1	2.139833	-1.523179	-3.042630
1	3.234415	-2.846247	-2.598496
1	4.693834	0.116087	-0.825533
1	4.966707	-1.091582	-2.098661
1	3.819464	0.244505	-2.375630
1	4.390227	-2.940204	-0.465086
1	4.094459	-1.750125	0.823547
1	2.831390	-2.926939	0.401625
1	1.667747	2.691800	-1.884417
1	0.402316	2.485842	-3.121818
1	0.979105	4.110534	-2.708806
1	-2.406476	3.941400	-1.096702
1	-1.437448	4.747921	-2.349119
1	-1.995068	3.073339	-2.599800
1	0.380338	5.239968	-0.654299
1	-0.571201	4.448641	0.622526
1	1.097639	3.921220	0.308918
1	0.237706	2.096335	1.987259
1	-3.237010	1.733508	-0.500651
1	-3.662775	1.810923	3.780358
1	0.180457	-3.651352	-0.193158
1	-2.112749	-0.685913	1.891656
1	0.011098	-3.701385	4.105870
1	3.209587	1.912177	-0.243695
1	1.507473	-1.303265	2.029091

1	3.120449	2.134437	4.052037
1	-1.458282	-1.694393	4.055888
1	0.823394	-4.683200	1.971234
1	-4.681929	1.673276	1.516896
1	-1.194093	2.019152	4.006776
1	3.732894	3.126153	1.856689

Gen-opt Structure 5Nb_S
B3LYP/GBS(1) = -1496.081186 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1502.864807 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1501.733427 a.u.
Enthalpy Correction = 0.710981
Gibbs Free Energy Correction = 0.599448

Atomic No	x-coord	y-coord	z-coord
41	0.144756	0.041777	-0.623519
7	-0.864627	1.757732	-0.231756
7	2.177422	-0.391419	-0.544144
7	-0.908038	-1.669923	-0.244924
6	-0.184723	0.312673	-2.614033
8	-0.366543	0.541407	-3.749610
6	-0.346577	3.170037	-0.215145
6	0.999027	3.209800	-0.973973
6	-1.339497	4.118001	-0.933070
6	-0.124935	3.653368	1.240841
6	-1.801338	-2.630732	-0.974070
6	-1.958240	-2.213264	-2.449667
6	-1.227561	-4.073670	-0.943144
6	-3.211228	-2.638823	-0.321178
6	3.085178	-1.031647	-1.537107
6	2.308428	-2.216173	-2.163881
6	3.493980	-0.074197	-2.692263
6	4.346354	-1.601847	-0.839708
6	2.689620	0.375496	0.519890
6	2.100434	0.208777	1.800808
6	3.695973	1.369505	0.397863
6	2.452053	1.028781	2.875377
6	4.066133	2.153794	1.487148
6	3.438086	2.005604	2.729168
6	-2.262120	1.600995	0.050091
6	-3.174699	1.414397	-1.003325
6	-2.749328	1.620931	1.370028
6	-4.534683	1.240884	-0.742143
6	-4.112067	1.454934	1.625137
6	-5.009368	1.262173	0.571858
6	-0.664142	-2.016217	1.128277
6	0.405734	-2.859560	1.497305
6	-1.453674	-1.463209	2.156321
6	0.674150	-3.134405	2.837855
6	-1.179102	-1.735326	3.498803
6	-0.116393	-2.572556	3.845719
1	1.508308	-3.776503	3.098572
1	1.744930	2.566586	-0.498747
1	0.861841	2.905863	-2.016325
1	1.389379	4.233637	-0.955575

1	-2.294706	4.169232	-0.404289
1	-0.903119	5.122000	-0.969376
1	-1.518921	3.776600	-1.957798
1	0.311760	4.658422	1.225320
1	-1.073635	3.700672	1.782567
1	0.561007	2.978029	1.761102
1	-0.994062	-2.228895	-2.966176
1	-2.628073	-2.924794	-2.945724
1	-2.384676	-1.211162	-2.529408
1	-1.148810	-4.444797	0.082377
1	-1.891120	-4.741890	-1.503603
1	-0.236112	-4.094083	-1.407955
1	-3.868074	-3.323337	-0.870445
1	-3.154885	-2.972534	0.719128
1	-3.640618	-1.632775	-0.349466
1	2.012245	-2.926118	-1.386918
1	1.405900	-1.863142	-2.675730
1	2.939109	-2.728276	-2.898818
1	4.124898	0.743763	-2.336667
1	4.053999	-0.631033	-3.452765
1	2.596371	0.349388	-3.153102
1	4.960088	-2.137927	-1.571737
1	4.948130	-0.806561	-0.392156
1	4.047945	-2.297886	-0.048435
1	1.424912	-0.623180	1.956942
1	4.171828	1.533510	-0.558387
1	3.727503	2.627488	3.567835
1	-2.801697	1.401604	-2.019939
1	-2.049745	1.739948	2.187485
1	-6.065711	1.128462	0.772812
1	1.037879	-3.264779	0.717933
1	-2.271038	-0.809489	1.881756
1	0.097398	-2.782838	4.887271
1	4.842428	2.901468	1.362381
1	1.979864	0.868581	3.838630
1	-4.471254	1.468390	2.648222
1	-5.223479	1.092216	-1.566116
1	-1.796777	-1.293836	4.273580

4 Geometric and Energetic details of Vanadium structures.

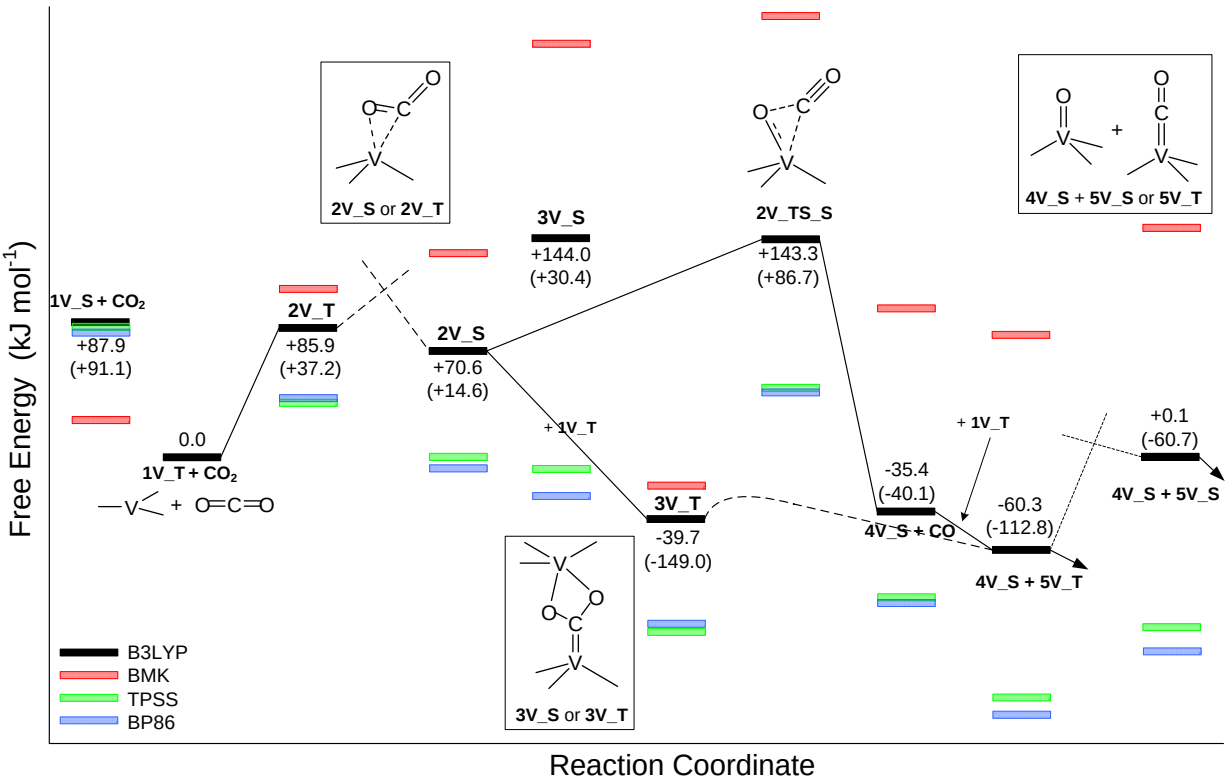

Figure S3. Potential energy surface displaying the reaction $V(NH_2)_3 + CO_2$. Values in normal script are at the Model-opt Gibbs corrected level of theory and those in parentheses are uncorrected electronic energies. All values in kJ mol^{-1}.

4.1 Model-opt level of theory (V)

Structure 1V_T
B3LYP/GBS(1) = -239.233670 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -239.339465 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -238.880755 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -239.323537 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -239.400563 a.u.
Enthalpy Correction = 0.082922
Gibbs Free Energy Correction = 0.042611

Atomic No	x-coord	y-coord	z-coord
23	-0.000040	-0.016263	-0.164613
7	-1.646982	-0.870384	0.126936
7	0.002339	1.834125	0.081544
7	1.645241	-0.873972	0.126154
1	0.834917	2.409842	0.177018
1	2.028198	-1.593143	-0.486750
1	-2.100657	-0.948347	1.034791
1	-0.830714	2.409591	0.174945
1	-2.036158	-1.583187	-0.489513

1	2.101162	-0.949107	1.033162

Structure 1V_S
B3LYP/GBS(1) = -239.197637 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -239.304766 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -238.870202 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -239.290226 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -239.369790 a.u.
Enthalpy Correction = 0.082249
Gibbs Free Energy Correction = 0.041389

Atomic No	x-coord	y-coord	z-coord
23	0.006544	-0.004870	-0.125675
7	-0.822220	1.623664	0.079221
7	1.839011	-0.095703	0.111313
7	-1.037325	-1.513647	0.110322
1	2.381795	-0.906163	-0.181914
1	-2.004957	-1.543156	0.415757
1	-1.042149	2.163298	0.909169
1	2.457986	0.621593	0.475571
1	-1.098718	2.133518	-0.763739
1	-0.700719	-2.457277	-0.070319

Structure 2V_T
B3LYP/GBS(1) = -427.798916 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -427.975601 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -427.419583 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -428.002244 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -428.060399 a.u.
Enthalpy Correction = 0.099071
Gibbs Free Energy Correction = 0.051429

Atomic No	x-coord	y-coord	z-coord
23	-0.505425	0.000084	-0.023689
7	-2.015047	-0.001291	1.036755
7	-0.625714	-1.571795	-0.995663
7	-0.625703	1.573817	-0.992718
1	0.139054	-1.961221	-1.542808
1	-1.516761	1.895533	-1.366801
1	-2.386338	-0.837214	1.485588
1	-1.517286	-1.893650	-1.368396
1	-2.387147	0.834167	1.485800
1	0.139877	1.965518	-1.537074
8	1.036638	-0.001050	1.249332
6	1.763025	0.000234	0.222531
8	2.893419	-0.000398	-0.159989

Structure 2V_S
B3LYP/GBS(1) = -427.808769 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -427.984205 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -427.413587 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -428.019827 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -428.082776 a.u.
Enthalpy Correction = 0.099836
Gibbs Free Energy Correction = 0.054181

Atomic No	x-coord	y-coord	z-coord
23	0.439500	-0.115849	0.000140
7	1.528771	1.335514	-0.000054
7	0.741104	-1.028653	-1.560961
7	0.736971	-1.028464	1.562473
1	0.360649	-1.957827	-1.735195
1	1.136521	-0.636080	2.409736
1	2.543350	1.249319	0.004384
1	1.154951	-0.641549	-2.403743
1	1.211457	2.302616	-0.000908
1	0.375366	-1.966211	1.730150
8	-0.991725	1.353708	-0.000204
6	-1.539101	0.220849	-0.000542
8	-2.596288	-0.348659	-0.001622

Structure 2V_TS_S
B3LYP/GBS(1) = -427.778786 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -427.956736 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -427.353306 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -428.002833 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -428.063123 a.u.
Enthalpy Correction = 0.098404
Gibbs Free Energy Correction = 0.054389

Atomic No	x-coord	y-coord	z-coord
23	-0.373260	-0.073095	-0.024940
7	-1.951093	0.247872	-0.943966
7	-0.557964	1.597581	0.767291
7	-0.691076	-1.408143	1.182400
1	0.197225	2.221024	1.030465
1	-0.232470	-2.311676	1.116298
1	-2.422506	-0.542494	-1.379281
1	-1.463048	2.059011	0.821385
1	-2.223230	1.122824	-1.381818
1	-1.194022	-1.289117	2.056575
8	0.775552	-0.780575	-1.083029
6	1.633127	0.194465	0.026835
8	2.790100	0.304782	-0.028356

Structure 3V_T
B3LYP/GBS(1) = -667.104133 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -667.385993 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -666.372370 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -667.406975 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -667.541163 a.u.
Enthalpy Correction = 0.184753
Gibbs Free Energy Correction = 0.117113

Atomic No	x-coord	y-coord	z-coord
23	2.392721	-0.005309	0.008159
7	2.579510	-0.174140	1.815250
7	2.947920	1.676327	-0.502898
7	2.899411	-1.577542	-0.811234
1	3.242878	1.928360	-1.444424
1	2.840003	-2.494262	-0.376837
1	3.432888	-0.237633	2.364217
1	2.921855	2.495342	0.097963
1	1.737617	-0.234946	2.385895
1	3.213867	-1.655724	-1.776543
8	-0.392257	-0.108941	0.912896
6	0.331186	0.035766	-0.170723
8	-0.296481	0.178576	-1.253714
23	-2.143155	-0.004088	0.036728
7	-2.640990	1.662785	-0.589682
7	-3.313340	-0.198746	1.440251
7	-2.622525	-1.454146	-1.006166
1	-3.583452	-1.097738	1.835342
1	-3.562284	-1.839201	-1.060924
1	-3.584267	2.040024	-0.541489
1	-3.593698	0.562306	2.056234
1	-2.126645	2.060125	-1.373024
1	-2.105909	-1.623983	-1.866577

Structure 3V_S
B3LYP/GBS(1) = -667.040380 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -667.317666 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -666.263833 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -667.368914 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -667.512089 a.u.
Enthalpy Correction = 0.184919
Gibbs Free Energy Correction = 0.118784

Atomic No	x-coord	y-coord	z-coord
23	-2.392408	-0.066249	-0.005987
7	-3.415320	1.435443	-0.358418
7	-3.026209	-0.725496	1.570830
7	-2.746479	-1.377263	-1.244725
1	-2.586473	-1.493606	2.075411
1	-2.368275	-1.434333	-2.186739

1	-4.337546	1.368110	-0.782327
1	-3.649406	-0.191168	2.169862
1	-3.000903	2.351525	-0.509532
1	-3.410981	-2.126124	-1.069670
8	-0.868281	1.273683	0.029259
6	-0.480747	0.053367	0.024675
8	0.670921	-0.448787	-0.047400
23	2.518102	-0.037880	0.001395
7	2.906980	1.743871	0.179186
7	3.243166	-0.613138	-1.610406
7	3.176377	-0.917054	1.498768
1	2.989030	-1.488284	-2.068580
1	4.125720	-0.775596	1.843808
1	2.903043	2.242339	1.067974
1	4.195446	-0.365472	-1.880209
1	2.892315	2.400896	-0.600308
1	2.850842	-1.837229	1.796364

Structure 4V_S
B3LYP/GBS(1) = -314.513739 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -314.653356 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -314.109240 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -314.671225 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -314.748409 a.u.
Enthalpy Correction = 0.088811
Gibbs Free Energy Correction = 0.048743

Atomic No	x-coord	y-coord	z-coord
23	-0.000012	-0.000116	0.077655
7	-1.570006	-0.753339	-0.535236
7	1.437460	-0.982796	-0.535674
7	0.132537	1.736017	-0.535628
1	1.979256	-1.588157	0.074205
1	-0.375663	2.066322	-1.350883
1	-1.603342	-1.356996	-1.351641
1	1.978263	-0.707899	-1.350508
1	-2.365120	-0.920496	0.074528
1	0.385300	2.508403	0.073870
8	0.000206	0.000289	1.661267

Structure 5V_T
B3LYP/GBS(1) = -352.570860 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -352.718834 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -352.203463 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -352.730907 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -352.793100 a.u.
Enthalpy Correction = 0.093434
Gibbs Free Energy Correction = 0.04672

Atomic No	x-coord	y-coord	z-coord
23	0.013412	-0.169689	2.261468
7	-1.654225	-0.865561	1.770999
7	0.355123	1.662657	2.440307
7	0.667820	-1.089612	3.761994
1	0.615593	2.305194	1.696427
1	0.477347	-2.070925	3.952566
1	-2.440069	-0.877140	2.419939
1	-0.003172	2.197744	3.230330
1	-2.005047	-0.986185	0.824185
1	1.483260	-0.793524	4.294038
6	0.951932	-0.447721	0.469929
8	1.570955	-0.702177	-0.462425

Structure 5V_S
B3LYP/GBS(1) = -352.553816 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -352.698985 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -352.180983 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -352.716462 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -352.782006 a.u.
Enthalpy Correction = 0.09414
Gibbs Free Energy Correction = 0.049863

Atomic No	x-coord	y-coord	z-coord
23	-0.371156	0.000108	-0.097241
7	-0.655609	-0.002338	1.726350
7	-0.885252	-1.676660	-0.710599
7	-0.888856	1.676749	-0.707684
1	-1.066715	-1.921347	-1.682940
1	-0.973240	2.498332	-0.116193
1	-1.602135	-0.005683	2.110069
1	-0.966349	-2.499361	-0.120224
1	0.022804	-0.001806	2.483273
1	-1.066670	1.923031	-1.680316
6	1.566811	0.001851	-0.040631
8	2.724506	0.001124	-0.083727

5 Geometric and Energetic details of Rhenium structures

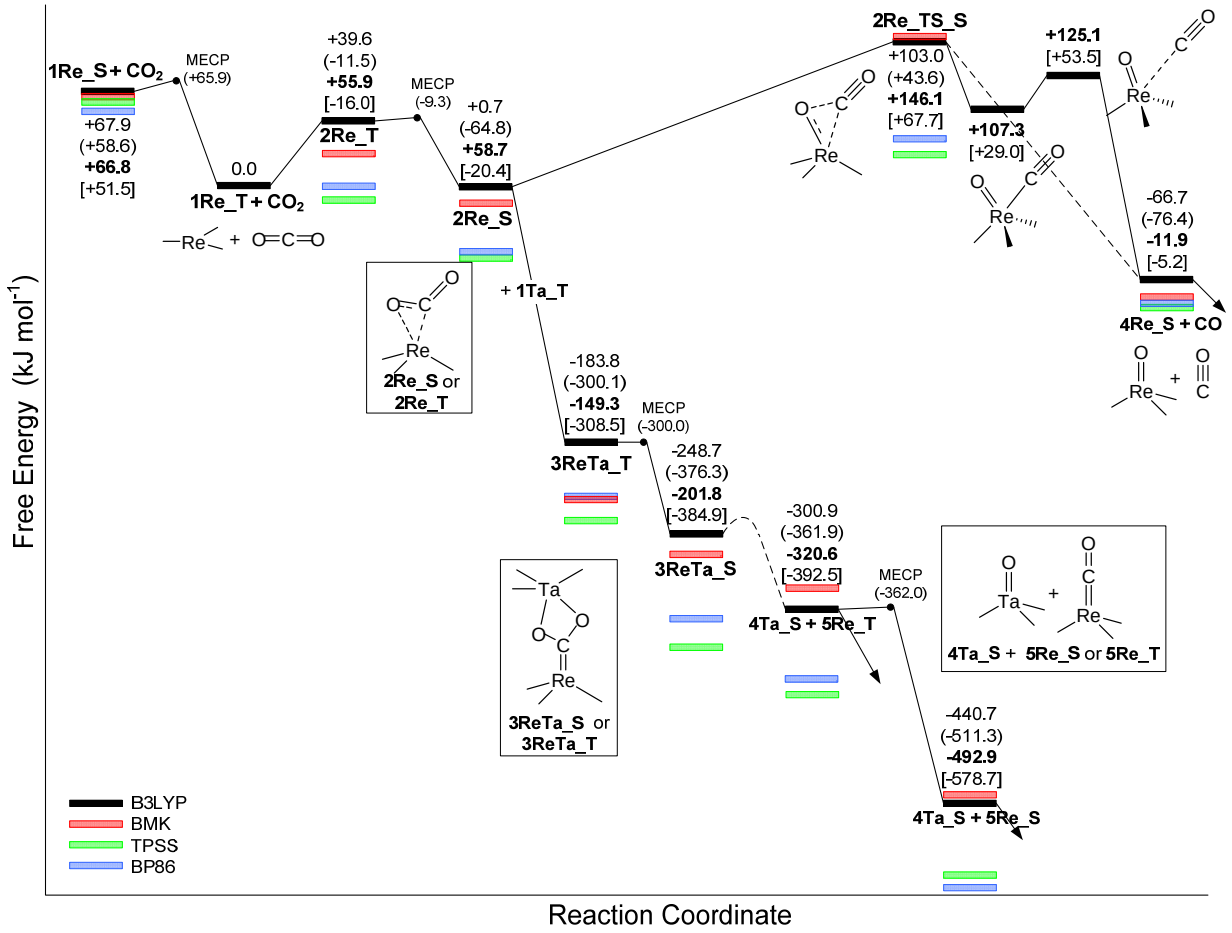

Figure S4. Potential energy surface displaying the reaction $Re(NR_2)_3 + CO_2$. Values in normal script are at the Model-opt Gibbs corrected level of theory and those in parentheses are uncorrected electronic energies. Values in bold are at the Full-opt Gibbs corrected level of theory and those in square brackets are uncorrected electronic energies All values in kJ mol^{-1}.

5.1 Model-opt level of theory (Re)

Structure 1Re_T
B3LYP/GBS(1) = -246.949028 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -247.054194 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -246.517298 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -247.035808 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -247.136993 a.u.
Enthalpy Correction = 0.083213
Gibbs Free Energy Correction = 0.042151

Atomic No	x-coord	y-coord	z-coord
75	-0.000252	-0.000189	-0.000159
7	1.304711	-1.402309	0.000581
7	-1.867140	-0.428520	0.000268
7	0.562713	1.830601	0.000369
1	0.731450	2.372056	0.843751
1	0.730698	2.372895	-0.842618
1	1.698135	-1.811691	-0.842338
1	1.697956	-1.811037	0.843902

1	-2.420853	-0.552959	-0.842825
1	-2.420504	-0.553521	0.843500

Structure 1Re_T to 1Re_S MECP
B3LYP/GBS(2)//B3LYP/GBS(1) = -247.029090 a.u.

Atomic No	x-coord	y-coord	z-coord
75	0.1411841	0.0374492	-0.2849902
7	1.3130168	-1.4115209	0.0474274
7	-1.7012138	-0.3961457	-0.2000303
7	0.5438622	1.8534794	0.0634973
1	1.0366199	2.2309227	0.8611835
1	0.0651860	2.5875460	-0.4564291
1	1.2174438	-2.2761814	-0.4833513
1	1.9078954	-1.5410216	0.8542949
1	-2.2571377	-0.5355022	-1.0406994
1	-2.2499431	-0.5336993	0.6435284

Structure 1Re_S
B3LYP/GBS(1) = -246.931001 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -247.031861 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -246.495754 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -247.016596 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -247.119585 a.u.
Enthalpy Correction = 0.084673
Gibbs Free Energy Correction = 0.045665

Atomic No	x-coord	y-coord	z-coord
75	0.002925	-0.001112	-0.100242
7	-1.203093	-1.419187	0.265384
7	-0.598893	1.760645	0.264623
7	1.828863	-0.342547	0.224558
1	2.228680	-1.271360	0.341907
1	2.537823	0.379589	0.335723
1	-1.948997	-1.655979	-0.397058
1	-1.395566	-1.834829	1.176260
1	-1.206074	2.255994	-0.396456
1	-0.623363	2.217619	1.175819

Structure 2Re_T

B3LYP/GBS(1) = -435.530976 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -435.708871 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -435.089748 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -435.734322 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -435.814228 a.u.
Enthalpy Correction = 0.100230
Gibbs Free Energy Correction = 0.051840

Atomic No	x-coord	y-coord	z-coord
75	-0.258803	0.000027	-0.046412
7	-0.459522	1.848607	-0.552730
7	-1.851746	-0.000098	1.106470
7	-0.459759	-1.848499	-0.552896
1	-1.356034	-2.331395	-0.579243
1	0.203587	-2.289365	-1.189111
1	0.203934	2.289317	-1.188933
1	-1.355686	2.331691	-0.579201
1	-2.160156	-0.831666	1.603400
1	-2.160469	0.831516	1.603131
6	1.790556	-0.000072	0.339506
8	1.680879	-0.000081	-0.947232
8	2.655230	-0.000135	1.168219

Structure 2Re_T to 2Re_S MECP
B3LYP/GBS(1) = -435.530618 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -435.708028 a.u.

GBS2 geometry

Atomic No	x-coord	y-coord	z-coord
75	-0.1301490	-0.0604279	0.0000283
7	-1.4500264	1.3781633	-0.0003363
7	-0.4214005	-0.6513443	1.8020601
7	-0.4219163	-0.6530133	-1.8013288
1	-1.3219007	-0.6265831	2.2690291
1	-1.3225728	-0.6287602	-2.2680612
1	-1.7270950	1.8890728	0.8298977
1	0.1759884	-1.3646656	2.2102338
1	-1.7269504	1.8887744	-0.8307773
1	0.1754222	-1.3666377	-2.2090940
8	1.6580434	-1.2399210	0.0003133
6	1.9462137	0.0110285	-0.0002745
8	2.9162576	0.7050122	-0.0006992

Structure 2Re_S
B3LYP/GBS(1) = -435.555844 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -435.729170 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -435.108517 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -435.755713 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -435.838421 a.u.

Enthalpy Correction = 0.102074
Gibbs Free Energy Correction = 0.05732

Atomic No	x-coord	y-coord	z-coord
75	-0.312479	0.005780	0.000009
7	-1.191047	1.699390	-0.000631
7	-0.538984	-0.920845	1.635850
7	-0.539541	-0.922438	-1.634857
1	-1.433743	-1.154483	2.063727
1	-1.434466	-1.156550	-2.062131
1	-1.306360	2.275267	0.833428
1	0.215580	-1.522799	1.974176
1	-1.306673	2.274490	-0.835182
1	0.214872	-1.524806	-1.972775
8	1.635068	-1.053691	0.000106
6	1.744167	0.219457	-0.000258
8	2.603520	1.061926	-0.000471

Structure 2Re_TS_S
B3LYP/GBS(1) = -435.506383 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -435.687886 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -435.061197 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -435.724747 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -435.804714 a.u.
Enthalpy Correction = 0.099465
Gibbs Free Energy Correction = 0.055003

Atomic No	x-coord	y-coord	z-coord
75	-0.215696	-0.072311	-0.123709
7	-0.631676	0.941809	1.550737
7	-1.594195	-1.241255	0.557099
7	-0.619140	1.545807	-1.065499
1	-2.179306	-1.085926	1.372770
1	-0.538292	2.484246	-0.677424
1	-0.422656	0.470801	2.430325
1	-1.752526	-2.153523	0.131839
1	-0.269533	1.892704	1.621679
1	-1.169144	1.555088	-1.921977
8	1.174948	-0.916432	-0.986371
6	1.729789	0.041383	0.268616
8	2.830673	0.077320	0.662986

Structure 4Re_S
B3LYP/GBS(1) = -322.241848 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -322.381897 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -321.815233 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -322.387955 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -322.483294 a.u.

Enthalpy Correction = 0.090289
Gibbs Free Energy Correction = 0.050178

Atomic No	x-coord	y-coord	z-coord
75	0.076010	0.069769	-0.000105
7	1.670583	-1.011949	-0.005067
7	-1.218599	-0.522535	-1.285833
7	-1.213576	-0.532567	1.285588
1	-1.110001	-0.394163	-2.286690
1	-2.185598	-0.745086	1.048348
1	1.725517	-2.026252	-0.006335
1	-2.189772	-0.736482	-1.046741
1	2.595720	-0.591268	-0.003407
1	-1.101442	-0.413189	2.287213
8	0.236997	1.767886	0.006584

Structure 5Re_T
B3LYP/GBS(1) = -360.29740 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -360.442232 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -359.845610 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -360.45537 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -360.542738 a.u.
Enthalpy Correction = 0.095255
Gibbs Free Energy Correction = 0.049896

Atomic No	x-coord	y-coord	z-coord
75	0.144737	0.073608	-0.000004
6	-1.687347	-0.447279	0.000014
8	-2.774809	-0.886576	0.000028
7	1.254040	-0.750666	-1.376033
7	-0.241094	1.973153	-0.000047
7	1.254047	-0.750601	1.376060
1	1.034807	-0.770343	-2.367748
1	2.093795	-1.299373	-1.189762
1	-1.154235	2.416483	-0.000120
1	0.495326	2.675228	0.000144
1	1.034829	-0.770211	2.367779
1	2.093818	-1.299291	1.189815

Structure 5Re_T to 5Re_S MECP
B3LYP/GBS(1) = -360.296913 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -360.442281 a.u.

Geometry from GBS2

Atomic No	x-coord	y-coord	z-coord
75	0.1559509	0.0804273	-0.0000112
6	-1.6593822	-0.4554352	0.0000531
8	-2.7396212	-0.8908463	-0.0000054

7	1.2455465	-0.7438026	-1.3898927
7	-0.2312566	1.9770124	-0.0000131
7	1.2454349	-0.7437484	1.3900308
1	0.9902847	-0.8079841	-2.3671895
1	2.0971631	-1.2699332	-1.2147542
1	-1.1427835	2.4158574	-0.0000189
1	0.4990307	2.6803330	-0.0000168
1	0.9902993	-0.8078820	2.3671453
1	2.0972475	-1.2698660	1.2147986

Structure 5Re_S
B3LYP/GBS(1) = -360.355102 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -360.499141 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -359.904865 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -360.512236 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -360.599765 a.u.
Enthalpy Correction = 0.096418
Gibbs Free Energy Correction = 0.053530

Atomic No	x-coord	y-coord	z-coord
75	-0.245293	0.000410	0.000000
6	1.569556	-0.001241	0.000000
8	2.748661	-0.002224	0.000000
7	-0.463124	-0.961091	1.663022
7	-0.459645	1.921776	0.000000
7	-0.463124	-0.961091	-1.663022
1	0.272857	-1.311228	2.267360
1	-1.378592	-1.185091	2.050655
1	0.277469	2.618988	0.000000
1	-1.374395	2.370945	0.000000
1	0.272857	-1.311229	-2.267359
1	-1.378592	-1.185091	-2.050655

5.2 Gen-opt level of theory (Re)

Gen-opt Structure 1Re_T
B3LYP/GBS(1) = -1405.470512 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1412.219785 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1411.128624 a.u.
Enthalpy Correction = 0.700447

Gibbs Free Energy Correction = 0.590806

Atomic No	x-coord	y-coord	z-coord
75	-0.059225	0.138578	-0.615519
7	-2.003190	0.024389	-0.528186
7	0.903521	1.801099	-0.344905
7	1.017875	-1.471342	-0.808392
6	-3.070768	0.586249	-1.409617
6	-2.412054	1.319539	-2.598761
6	-3.983968	-0.537671	-1.962455
6	-3.927317	1.602695	-0.612240
1	-1.768706	2.129806	-2.241628
1	-1.807612	0.627233	-3.193835
1	-3.194369	1.742031	-3.239897
1	-4.492803	-1.062219	-1.149101
1	-4.740756	-0.104360	-2.625837
1	-3.386425	-1.257413	-2.532871
1	-4.700526	2.029174	-1.261052
1	-4.412157	1.116988	0.239645
1	-3.289442	2.411771	-0.240326
6	1.195041	-2.308700	-2.039470
6	0.309924	-1.737536	-3.169701
6	2.669306	-2.316506	-2.519551
6	0.739432	-3.762927	-1.751865
1	0.606769	-0.713561	-3.422267
1	0.420203	-2.359844	-4.065491
1	-0.743450	-1.741000	-2.869721
1	3.322672	-2.757731	-1.762174
1	2.756046	-2.904683	-3.440418
1	3.000107	-1.292118	-2.723617
1	0.844066	-4.372778	-2.656312
1	1.341079	-4.207796	-0.954285
1	-0.311264	-3.765443	-1.441200
6	1.750500	2.648330	-1.238041
6	1.793826	2.003431	-2.638345
6	1.168309	4.079347	-1.363688
6	3.193689	2.724069	-0.677697
1	2.225334	0.998696	-2.580653
1	0.786192	1.931949	-3.060273
1	2.414364	2.615100	-3.302992
1	1.159072	4.582378	-0.392600
1	1.780762	4.669442	-2.054886
1	0.144610	4.031511	-1.751443
1	3.822746	3.325689	-1.343278
1	3.199545	3.177843	0.317707
1	3.615131	1.715459	-0.605469
6	0.805605	2.188784	1.036224
6	1.595093	1.559401	2.017963
6	-0.140737	3.150183	1.449746
6	1.437645	1.878431	3.368478
1	2.308396	0.804034	1.711734
6	-0.283046	3.474527	2.798602
1	-0.771990	3.616893	0.703145
6	0.505322	2.839462	3.764105
1	0.388044	3.087936	4.812600
6	-2.421088	-0.671875	0.658194
6	-2.750693	-2.041110	0.609707
6	-2.458686	-0.014408	1.902183
6	-3.118599	-2.725723	1.768216
1	-2.693707	-2.557283	-0.340983

6	-2.818178	-0.706534	3.059791
1	-2.180336	1.031456	1.949903
6	-3.154616	-2.060783	2.997546
1	-3.434556	-2.595478	3.897833
6	1.706442	-1.918465	0.368628
6	3.057235	-1.584733	0.587600
6	1.027990	-2.648542	1.361519
6	3.709465	-1.980025	1.757655
1	3.576578	-0.993685	-0.157297
6	1.682065	-3.037766	2.530182
1	-0.021377	-2.873040	1.213916
6	3.026530	-2.711252	2.732390
1	3.532373	-3.015511	3.641410
1	4.749080	-1.710440	1.910137
1	1.139192	-3.592407	3.287572
1	2.043774	1.370660	4.110321
1	-1.015551	4.215961	3.099000
1	-2.830076	-0.187246	4.011444
1	-3.368591	-3.779698	1.714100

Gen-opt Structure 1Re_S
B3LYP/GBS(1) = -1405.453335 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1412.199066 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1411.108989 a.u.
Enthalpy Correction = 0.701748
Gibbs Free Energy Correction = 0.596626

Atomic No	x-coord	y-coord	z-coord
75	0.053157	-0.366340	0.149081
7	1.821865	-0.989931	0.536054
7	-0.340320	1.377179	0.880675
7	-1.513633	-1.442073	-0.210672
6	2.646983	-1.423162	1.702871
6	1.717152	-1.804119	2.869870
6	3.519779	-2.650373	1.335990
6	3.563062	-0.253478	2.143431
1	1.098348	-0.952205	3.156932
1	1.056887	-2.625099	2.579595
1	2.323070	-2.117024	3.727866
1	4.207174	-2.413641	0.518933
1	4.107800	-2.952178	2.209863
1	2.883100	-3.489208	1.035370
1	4.166594	-0.551788	3.008121
1	4.234771	0.036683	1.329447
1	2.947328	0.609050	2.420466
6	-1.638706	-2.929610	-0.410031
6	-0.344182	-3.624388	0.053400
6	-2.815424	-3.498912	0.422004
6	-1.865318	-3.241465	-1.911062
1	-0.162249	-3.426505	1.111835
1	-0.447402	-4.704364	-0.100035
1	0.516957	-3.269092	-0.517736
1	-3.772619	-3.094976	0.083488
1	-2.839636	-4.588061	0.306520
1	-2.674841	-3.259964	1.481507

1	-1.941878	-4.325410	-2.050761
1	-2.785971	-2.775364	-2.272221
1	-1.022043	-2.864705	-2.499092
6	-1.085560	1.774002	2.134868
6	-1.542603	0.517384	2.902208
6	-0.203991	2.614945	3.097459
6	-2.332945	2.607582	1.739521
1	-2.150419	-0.126651	2.268231
1	-0.680941	-0.056231	3.248118
1	-2.135162	0.832058	3.769659
1	0.065094	3.577515	2.656374
1	-0.765446	2.803301	4.019689
1	0.709160	2.065099	3.351495
1	-2.880238	2.903951	2.642053
1	-2.036689	3.511252	1.198594
1	-2.992543	2.013260	1.101690
6	0.167255	2.488209	0.115605
6	-0.497725	2.898111	-1.054359
6	1.342181	3.171706	0.489147
6	0.001685	3.943371	-1.831992
1	-1.402259	2.376186	-1.340446
6	1.839125	4.217536	-0.291349
1	1.872671	2.859908	1.380396
6	1.172158	4.607789	-1.455277
1	1.559095	5.419763	-2.060168
6	2.496314	-0.701159	-0.710323
6	2.750601	-1.733541	-1.645618
6	2.872323	0.612547	-1.052780
6	3.336650	-1.453060	-2.873293
1	2.468180	-2.747689	-1.392123
6	3.434001	0.892476	-2.303351
1	2.694744	1.415614	-0.352727
6	3.672689	-0.134002	-3.213306
1	4.115284	0.081859	-4.178822
6	-2.662911	-0.679072	-0.629491
6	-3.788229	-0.522114	0.199983
6	-2.670339	-0.065119	-1.896424
6	-4.885144	0.228601	-0.225582
1	-3.790688	-0.978135	1.180547
6	-3.769440	0.686844	-2.316317
1	-1.799294	-0.182857	-2.529533
6	-4.880706	0.837493	-1.483281
1	-5.732312	1.423455	-1.808566
1	-3.757277	1.152576	-3.295583
1	-5.741707	0.342745	0.429381
1	3.682077	1.917396	-2.554885
1	3.522806	-2.256601	-3.577537
1	2.749067	4.725865	0.009200
1	-0.523177	4.239367	-2.733697

Gen-opt Structure 2Re_T
B3LYP/GBS(1) = -1594.047793 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1600.862122 a.u.

M06/GBS(2)//B3LYP/GBS(1) = -1599.696837 a.u.
Enthalpy Correction = 0.718259
Gibbs Free Energy Correction = 0.608463

Atomic No	x-coord	y-coord	z-coord
75	-0.121139	-0.571696	-0.571716
8	-0.845642	-0.788531	-2.741964
6	-0.190120	-1.767069	-2.246567
8	0.180546	-2.861620	-2.618821
7	0.959759	-1.370742	0.828766
7	-1.984245	-0.431187	0.024549
7	1.112394	0.813824	-1.276880
6	0.961930	-2.836666	1.223961
6	-0.349435	-3.516322	0.766466
6	2.142121	-3.566289	0.533919
6	1.076872	-2.973044	2.762636
6	2.240412	0.777016	-2.275501
6	2.853767	-0.638821	-2.346100
6	1.736421	1.176278	-3.687433
6	3.352444	1.762784	-1.827998
6	-3.323443	-0.685340	-0.659190
6	-3.588856	0.399901	-1.730728
6	-3.336805	-2.091114	-1.303407
6	-4.477751	-0.639721	0.378180
6	-2.070816	0.302317	1.261859
6	-2.064847	1.706300	1.278701
6	-2.167742	-0.390284	2.483158
6	-2.158485	2.398267	2.489045
6	-2.266729	0.304002	3.687828
6	-2.262409	1.703294	3.694947
6	1.833060	-0.519703	1.595866
6	3.224086	-0.507876	1.388889
6	1.291719	0.329060	2.575641
6	4.046547	0.335680	2.137484
6	2.118513	1.173118	3.319967
6	3.497942	1.182421	3.105123
6	0.559200	2.112362	-1.018426
6	-0.472292	2.630662	-1.826459
6	1.023420	2.877813	0.066345
6	-1.018390	3.886698	-1.555862
6	0.478222	4.135900	0.325961
6	-0.541841	4.645463	-0.482547
1	0.847190	4.716296	1.164102
1	-1.814157	4.272401	-2.183430
1	-1.219441	-3.003668	1.183674
1	-0.424542	-3.536946	-0.323975
1	-0.346414	-4.552172	1.124183
1	3.104662	-3.177824	0.876061
1	2.099471	-4.633984	0.778414
1	2.057012	-3.451106	-0.550585
1	1.020526	-4.034365	3.027150
1	2.024561	-2.571004	3.129428
1	0.256304	-2.441879	3.255820
1	2.150036	-1.371748	-2.742780
1	3.724332	-0.607852	-3.010587
1	3.183188	-0.963593	-1.357851
1	1.374998	2.208686	-3.693882
1	2.565416	1.095014	-4.399788
1	0.928536	0.508657	-3.998635
1	4.180419	1.710415	-2.543457

1	2.980898	2.790272	-1.800166
1	3.721014	1.489668	-0.834581
1	-3.573579	1.395487	-1.275417
1	-2.830744	0.342939	-2.512579
1	-4.576398	0.236268	-2.178079
1	-3.107077	-2.852413	-0.551628
1	-4.337279	-2.286908	-1.705433
1	-2.622146	-2.159797	-2.121541
1	-5.409411	-0.871611	-0.148600
1	-4.330600	-1.382778	1.167273
1	-4.572877	0.347921	0.835704
1	-1.966296	2.246164	0.346338
1	-2.160801	-1.472978	2.471234
1	-2.337205	2.242673	4.632054
1	3.654895	-1.144207	0.629401
1	0.225757	0.313638	2.751824
1	4.138832	1.837363	3.683726
1	-0.843498	2.030902	-2.647540
1	1.797915	2.469895	0.702026
1	-0.962654	5.623313	-0.278176
1	-2.342805	-0.243888	4.620459
1	-2.142521	3.481726	2.483429
1	1.678635	1.819882	4.070689
1	5.116425	0.333795	1.961086

Gen-opt Structure 2Re_S
B3LYP/GBS(1) = -1594.057595 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1600.869623 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1599.698513 a.u.
Enthalpy Correction = 0.719173
Gibbs Free Energy Correction = 0.611197

Atomic No	x-coord	y-coord	z-coord
75	-0.036493	-0.078871	-0.660273
8	-0.184778	0.587067	-2.836685
6	0.423843	-0.510652	-2.591058
8	1.006830	-1.355440	-3.244176
7	0.792553	-1.620790	0.166376
7	-1.986025	0.040186	-0.566539
7	0.892865	1.561764	-0.214891
6	0.302353	-3.065519	0.202093
6	-0.724775	-3.279852	-0.932012
6	1.462394	-4.066740	-0.028917
6	-0.329588	-3.330505	1.587834
6	1.703109	2.541269	-1.068552
6	2.606424	1.770308	-2.058627
6	0.800663	3.522698	-1.851770
6	2.645429	3.360191	-0.141217
6	-3.036992	0.614914	-1.521199
6	-2.642263	2.050080	-1.944026
6	-3.173586	-0.297327	-2.763500
6	-4.427431	0.736805	-0.835030
6	-2.508382	-0.437544	0.688531
6	-2.255581	0.242388	1.890679
6	-3.296812	-1.605827	0.735248

6	-2.746106	-0.247240	3.103908
6	-3.804663	-2.076099	1.944738
6	-3.523320	-1.405446	3.138849
6	2.192975	-1.475952	0.476480
6	3.154560	-1.447201	-0.546329
6	2.611040	-1.425962	1.816602
6	4.510800	-1.340708	-0.228519
6	3.968886	-1.329953	2.126063
6	4.922284	-1.280462	1.104770
6	0.603115	2.059420	1.108560
6	-0.414531	3.009804	1.312538
6	1.342533	1.614085	2.213129
6	-0.680065	3.500661	2.591558
6	1.065274	2.097327	3.493190
6	0.056714	3.043948	3.688279
1	1.644054	1.739678	4.337493
1	-1.469828	4.229947	2.733361
1	-1.554714	-2.578327	-0.846984
1	-0.240156	-3.145996	-1.903132
1	-1.125215	-4.297545	-0.864324
1	2.206109	-4.019549	0.769923
1	1.034314	-5.075243	-0.047108
1	1.953311	-3.879196	-0.987603
1	-0.708878	-4.358643	1.623909
1	0.422524	-3.215350	2.374661
1	-1.155155	-2.643227	1.772055
1	2.019181	1.283219	-2.834689
1	3.282735	2.485549	-2.540817
1	3.205604	1.029598	-1.523374
1	0.192631	4.128758	-1.174176
1	1.435751	4.198163	-2.437132
1	0.154097	2.969840	-2.532413
1	3.282567	3.982820	-0.778034
1	2.089142	4.012179	0.536229
1	3.283498	2.694359	0.447710
1	-2.552278	2.687057	-1.057460
1	-1.703999	2.047063	-2.489671
1	-3.427720	2.461094	-2.588556
1	-3.462051	-1.310192	-2.461836
1	-3.950038	0.101328	-3.427161
1	-2.228462	-0.336555	-3.305054
1	-5.099172	1.235611	-1.541870
1	-4.855272	-0.233565	-0.579784
1	-4.366675	1.340716	0.075374
1	-1.685046	1.157580	1.866553
1	-3.513890	-2.137710	-0.182211
1	-3.910195	-1.779075	4.079586
1	2.824514	-1.519288	-1.576712
1	1.864316	-1.457551	2.600545
1	5.975636	-1.202929	1.347329
1	-1.006016	3.336647	0.467504
1	2.124412	0.885635	2.052924
1	-0.152626	3.422953	4.681744
1	-4.411308	-2.974802	1.956536
1	-2.528522	0.293360	4.018034
1	4.282678	-1.294462	3.163406
1	5.245174	-1.315231	-1.025780

Gen-opt Structure 2Re_TS_S
B3LYP/GBS(1) = -1594.019295 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1599.664926 a.u.
Enthalpy Correction = 0.716800
Gibbs Free Energy Correction = 0.610904

Atomic No	x-coord	y-coord	z-coord
75	-0.035342	-0.300387	-0.855213
8	-0.475215	0.015601	-2.620852
6	0.038963	-1.697434	-2.281103
8	0.016076	-2.477482	-3.153558
7	-0.667624	1.559425	-0.439970
7	1.879592	-0.352724	-0.391143
7	-0.958052	-1.444477	0.456733
6	-0.116445	2.913707	-0.891717
6	0.905923	2.711708	-2.033869
6	-1.227235	3.838271	-1.468371
6	0.533364	3.638612	0.312014
6	-1.930434	-2.589522	0.201506
6	-1.176411	-3.921630	-0.032779
6	-2.872972	-2.766181	1.424550
6	-2.834473	-2.273383	-1.012897
6	2.914464	-1.393409	-0.850817
6	2.397334	-2.842800	-0.668733
6	3.282350	-1.151269	-2.335425
6	4.213144	-1.319238	0.007161
6	2.461180	0.696787	0.408123
6	2.159896	0.789016	1.775143
6	3.403475	1.597508	-0.127699
6	2.763581	1.760054	2.577464
6	4.010036	2.560537	0.676895
6	3.690448	2.650186	2.034539
6	-2.081594	1.641567	-0.182712
6	-3.020635	1.219297	-1.139528
6	-2.554665	2.210115	1.016052
6	-4.391206	1.329931	-0.887837
6	-3.923748	2.320322	1.260756
6	-4.849614	1.874297	0.312651
6	-0.635061	-1.255922	1.847300
6	0.339517	-2.061783	2.464112
6	-1.306994	-0.305046	2.629001
6	0.635263	-1.914119	3.819642
6	-1.000716	-0.149778	3.981811
6	-0.029899	-0.952823	4.584741
1	-1.529221	0.594772	4.566688
1	1.392482	-2.542792	4.274428
1	1.715511	2.057842	-1.724884
1	0.414309	2.272828	-2.904485
1	1.329403	3.686267	-2.302429
1	-1.965380	4.116857	-0.713475
1	-0.742194	4.750550	-1.833317
1	-1.740271	3.357620	-2.305920
1	0.981988	4.578311	-0.031822
1	-0.225102	3.879208	1.063938

1	1.304326	3.025594	0.770712
1	-0.555315	-4.173252	0.831439
1	-1.906807	-4.726017	-0.177216
1	-0.549155	-3.862233	-0.923677
1	-3.410634	-1.837143	1.635023
1	-3.602782	-3.544617	1.178423
1	-2.326854	-3.071727	2.319841
1	-3.569078	-3.079069	-1.121493
1	-3.361799	-1.331662	-0.845720
1	-2.272147	-2.207387	-1.944893
1	2.139086	-3.020771	0.377064
1	1.536270	-3.065259	-1.291060
1	3.200578	-3.533293	-0.948315
1	3.735843	-0.164287	-2.463957
1	4.002374	-1.909038	-2.665145
1	2.397658	-1.213183	-2.972518
1	4.863201	-2.144926	-0.300890
1	4.754596	-0.383854	-0.130474
1	3.980121	-1.432585	1.070186
1	1.465944	0.084625	2.204957
1	3.668933	1.533115	-1.174621
1	4.160401	3.401982	2.657714
1	-2.658560	0.823351	-2.080575
1	-1.837515	2.562094	1.747134
1	-5.912633	1.961721	0.504299
1	0.874298	-2.788587	1.870192
1	-2.062876	0.308471	2.163360
1	0.203775	-0.834011	5.636243
1	4.730896	3.243754	0.241932
1	2.510194	1.809423	3.630268
1	-4.268857	2.759207	2.190641
1	-5.099676	1.001107	-1.640506

Gen-opt Structure - IRC minimum after 2Re_TS_S
B3LYP/GBS(1) = -1594.027132 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1599.679674 a.u.
Enthalpy Correction = 0.717908
Gibbs Free Energy Correction = 0.610885

Atomic No	x-coord	y-coord	z-coord
75	-0.053644	-0.326017	-0.928733
8	-0.375170	0.009438	-2.618430
6	0.070920	-2.147818	-1.913521
8	-0.052107	-3.035792	-2.635517
7	-0.685580	1.533180	-0.402970
7	1.885645	-0.364233	-0.469300
7	-1.038902	-1.346302	0.494630
6	-0.129272	2.908292	-0.780665
6	0.823127	2.774172	-1.992856
6	-1.244033	3.893603	-1.247802
6	0.577422	3.552624	0.434874
6	-2.158932	-2.362699	0.379218
6	-1.618548	-3.809075	0.535507
6	-3.215729	-2.111811	1.492073
6	-2.912394	-2.231062	-0.966384
6	2.912023	-1.421008	-0.917365
6	2.546237	-2.831826	-0.380687
6	3.056284	-1.400823	-2.459689

```
6     4.336859   -1.162824   -0.331875
6     2.500537    0.694036    0.288990
6     2.326502    0.748499    1.680081
6     3.378336    1.619041   -0.308872
6     2.995210    1.705536    2.447139
6     4.047697    2.570633    0.458735
6     3.857810    2.620477    1.842312
6    -2.101508    1.602637   -0.185641
6    -3.008976    1.189168   -1.178839
6    -2.629035    2.177516    0.990215
6    -4.389414    1.295590   -0.982546
6    -4.006369    2.277950    1.185286
6    -4.895671    1.827794    0.203600
6    -0.578823   -1.170478    1.848053
6     0.385530   -2.044223    2.382723
6    -1.100781   -0.168602    2.679954
6     0.815611   -1.915112    3.704436
6    -0.661605   -0.032154    3.997238
6     0.298147   -0.904028    4.517356
1    -1.077189    0.751938    4.620380
1     1.562209   -2.598031    4.094246
1     1.600833    2.042040   -1.807670
1     0.261921    2.461555   -2.877054
1     1.292955    3.745678   -2.185687
1    -1.934069    4.152151   -0.442571
1    -0.749708    4.810299   -1.588960
1    -1.815613    3.474823   -2.080440
1     1.019554    4.511972    0.139152
1    -0.151186    3.743464    1.230325
1     1.357918    2.908489    0.825776
1    -1.184460   -3.953380    1.528221
1    -2.445893   -4.517281    0.415093
1    -0.863441   -4.030419   -0.223769
1    -3.613084   -1.095456    1.412984
1    -4.038308   -2.821809    1.353617
1    -2.794280   -2.256984    2.488902
1    -3.736223   -2.953467   -0.968215
1    -3.329973   -1.227960   -1.058079
1    -2.286040   -2.443178   -1.831898
1     2.706468   -2.857561    0.701000
1     1.516511   -3.120120   -0.577896
1     3.203482   -3.573796   -0.847082
1     3.408880   -0.414845   -2.779272
1     3.789852   -2.153011   -2.771529
1     2.115580   -1.601485   -2.972364
1     4.957934   -2.024623   -0.600464
1     4.801288   -0.265249   -0.738999
1     4.307009   -1.077600    0.757133
1     1.679840    0.027202    2.154054
1     3.546530    1.578888   -1.377597
1     4.376617    3.362281    2.438255
1    -2.615357    0.813332   -2.115929
1    -1.943034    2.559921    1.736335
1    -5.965471    1.909366    0.356229
1     0.806736   -2.809806    1.748445
1    -1.856073    0.486799    2.278283
1     0.635373   -0.799836    5.542029
1     4.716999    3.273990   -0.023899
1     2.840567    1.727190    3.519859
1    -4.388289    2.719563    2.099466
1    -5.066916    0.974426   -1.766681
```

Gen-opt Structure - TS just prior to 4Re_S + CO (located using IRC)
B3LYP/GBS(1) = -1594.019867 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1599.670345 a.u.
Enthalpy Correction = 0.716328
Gibbs Free Energy Correction = 0.608323

Atomic No	x-coord	y-coord	z-coord
75	-0.090069	-0.360560	-0.842260
8	-0.464884	-0.321201	-2.534423
6	-0.044434	-2.693832	-2.009939
8	-0.225273	-3.389476	-2.896626
7	-0.659147	1.508939	-0.529736
7	1.859191	-0.406192	-0.434693
7	-0.996785	-1.303148	0.665524
6	-0.056210	2.813240	-1.067663
6	0.877746	2.508212	-2.261237
6	-1.149507	3.768420	-1.634438
6	0.679113	3.564834	0.065064
6	-2.100507	-2.341708	0.631752
6	-1.523986	-3.772071	0.797342
6	-3.112650	-2.088793	1.784550
6	-2.914950	-2.247366	-0.680124
6	2.821156	-1.546288	-0.806462
6	2.383431	-2.885346	-0.151892
6	2.930632	-1.649452	-2.348670
6	4.267682	-1.322640	-0.265280
6	2.536800	0.683802	0.213828
6	2.377794	0.882585	1.594066
6	3.442384	1.513761	-0.476471
6	3.084545	1.887582	2.258966
6	4.150170	2.512978	0.189688
6	3.972632	2.707843	1.562087
6	-2.078065	1.634989	-0.323134
6	-3.005676	1.142739	-1.258271
6	-2.571170	2.337188	0.795306
6	-4.379777	1.303846	-1.056324
6	-3.942731	2.494923	0.993918
6	-4.855727	1.969906	0.073882
6	-0.566442	-0.976483	2.000698
6	0.390574	-1.778180	2.649551
6	-1.101455	0.115227	2.701042
6	0.799831	-1.492554	3.953363
6	-0.682071	0.408394	3.999110
6	0.270386	-0.393349	4.633072
1	-1.107049	1.260061	4.518804
1	1.541067	-2.122576	4.432419
1	1.635008	1.779394	-1.995398
1	0.296363	2.111413	-3.097644
1	1.373308	3.435473	-2.570681
1	-1.824718	4.133097	-0.858240
1	-0.634333	4.627806	-2.078269
1	-1.739054	3.275431	-2.412017
1	1.145733	4.472238	-0.337013
1	-0.036960	3.862901	0.838681
1	1.444246	2.944268	0.519512

1	-1.035011	-3.879935	1.769229
1	-2.337686	-4.503659	0.737405
1	-0.799590	-3.995099	0.009371
1	-3.530370	-1.080503	1.707277
1	-3.928216	-2.814515	1.692949
1	-2.647271	-2.208485	2.765251
1	-3.707244	-3.003756	-0.655717
1	-3.372538	-1.259699	-0.757867
1	-2.310703	-2.422564	-1.569820
1	2.595467	-2.845598	0.920646
1	1.324433	-3.091413	-0.281463
1	2.959676	-3.708943	-0.588371
1	3.406995	-0.744363	-2.740372
1	3.543028	-2.514565	-2.627046
1	1.954454	-1.736812	-2.826219
1	4.838207	-2.233332	-0.480823
1	4.769593	-0.481280	-0.742278
1	4.262617	-1.158863	0.815402
1	1.709808	0.234705	2.140091
1	3.598796	1.364454	-1.537397
1	4.521170	3.486951	2.078546
1	-2.635674	0.653419	-2.151476
1	-1.864134	2.769780	1.492787
1	-5.921005	2.093351	0.229875
1	0.822832	-2.612785	2.117790
1	-1.850121	0.719798	2.214347
1	0.592791	-0.167310	5.642794
1	4.839649	3.140939	-0.363629
1	2.939824	2.020805	3.325093
1	-4.300407	3.036258	1.863087
1	-5.076445	0.919295	-1.793625

Gen-opt Structure 4Re_S
B3LYP/GBS(1) = -1480.742626 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1487.522946 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1486.404291 a.u.
Enthalpy Correction = 0.706957
Gibbs Free Energy Correction = 0.602573

Atomic No	x-coord	y-coord	z-coord
7	-0.660240	1.612725	-0.090636
7	1.870026	-0.342315	-0.630896
7	-0.967060	-1.518895	0.016900
6	0.006703	2.981826	-0.012048
6	1.062952	3.100409	-1.132790
6	-1.019367	4.125231	-0.245831
6	0.662687	3.172841	1.374712
6	-1.979078	-2.474229	-0.565854
6	-2.165275	-2.212940	-2.077159
6	-1.531750	-3.946185	-0.368543
6	-3.352020	-2.270466	0.129439
6	2.626479	-1.292755	-1.543029
6	1.714079	-2.479090	-1.938952
6	3.054485	-0.572240	-2.849604
6	3.864994	-1.883028	-0.821806
6	2.673274	0.359749	0.324008
6	2.454098	0.135297	1.693809
6	3.704995	1.246697	-0.045393

6	3.223942	0.783861	2.660900
6	4.473059	1.891727	0.924162
6	4.236610	1.666463	2.282610
6	-2.090910	1.653230	0.041243
6	-2.931698	1.475183	-1.072515
6	-2.685658	1.888011	1.297263
6	-4.321917	1.493710	-0.926538
6	-4.073062	1.919267	1.434996
6	-4.899264	1.712145	0.325522
6	-0.715193	-1.693444	1.421679
6	0.305485	-2.563052	1.848891
6	-1.461179	-1.007544	2.394010
6	0.562142	-2.750767	3.207679
6	-1.195979	-1.190211	3.752613
6	-0.187977	-2.064253	4.166016
1	1.352718	-3.425435	3.516499
1	1.854140	2.369698	-0.992194
1	0.597059	2.943675	-2.110056
1	1.507707	4.101805	-1.100397
1	-1.776376	4.166169	0.539847
1	-0.471174	5.073748	-0.250559
1	-1.520912	4.005952	-1.211045
1	1.186014	4.135917	1.409339
1	-0.101694	3.168966	2.159337
1	1.375334	2.374371	1.575688
1	-1.237950	-2.373446	-2.632350
1	-2.918837	-2.911572	-2.456982
1	-2.513149	-1.194041	-2.262846
1	-1.418580	-4.182477	0.692552
1	-2.292220	-4.610197	-0.793721
1	-0.582504	-4.131534	-0.879892
1	-4.083166	-2.955658	-0.314297
1	-3.281800	-2.483947	1.199284
1	-3.699143	-1.243033	-0.010763
1	1.365174	-3.011656	-1.051893
1	0.850133	-2.145152	-2.522032
1	2.286666	-3.170166	-2.567481
1	3.801301	0.200356	-2.652751
1	3.491374	-1.298391	-3.545214
1	2.179379	-0.111535	-3.318637
1	4.331631	-2.627511	-1.476083
1	4.600626	-1.111026	-0.588700
1	3.563737	-2.369434	0.111838
1	1.685181	-0.564907	1.986371
1	3.899735	1.437494	-1.091752
1	4.835023	2.170264	3.032596
1	-2.483278	1.335772	-2.049823
1	-2.044939	2.045460	2.156232
1	-5.977069	1.730316	0.436471
1	0.900207	-3.076616	1.104784
1	-2.234805	-0.326606	2.070104
1	0.013187	-2.207157	5.221300
1	5.256661	2.575179	0.616164
1	3.031701	0.591237	3.710465
1	-4.511866	2.102853	2.409808
1	-4.952522	1.353976	-1.797992
1	-1.780726	-0.650119	4.488939
8	-0.276423	0.346205	-2.585116
75	-0.048848	-0.052860	-0.922983

Gen-opt Structure 5Re_T
B3LYP/GBS(1) = -1518.808956 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1525.595709 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1524.455673 a.u.
Enthalpy Correction = 0.711998
Gibbs Free Energy Correction = 0.601269

Atomic No	x-coord	y-coord	z-coord
75	-0.064276	-0.329745	-0.717681
7	0.485015	1.629523	-0.739166
7	1.607905	-1.211381	0.005458
7	-1.747620	-1.133145	-0.097452
6	-0.337957	-0.255124	-2.574764
8	-0.319283	-0.256996	-3.753803
6	1.648989	2.397561	-1.295441
6	2.604037	1.431586	-2.025643
6	1.139869	3.443425	-2.325115
6	2.415698	3.131114	-0.164830
6	-2.963803	-1.763163	-0.726008
6	-2.752991	-1.984013	-2.235679
6	-3.238702	-3.145462	-0.074678
6	-4.204213	-0.851970	-0.534878
6	2.138994	-2.525575	-0.497249
6	0.941782	-3.415460	-0.918908
6	3.042396	-2.345669	-1.747942
6	2.899661	-3.289028	0.618510
6	2.363947	-0.516037	0.987914
6	1.698106	-0.017973	2.129279
6	3.750361	-0.255858	0.882780
6	2.370182	0.735472	3.092543
6	4.420563	0.483088	1.857272
6	3.736490	0.993637	2.963713
6	-0.620117	2.414706	-0.282592
6	-1.736143	2.646035	-1.110446
6	-0.621238	2.942549	1.021933
6	-2.823957	3.382696	-0.639897
6	-1.704993	3.694251	1.478959
6	-2.810834	3.913729	0.653973
6	-1.843535	-0.978214	1.333706
6	-1.336035	-1.968788	2.196428
6	-2.407650	0.179800	1.899935
6	-1.396063	-1.809076	3.580774
6	-2.461608	0.337612	3.286135
6	-1.959978	-0.654608	4.131610
1	-0.995061	-2.580335	4.228714
1	2.973632	0.670759	-1.340877
1	2.093726	0.948322	-2.863391
1	3.454834	2.002270	-2.414479
1	0.496169	4.188596	-1.850966
1	2.005083	3.953375	-2.762535
1	0.584499	2.946869	-3.127476
1	3.273840	3.656349	-0.600266
1	1.770959	3.870426	0.319014
1	2.777805	2.418401	0.578815
1	-1.857699	-2.584435	-2.422032
1	-3.620135	-2.521713	-2.634525
1	-2.662512	-1.034524	-2.765654

1	-3.435684	-3.046362	0.995596
1	-4.114108	-3.600619	-0.550443
1	-2.377207	-3.805935	-0.220120
1	-5.065514	-1.294726	-1.047521
1	-4.449996	-0.741433	0.524710
1	-4.006197	0.137181	-0.960498
1	0.270782	-3.578351	-0.071153
1	0.374409	-2.950161	-1.731645
1	1.315707	-4.383172	-1.271861
1	3.954493	-1.791088	-1.515380
1	3.330352	-3.327330	-2.141925
1	2.489262	-1.802539	-2.520462
1	3.177173	-4.281415	0.246901
1	3.805987	-2.766298	0.928911
1	2.252307	-3.407074	1.494086
1	0.653527	-0.265477	2.267667
1	4.303225	-0.618685	0.027957
1	4.261892	1.571233	3.715049
1	-1.735801	2.240030	-2.114160
1	0.219335	2.731816	1.670433
1	-3.653351	4.493269	1.013038
1	-0.883753	-2.853193	1.765981
1	-2.781458	0.957577	1.247699
1	-2.002282	-0.528728	5.207278
1	5.482840	0.671114	1.743763
1	1.825994	1.098002	3.957965
1	-1.690380	4.097261	2.485524
1	-3.676587	3.552756	-1.287853
1	-2.889837	1.242391	3.702366

Gen-opt Structure 5Re_S
B3LYP/GBS(1) = -1518.884586 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -1525.667218 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1524.526587 a.u.
Enthalpy Correction = 0.713194
Gibbs Free Energy Correction = 0.606497

Atomic No	x-coord	y-coord	z-coord
75	0.719488	0.036777	0.082221
7	0.237487	-0.550967	1.887690
7	0.678153	-1.295529	-1.354777
7	0.411370	1.915056	-0.385105
6	2.514006	0.117197	0.310624
8	3.690243	0.171199	0.461758
6	1.045311	-1.097759	3.039374
6	1.969753	-2.223540	2.515385
6	1.904170	0.011908	3.694664
6	0.111467	-1.720854	4.109853
6	1.272698	3.150860	-0.292573
6	1.864079	3.240738	1.135228
6	2.422833	3.107886	-1.328428
6	0.423057	4.427514	-0.526547
6	1.749549	-1.877036	-2.244966
6	2.562969	-0.718944	-2.872334
6	2.700578	-2.800760	-1.444379

6	1.115293	-2.682903	-3.409058
6	-0.608034	-1.933283	-1.392848
6	-1.708080	-1.283892	-1.977217
6	-0.806928	-3.202592	-0.807795
6	-2.973826	-1.877418	-1.962143
6	-2.066139	-3.798539	-0.814357
6	-3.158399	-3.134855	-1.387543
6	-1.132705	-0.221312	2.166838
6	-1.461966	0.928730	2.915326
6	-2.175433	-1.019300	1.667349
6	-2.793084	1.262226	3.157171
6	-3.509282	-0.669549	1.896750
6	-3.824286	0.465757	2.643636
6	-0.828343	2.043376	-1.098938
6	-0.850020	2.138074	-2.506921
6	-2.050836	2.034908	-0.407303
6	-2.059256	2.224082	-3.194001
6	-3.261544	2.101253	-1.102832
6	-3.272360	2.200221	-2.494127
1	-2.059385	2.297691	-4.276071
1	1.372651	-2.981173	1.997794
1	2.720181	-1.830548	1.828516
1	2.487544	-2.692734	3.359782
1	1.267168	0.798687	4.110527
1	2.504314	-0.414111	4.507316
1	2.578175	0.451849	2.955980
1	0.729904	-2.177889	4.889597
1	-0.532209	-0.967794	4.571066
1	-0.521300	-2.495180	3.664242
1	2.526975	2.398909	1.340139
1	2.440539	4.167544	1.234806
1	1.053599	3.245163	1.871547
1	2.021991	3.067277	-2.346086
1	3.041573	4.008054	-1.234112
1	3.052960	2.232139	-1.157886
1	1.059991	5.304332	-0.368332
1	0.023263	4.465619	-1.542833
1	-0.412909	4.468456	0.179064
1	1.896674	-0.065158	-3.444552
1	3.067752	-0.130836	-2.104713
1	3.321434	-1.130550	-3.548018
1	2.149881	-3.644249	-1.016721
1	3.479513	-3.195802	-2.107206
1	3.178953	-2.241493	-0.637624
1	1.914653	-3.011031	-4.082059
1	0.580616	-3.564558	-3.047295
1	0.415844	-2.057340	-3.972946
1	-1.564023	-0.313931	-2.434516
1	0.031521	-3.701429	-0.337211
1	-4.138499	-3.597735	-1.385259
1	-0.662700	1.559191	3.285431
1	-1.932259	-1.905162	1.095499
1	-4.859207	0.730395	2.827573
1	0.088960	2.126987	-3.046804
1	-2.043400	1.967102	0.672421
1	-4.211564	2.260289	-3.031893
1	-2.201689	-4.774970	-0.362100
1	-3.810767	-1.351485	-2.406762
1	-4.298036	-1.292342	1.490665
1	-3.029690	2.148648	3.735585
1	-4.193047	2.078211	-0.549177

6 Geometric and Energetic details of mixed metal structures

6.1 Model-opt level of theory (Re-Ta)

Structure 3ReTa_T
B3LYP/GBS(1) = -661.36202 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -661.635092 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -660.582700 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -661.648465 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -661.799225 a.u.
Enthalpy Correction = 0.185508
Gibbs Free Energy Correction = 0.116419

Atomic No	x-coord	y-coord	z-coord
7	-2.444220	1.710806	-0.940818
7	-2.545526	0.043372	1.914033
7	-2.643119	-1.609924	-0.947105
1	-3.435211	0.101624	2.407288
1	-1.892380	-2.292825	-1.034599
1	-3.278433	2.153216	-1.317016
1	-1.774240	-0.008119	2.574474
1	-1.621161	2.305853	-1.020160
1	-3.527886	-1.961356	-1.303526
8	0.239341	-1.209362	-0.049256
6	-0.393125	-0.103730	-0.055468
8	0.350275	0.986838	-0.055219
7	3.450908	1.572343	0.033828
7	2.833288	-0.915252	-1.647603
7	2.696364	-0.925620	1.692778
1	2.333969	-1.707943	-2.046929
1	3.608030	-0.897733	2.145094
1	3.725950	2.093611	0.866566
1	3.778355	-0.884515	-2.025397
1	3.780345	2.080544	-0.787527
1	2.177344	-1.736015	2.027154
75	-2.366775	0.038301	-0.002804
73	2.217006	0.015803	0.002160

Structure 3ReTa_T to 3ReTa_S MECP
B3LYP/GBS(1) = -661.360643 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -661.634982 a.u.

Geometry GBS2

Atomic No	x-coord	y-coord	z-coord
7	-2.4283043	1.7090044	-0.9347630
7	-2.5477364	0.0440761	1.9168052
7	-2.6177121	-1.6118858	-0.9397463
1	-3.4423723	0.0965431	2.3944117
1	-1.8580767	-2.2684617	-1.0872866
1	-3.2665597	2.1693796	-1.2689668
1	-1.7922006	-0.0056676	2.5892663
1	-1.6012479	2.2795020	-1.0766783
1	-3.5046102	-1.9829441	-1.2607927
8	0.2710618	-1.1914268	-0.0566212
6	-0.3867924	-0.0970597	-0.0507265
8	0.3659299	0.9915005	-0.0481826
7	3.4328307	1.5551531	0.0324431
7	2.8197560	-0.9185580	-1.6498521
7	2.6837210	-0.9283584	1.6928471
1	2.3147691	-1.6849323	-2.0819927
1	3.5877646	-0.8844236	2.1509248
1	3.7080875	2.0789795	0.8588511
1	3.7600555	-0.8805940	-2.0287969
1	3.7644225	2.0613532	-0.7849853
1	2.1598459	-1.7161548	2.0599782
75	-2.3520938	0.0369829	0.0027648
73	2.1985607	-0.0020909	0.0010469

Structure 3ReTa_S
B3LYP/GBS(1) = -661.388203 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -661.664121 a.u.
BMK/GBS(2)//B3LYP/GBS(1) = -660.602264 a.u.
TPSS/GBS(2)//B3LYP/GBS(1) = -661.686793 a.u.
BP86/GBS(2)//B3LYP/GBS(1) = -661.837271 a.u.
Enthalpy Correction = 0.186329
Gibbs Free Energy Correction = 0.120732

Atomic No	x-coord	y-coord	z-coord
75	-2.287885	0.001325	-0.021521
7	-3.069075	-0.134448	1.794443
7	-2.422468	-1.617937	-1.037725
7	-2.460980	1.737265	-0.817688
1	-3.302834	-2.024531	-1.353446
1	-3.350785	2.156781	-1.086750
1	-2.873157	-0.978829	2.334548
1	-1.627784	-2.055560	-1.500727
1	-2.921313	0.653257	2.427670
1	-1.677604	2.249826	-1.218577
8	0.452763	1.097194	-0.027596
6	-0.409081	0.031999	-0.122339
8	0.465405	-1.056567	-0.206027
7	2.946782	1.775268	0.262476

7	2.715396	-0.966576	1.649534
7	3.291979	-0.680328	-1.463889
1	3.219932	-0.412049	-2.442080
1	3.931714	-1.463052	-1.361969
1	2.401910	2.595032	0.515793
1	3.872989	2.036605	-0.063840
1	3.331464	-0.579055	2.357140
1	2.176553	-1.745869	2.020055
73	2.143945	-0.025229	0.012044

6.2 Gen-opt level of theory (Re-Ta)

Gen-opt Structure 3ReTa_T
B3LYP/GBS(1) = -2978.363523 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2991.903530 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2989.692725 a.u.
Enthalpy Correction = 1.422826
Gibbs Free Energy Correction = 1.23328

Atomic No	x-coord	y-coord	z-coord
75	-2.441772	-0.036710	-0.150425
73	2.276623	0.045215	-0.041140
6	-0.419747	-0.004358	-0.142415
8	0.339668	-0.433296	0.841141
8	0.297804	0.441781	-1.118829
7	-2.819108	1.871484	0.078605
7	-2.764627	-1.116200	1.444209
7	-3.067643	-0.725946	-1.872523
7	3.041596	-0.646315	1.735219
7	3.168421	-1.083900	-1.482382
7	2.933180	1.930507	-0.498390
6	2.904509	-0.042886	3.124858
6	2.588136	-2.236138	-2.275802
6	2.779172	2.843034	-1.710186
6	-2.658222	-0.608306	-3.323548
6	-2.029638	3.115324	0.431655
6	-4.281022	-1.480184	-1.649618
6	-4.254980	-2.888114	-1.608469
6	-5.512596	-0.826778	-1.464465
6	-5.420467	-3.616367	-1.371848
6	-6.675621	-1.560798	-1.216702
6	-6.636169	-2.955181	-1.167028
6	-4.199035	2.168216	-0.238836
6	-4.572124	2.531140	-1.547311
6	-5.196976	2.106628	0.747723
6	-5.901821	2.818036	-1.858599
6	-6.528417	2.384066	0.430960
6	-6.887831	2.741692	-0.870046
6	3.875537	2.486641	0.438801
6	3.507109	3.514568	1.330400
6	5.214572	2.052960	0.449812
6	4.443287	4.088277	2.192562
6	6.147727	2.626765	1.314580
6	5.769636	3.651124	2.186087
6	4.535135	-0.803985	-1.842578

6	4.870463	-0.127951	-3.033182
6	5.587991	-1.238091	-1.020145
6	6.203500	0.103581	-3.377866
6	6.920456	-0.994074	-1.358312
6	7.237321	-0.322854	-2.540947
6	-2.241819	-2.466261	1.891260
6	3.495261	-2.004221	1.789727
6	2.587053	-3.074633	1.695552
6	4.856726	-2.312108	1.989045
6	3.024675	-4.399976	1.747655
6	5.291091	-3.637106	2.054042
6	4.379757	-4.688626	1.923684
6	-3.733956	-0.542936	2.340949
6	-3.315272	0.339613	3.352094
6	-5.099424	-0.857233	2.236283
6	-4.240614	0.895250	4.236576
6	-6.020630	-0.309323	3.131830
6	-5.596964	0.568201	4.132436
6	2.377177	-1.081073	4.152387
6	-1.368310	-2.280305	3.154356
6	4.170144	3.200236	-2.303810
6	-3.907042	-0.394672	-4.219460
6	3.566509	-3.441174	-2.267052
6	-2.849024	4.015121	1.398944
6	4.266479	0.493920	3.633712
6	-3.411495	-3.434620	2.206557
6	2.070046	4.172442	-1.338031
6	-1.921709	-1.892641	-3.777399
6	2.282975	-1.838798	-3.745237
6	-1.703975	3.918363	-0.851358
6	1.881997	1.112644	3.084514
6	-1.388930	-3.102979	0.776914
6	-1.721002	0.601265	-3.505714
6	1.938009	2.159088	-2.808636
6	1.272133	-2.704796	-1.626027
6	-0.721240	2.747647	1.152367
1	-0.264264	3.665515	1.539705
1	-3.314209	-3.401924	-1.751738
1	-5.552081	0.250797	-1.530608
1	-5.379934	-4.699701	-1.343509
1	-7.612997	-1.035101	-1.072438
1	-7.540450	-3.522585	-0.979746
1	-3.814816	2.562538	-2.318717
1	-4.923636	1.844621	1.759024
1	-6.168747	3.093167	-2.873175
1	-7.282346	2.322567	1.207666
1	-7.921306	2.961132	-1.112247
1	2.479360	3.854903	1.343507
1	5.514420	1.266453	-0.229960
1	4.135269	4.876362	2.871355
1	7.173619	2.274542	1.301912
1	6.496267	4.098560	2.854497
1	4.083001	0.232637	-3.678574
1	5.340864	-1.783094	-0.122750
1	6.432889	0.628870	-4.298849
1	7.710757	-1.343907	-0.702315
1	8.271050	-0.137705	-2.809124
1	1.532403	-2.846647	1.608597
1	5.566020	-1.498778	2.080248
1	2.303984	-5.207062	1.665691
1	6.344367	-3.849707	2.203293

1	4.720295	-5.716604	1.968425
1	-2.263151	0.586491	3.420595
1	-5.430762	-1.515453	1.443837
1	-3.904058	1.577771	5.009005
1	-7.071118	-0.561921	3.039804
1	-6.314012	0.994644	4.824399
1	3.090030	-1.894640	4.308704
1	2.216909	-0.571446	5.109687
1	1.426491	-1.502616	3.816758
1	-1.960013	-1.878217	3.982180
1	-0.957544	-3.249446	3.461059
1	-0.546538	-1.598648	2.924712
1	4.025223	3.782793	-3.221186
1	4.756912	3.799639	-1.603189
1	4.727141	2.292844	-2.539382
1	-3.572198	-0.227968	-5.249131
1	-4.570132	-1.263564	-4.205418
1	-4.470346	0.482774	-3.887184
1	3.098266	-4.284747	-2.787613
1	4.504702	-3.197772	-2.771665
1	3.784497	-3.737103	-1.236319
1	-2.231020	4.875095	1.678693
1	-3.766230	4.383263	0.934549
1	-3.107785	3.458492	2.305101
1	4.119143	1.013013	4.588815
1	4.964034	-0.331667	3.803421
1	4.700512	1.189104	2.915876
1	-2.988020	-4.408273	2.477190
1	-4.018151	-3.077948	3.042031
1	-4.049196	-3.560557	1.326517
1	2.695690	4.785069	-0.684517
1	1.874631	4.740752	-2.255432
1	1.118213	3.966987	-0.844288
1	-2.588812	-2.759051	-3.745853
1	-1.571034	-1.768454	-4.808428
1	-1.059935	-2.073906	-3.131986
1	3.201605	-1.637206	-4.301371
1	1.761526	-2.665212	-4.242357
1	1.640106	-0.953455	-3.768051
1	-2.620286	4.270824	-1.333424
1	-1.093929	4.791858	-0.595933
1	-1.143439	3.288184	-1.547755
1	2.197714	1.880205	2.377816
1	0.895736	0.735328	2.808484
1	1.826210	1.577939	4.075646
1	-1.974976	-3.225268	-0.136891
1	-0.513428	-2.491893	0.572238
1	-1.059720	-4.093892	1.110471
1	-2.235836	1.527025	-3.230784
1	-0.827592	0.501355	-2.889832
1	-1.427556	0.668114	-4.559454
1	2.334669	1.169882	-3.043892
1	0.903239	2.044244	-2.490943
1	1.971076	2.778202	-3.712373
1	1.454805	-3.039782	-0.603832
1	0.527874	-1.907978	-1.630625
1	0.875109	-3.550974	-2.199099
1	-0.919168	2.075411	1.991084
1	-0.010902	2.280463	0.473671

Gen-opt Structure 3ReTa_S
B3LYP/GBS(1) = -2978.393338 a.u.
B3LYP/GBS(2)//B3LYP/GBS(1) = -2991.931819 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -2989.721805 a.u.
Enthalpy Correction = 1.423565
Gibbs Free Energy Correction = 1.242596

Atomic No	x-coord	y-coord	z-coord
75	-2.392004	-0.063280	-0.023790
73	2.148756	-0.027414	-0.014131
6	-0.478272	-0.126009	0.010063
8	0.410643	-0.138105	-1.046369
8	0.388125	-0.090728	1.074853
7	-2.846866	-0.517124	1.836048
7	-3.015276	-1.457443	-1.279005
7	-2.687065	1.808640	-0.618192
7	3.014041	-1.624775	-0.858397
7	2.902634	1.592036	-0.979497
7	3.048536	0.110299	1.818218
6	2.534243	-3.062276	-0.764925
6	2.580405	2.235697	-2.340000
6	2.692027	0.918683	3.063156
6	-2.014809	3.143971	-0.478451
6	-2.305182	-1.393672	2.939542
6	-3.973604	1.901867	-1.261325
6	-4.071298	1.758612	-2.660086
6	-5.150318	2.147242	-0.531858
6	-5.302158	1.864827	-3.307007
6	-6.382776	2.249650	-1.182339
6	-6.465153	2.114076	-2.569040
6	-4.026628	0.212888	2.236660
6	-3.896378	1.477311	2.845007
6	-5.320809	-0.299294	2.035593
6	-5.020699	2.206041	3.234080
6	-6.444583	0.434968	2.421742
6	-6.302678	1.687115	3.023172
6	4.122070	-0.812197	2.112704
6	3.870006	-2.059284	2.713312
6	5.458624	-0.447104	1.881491
6	4.917555	-2.917832	3.052129
6	6.505979	-1.307048	2.220989
6	6.241742	-2.547320	2.805568
6	3.998102	2.300340	-0.351385
6	3.780598	3.477746	0.384225
6	5.321228	1.869895	-0.543546
6	4.851809	4.191613	0.925316
6	6.392049	2.586611	-0.003773
6	6.162946	3.749494	0.734722
6	-2.442884	-2.231527	-2.442795
6	4.110228	-1.472698	-1.783357
6	3.877763	-1.341317	-3.163297
6	5.437910	-1.528104	-1.328696
6	4.943222	-1.262191	-4.061826
6	6.501666	-1.443143	-2.230328
6	6.260177	-1.311152	-3.599487
6	-4.351021	-1.880806	-0.929859
6	-4.544296	-3.004087	-0.100632

6	-5.484107	-1.207218	-1.413374
6	-5.827494	-3.444204	0.222626
6	-6.768915	-1.643110	-1.078877
6	-6.948261	-2.763242	-0.265953
6	1.976606	-3.547503	-2.126262
6	-1.757272	-3.525141	-1.942781
6	3.945392	1.685023	3.567381
6	-2.921462	4.158074	0.274999
6	3.851439	2.233360	-3.234032
6	-3.446111	-2.202576	3.617556
6	3.692502	-3.993773	-0.330171
6	-3.555012	-2.622971	-3.455673
6	2.175686	0.009458	4.208062
6	-1.677811	3.732579	-1.873020
6	2.116674	3.706292	-2.172700
6	-1.602142	-0.528912	4.015073
6	1.405978	-3.142476	0.279197
6	-1.432029	-1.347738	-3.200239
6	-0.722777	2.986159	0.335065
6	1.593478	1.957703	2.753199
6	1.473910	1.475358	-3.099889
6	-1.299444	-2.406535	2.363112
1	-0.960626	-3.071262	3.167166
1	-3.168757	1.546350	-3.219963
1	-5.093040	2.254542	0.542069
1	-5.356962	1.749214	-4.384219
1	-7.277872	2.432528	-0.598111
1	-7.422006	2.198021	-3.071939
1	-2.901889	1.882502	2.985287
1	-5.438097	-1.269482	1.575154
1	-4.897972	3.179537	3.696815
1	-7.432513	0.022543	2.248542
1	-7.176886	2.252904	3.324897
1	2.848288	-2.348023	2.918824
1	5.659942	0.515202	1.434174
1	4.697623	-3.874928	3.512414
1	7.529992	-1.001382	2.034169
1	7.054466	-3.213034	3.071713
1	2.768803	3.831501	0.527895
1	5.498840	0.969442	-1.115771
1	4.660305	5.094457	1.494620
1	7.405748	2.236530	-0.167288
1	6.993664	4.306400	1.152130
1	2.859207	-1.295512	-3.523669
1	5.623579	-1.632503	-0.269302
1	4.742403	-1.158239	-5.122307
1	7.520109	-1.488275	-1.860057
1	7.086741	-1.249342	-4.297646
1	-3.675137	-3.507306	0.302679
1	-5.351612	-0.347187	-2.053359
1	-5.954737	-4.310959	0.862540
1	-7.627884	-1.102027	-1.459866
1	-7.946119	-3.102744	-0.012109
1	2.768454	-3.610939	-2.876352
1	1.544264	-4.545641	-1.995263
1	1.192721	-2.871411	-2.477244
1	-2.493967	-4.202449	-1.499482
1	-1.268905	-4.044485	-2.775768
1	-1.008697	-3.273791	-1.190584
1	3.654030	2.289953	4.433502
1	4.736041	0.998246	3.877895

1	4.328278	2.346585	2.787523
1	-2.371120	5.096288	0.410594
1	-3.834440	4.369616	-0.286830
1	-3.195701	3.761278	1.256386
1	3.583171	2.649142	-4.211765
1	4.643635	2.849953	-2.804406
1	4.223173	1.216995	-3.372936
1	-3.003295	-2.866037	4.369036
1	-4.167625	-1.548799	4.113111
1	-3.972631	-2.811667	2.876350
1	3.298408	-5.009542	-0.211589
1	4.484462	-4.015734	-1.083272
1	4.113876	-3.662563	0.620892
1	-3.080111	-3.105396	-4.317686
1	-4.279389	-3.317170	-3.023106
1	-4.084770	-1.730083	-3.801379
1	2.964932	-0.643940	4.587773
1	1.830847	0.644016	5.032453
1	1.334909	-0.593959	3.858558
1	-2.590114	3.906751	-2.450530
1	-1.153240	4.688388	-1.758559
1	-1.036355	3.039430	-2.423585
1	2.921670	4.336445	-1.788298
1	1.819975	4.090668	-3.154983
1	1.255707	3.765638	-1.504410
1	-2.318739	0.134017	4.509785
1	-1.147981	-1.174401	4.776697
1	-0.821241	0.068656	3.541255
1	1.741881	-2.778493	1.251719
1	0.532763	-2.572281	-0.039731
1	1.097050	-4.186650	0.396835
1	-1.945600	-0.467875	-3.603259
1	-0.635893	-1.009444	-2.540198
1	-1.005619	-1.917579	-4.035218
1	-0.937871	2.539963	1.308774
1	-0.012845	2.347692	-0.188618
1	-0.268355	3.972404	0.486665
1	1.862210	2.559189	1.883693
1	0.642384	1.466565	2.564443
1	1.494556	2.627313	3.615034
1	1.726498	0.422026	-3.225921
1	0.515862	1.531873	-2.588182
1	1.378399	1.929520	-4.092422
1	-1.773607	-3.010906	1.583001
1	-0.444486	-1.881581	1.945341

7. Extra calculations to determine effect of methyl groups in the experimental structure

7.1 Optimisation of Tantalum structures with Ar=3,5-$C_6H_3Me_2$

Gen-opt Structure 1Ta_T with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -1618.859382 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1625.667401 a.u.

Atomic No x-coord y-coord z-coord

Ta	0.109137	-0.531842	-0.539508
N	-1.726329	-1.221545	-0.984140
N	0.461933	1.333203	-1.271025
N	1.566779	-1.757399	0.119059
C	-2.483745	-1.569924	-2.216397
C	-1.478546	-1.695706	-3.381838
C	-3.230847	-2.919275	-2.058446
C	-3.509420	-0.456310	-2.551366
H	-0.950985	-0.748391	-3.534386
H	-0.742946	-2.478366	-3.167288
H	-2.010972	-1.952844	-4.304580
H	-3.958202	-2.866920	-1.243210
H	-3.762021	-3.157904	-2.986919
H	-2.516219	-3.721684	-1.846022
H	-4.056814	-0.706256	-3.467634
H	-4.226947	-0.338988	-1.733144
H	-2.985454	0.494195	-2.697572
C	1.678659	-3.234499	0.320456
C	0.659835	-3.932577	-0.606356
C	3.091686	-3.763304	-0.031054
C	1.355059	-3.577779	1.797168
H	0.903101	-3.727905	-1.654923
H	0.692269	-5.014953	-0.438784
H	-0.354338	-3.573687	-0.412339
H	3.853365	-3.320765	0.616419
H	3.110144	-4.850913	0.099529
H	3.333512	-3.533017	-1.074231
H	1.428541	-4.659203	1.960132
H	2.060161	-3.074368	2.466387
H	0.339615	-3.245820	2.037540
C	1.354918	1.821205	-2.367560
C	1.963761	0.604429	-3.100098
C	0.578963	2.670441	-3.408869
C	2.508536	2.674225	-1.776783
H	2.522924	-0.024553	-2.401523
H	1.178673	0.003269	-3.570468
H	2.649161	0.956189	-3.880166
H	0.161178	3.570335	-2.949382
H	1.258523	2.973749	-4.213622
H	-0.236936	2.079887	-3.840407
H	3.167882	3.024626	-2.579733
H	2.106677	3.544580	-1.248998
H	3.089975	2.071300	-1.072434
C	-0.227045	2.347413	-0.527819
C	0.278539	2.792795	0.708644
C	-1.447228	2.888077	-0.982489
C	-0.402200	3.746793	1.472626
H	1.213421	2.371629	1.061233
C	-2.142506	3.843883	-0.234261
H	-1.854041	2.535097	-1.923142
C	-1.610969	4.268281	0.991260
H	-2.143331	5.013561	1.575582
C	-2.450344	-1.129703	0.254697
C	-2.661126	-2.279410	1.052797
C	-2.914166	0.110044	0.736549
C	-3.291990	-2.194794	2.292349
H	-2.303420	-3.236343	0.691716
C	-3.539263	0.213030	1.988845

H	-2.756787	0.999356	0.137581
C	-3.722831	-0.939578	2.755354
H	-4.203232	-0.865477	3.726556
C	2.612733	-0.940630	0.670681
C	3.817871	-0.714960	-0.026602
C	2.419124	-0.294139	1.903304
C	4.801211	0.130278	0.487175
H	3.966638	-1.202239	-0.982385
C	3.394543	0.567455	2.432688
H	1.499298	-0.476921	2.449062
C	4.576772	0.768462	1.719532
H	5.337621	1.430374	2.122214
C	6.094116	0.377196	-0.272933
H	6.177663	1.431310	-0.563970
H	6.963981	0.128479	0.346506
H	6.135142	-0.231100	-1.181392
C	3.147198	1.272995	3.755523
H	4.063423	1.740785	4.128572
H	2.389625	2.057304	3.635266
H	2.782681	0.570243	4.513143
C	0.173543	4.236687	2.791502
H	0.923014	3.535511	3.170879
H	0.658651	5.213156	2.664107
H	-0.611120	4.344650	3.548366
C	-3.478522	4.384461	-0.718672
H	-4.307189	3.871970	-0.212593
H	-3.567717	5.455986	-0.509272
H	-3.594992	4.232485	-1.796202
C	-4.026149	1.565465	2.483413
H	-3.294135	2.345888	2.252240
H	-4.973547	1.834183	1.997137
H	-4.195074	1.549171	3.564953
C	-3.512002	-3.435716	3.142499
H	-3.101398	-3.297128	4.149611
H	-4.582843	-3.652394	3.243510
H	-3.028916	-4.308341	2.692183

Gen-opt Structure 1Ta_S with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -1618.850751 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1625.658591 a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	0.017751	-0.314636	-0.755967
N	-1.940613	-0.541840	-1.064201
N	0.840903	1.449275	-1.202970
N	1.181563	-1.893095	-0.332466
C	-2.915378	-0.292050	-2.168223
C	-2.138963	0.177588	-3.417839
C	-3.675102	-1.597879	-2.516163
C	-3.942319	0.800210	-1.773525
H	-1.593406	1.102366	-3.204221
H	-1.415083	-0.583447	-3.723307
H	-2.843908	0.360093	-4.237603
H	-4.257163	-1.946407	-1.657870
H	-4.359964	-1.416342	-3.352267

H	-2.960419	-2.375276	-2.805384
H	-4.630786	0.975006	-2.607966
H	-4.521597	0.492906	-0.897978
H	-3.426053	1.736585	-1.539319
C	1.084708	-3.370441	-0.532916
C	0.050300	-3.643810	-1.646662
C	2.436998	-3.983411	-0.975571
C	0.625865	-4.043751	0.785912
H	0.387383	-3.199570	-2.588283
H	-0.071258	-4.725028	-1.778083
H	-0.918962	-3.208304	-1.391088
H	3.206022	-3.843172	-0.211348
H	2.304015	-5.057835	-1.144574
H	2.772258	-3.520672	-1.909916
H	0.535544	-5.127386	0.646820
H	1.353392	-3.851843	1.581182
H	-0.343412	-3.636280	1.090596
C	1.863055	1.991501	-2.145892
C	2.300753	0.858151	-3.099701
C	1.264924	3.144646	-2.990880
C	3.101571	2.509471	-1.371638
H	2.719051	0.022379	-2.531635
H	1.444272	0.491340	-3.671789
H	3.064934	1.236637	-3.789041
H	0.944877	3.971961	-2.350700
H	2.019667	3.516513	-3.693091
H	0.402394	2.780295	-3.559281
H	3.855347	2.874241	-2.078846
H	2.822659	3.331081	-0.704816
H	3.531669	1.698764	-0.775249
C	0.275775	2.375209	-0.246837
C	0.867710	2.576675	1.016098
C	-0.893658	3.092641	-0.562515
C	0.304736	3.454479	1.945679
H	1.754700	2.007304	1.267710
C	-1.475780	3.974540	0.357627
H	-1.352560	2.938374	-1.532053
C	-0.871074	4.143020	1.608177
H	-1.319332	4.818316	2.330873
C	-2.497010	-0.851750	0.237457
C	-2.806133	-2.175385	0.592146
C	-2.731828	0.171221	1.180100
C	-3.324635	-2.483855	1.859053
H	-2.620482	-2.968760	-0.121134
C	-3.244264	-0.116051	2.445421
H	-2.482870	1.190892	0.912371
C	-3.536226	-1.450127	2.773996
H	-3.926203	-1.683172	3.760386
C	2.260447	-1.413450	0.491388
C	3.550555	-1.215424	-0.041230
C	2.029253	-1.076969	1.837181
C	4.584314	-0.694912	0.740765
H	3.727523	-1.456663	-1.081958
C	3.052899	-0.542203	2.634893
H	1.036805	-1.226176	2.245093
C	4.321015	-0.358066	2.077772
H	5.117959	0.054949	2.689282
C	2.766637	-0.145779	4.073419

H	3.693973	-0.040933	4.645356
H	2.236996	0.814863	4.105378
H	2.134565	-0.891185	4.568062
C	5.977793	-0.505544	0.162970
H	6.396718	0.462981	0.457615
H	6.655613	-1.289644	0.524124
H	5.957136	-0.552935	-0.930168
C	-3.481113	0.998430	3.451217
H	-2.902150	1.887479	3.182436
H	-4.542938	1.276198	3.480999
H	-3.187568	0.685410	4.459428
C	-3.633716	-3.927763	2.220830
H	-4.001302	-4.002919	3.248714
H	-4.398324	-4.342603	1.552739
H	-2.735191	-4.550277	2.131471
C	0.958656	3.660603	3.302174
H	1.367224	2.718667	3.682315
H	1.784599	4.380077	3.229748
H	0.238196	4.043444	4.032119
C	-2.735975	4.740458	-0.011866
H	-3.461669	4.083216	-0.504123
H	-3.208087	5.170516	0.876979
H	-2.502311	5.560651	-0.702573

Gen-opt Structure 2Ta_S with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -1807.504286 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1814.301834 a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	1.283368	-0.216255	-0.451748
O	2.680763	-0.896573	-1.768704
C	3.370591	-0.378276	-0.733544
O	4.567861	-0.287894	-0.589121
N	0.279626	0.879185	-1.785582
N	1.337706	0.840047	1.267402
N	0.523040	-2.013568	0.016722
C	0.832807	1.918979	-2.729612
C	2.235038	2.362094	-2.244024
C	0.968237	1.322794	-4.152497
C	-0.086719	3.164315	-2.773713
C	0.946858	-3.392172	-0.499139
C	2.385114	-3.710654	-0.021371
C	0.005014	-4.502397	0.036275
C	0.875148	-3.424720	-2.044431
C	2.410575	0.989623	2.330913
C	3.177552	-0.342453	2.513207
C	3.423872	2.091926	1.930570
C	1.772489	1.352662	3.697912
C	0.217317	1.736772	1.436734
C	-0.955369	1.288342	2.061540
C	0.289170	3.081113	1.021447
C	-2.035616	2.156757	2.279216
C	-0.778740	3.958707	1.221076
C	-1.939811	3.483981	1.851280
C	-1.090275	0.508232	-2.017431

C	-1.408869	-0.545703	-2.887356
C	-2.129184	1.199913	-1.371060
C	-2.741642	-0.910504	-3.119654
C	-3.465693	0.860490	-1.602972
C	-3.759966	-0.197046	-2.476704
C	-0.543606	-2.026598	0.981555
C	-0.274236	-2.199845	2.347206
C	-1.877550	-1.911433	0.557944
C	-1.310892	-2.259260	3.285520
C	-2.929571	-1.987248	1.478417
C	-2.634183	-2.157746	2.838344
H	2.203839	2.683662	-1.198079
H	2.971291	1.563453	-2.359024
H	2.568310	3.210962	-2.850951
H	-0.010577	1.032080	-4.544528
H	1.404478	2.071784	-4.823355
H	1.623673	0.446623	-4.126202
H	0.360398	3.911422	-3.438879
H	-1.079108	2.907776	-3.153078
H	-0.190938	3.593977	-1.773484
H	2.432383	-3.683613	1.072426
H	2.673450	-4.712646	-0.360389
H	3.098332	-2.991208	-0.426989
H	-1.028232	-4.331244	-0.276955
H	0.345666	-5.457163	-0.378416
H	0.032870	-4.563990	1.126756
H	1.160884	-4.421173	-2.400878
H	-0.149260	-3.216203	-2.369743
H	1.556117	-2.691712	-2.480490
H	2.479253	-1.157889	2.719674
H	3.776324	-0.580328	1.633874
H	3.856931	-0.242667	3.367647
H	2.926583	3.061354	1.831499
H	4.194822	2.180452	2.705257
H	3.910036	1.823224	0.988555
H	2.565280	1.383365	4.452862
H	1.280413	2.327676	3.668580
H	1.037056	0.595844	3.989819
H	-1.012309	0.260072	2.391600
H	1.187169	3.435426	0.532683
H	-2.771639	4.162561	2.017872
H	-0.604453	-1.086129	-3.371350
H	-1.882773	1.998101	-0.682982
H	-4.796183	-0.467266	-2.658238
H	0.756139	-2.278702	2.671410
H	-2.082695	-1.769188	-0.496010
H	-3.445430	-2.215355	3.558114
C	-3.276318	1.666562	3.007916
H	-3.382871	0.584484	2.895713
H	-3.204097	1.893256	4.079791
H	-4.178612	2.152851	2.621371
C	-0.696144	5.405666	0.761314
H	-1.435497	5.608343	-0.023288
H	-0.893985	6.090490	1.594229
H	0.296546	5.632688	0.360829
C	-3.063363	-2.053827	-4.068222
H	-2.419618	-2.917968	-3.868628
H	-4.106032	-2.368985	-3.963161

H	-2.903099	-1.749425	-5.110093
C	-4.584754	1.641084	-0.933122
H	-5.380648	0.972036	-0.588002
H	-4.202113	2.197928	-0.073163
H	-5.027862	2.357927	-1.636453
C	-4.373010	-1.916533	1.007795
H	-4.979014	-1.307757	1.688177
H	-4.426095	-1.479691	0.007268
H	-4.814375	-2.920922	0.970623
C	-0.992107	-2.414900	4.763757
H	-0.416712	-1.554182	5.126611
H	-1.908927	-2.486918	5.356511
H	-0.395518	-3.317007	4.942939

Gen-opt Structure 3Ta_S with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -3426.420000 a.u.
M06/GBS(2)//B3LYP/GBS(1) = a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	2.131291	-0.045495	-0.181362
Ta	-2.508092	-0.224537	-0.049591
C	-0.471169	-0.125825	-0.089328
O	0.393547	0.272781	0.885639
O	0.375591	-0.512831	-1.101123
N	-3.131576	1.070553	-1.489703
N	-2.911554	0.563450	1.756916
N	-3.145027	-2.094333	-0.573600
N	2.961688	1.104710	1.263138
N	2.912143	-1.880945	0.045470
N	2.963057	0.748677	-1.876379
C	2.477879	2.453441	1.765141
C	2.234146	-3.146502	0.544771
C	2.613621	0.650065	-3.360296
C	-2.735540	-3.080574	-1.630308
C	-2.460657	2.116543	-2.356550
C	-4.239811	-2.511068	0.258552
C	-4.089366	-3.512795	1.242611
C	-5.502060	-1.908067	0.113283
C	-5.155775	-3.894733	2.058820
C	-6.578700	-2.267842	0.936352
C	-6.397778	-3.263080	1.900734
C	-4.514548	0.867274	-1.855815
C	-4.875480	0.040339	-2.936051
C	-5.537422	1.521207	-1.148539
C	-6.212937	-0.129676	-3.309578
C	-6.882526	1.366265	-1.506707
C	-7.209742	0.539827	-2.588249
C	4.134384	1.577482	-1.676556
C	4.058680	2.979228	-1.705099
C	5.397500	0.980841	-1.524330
C	5.204205	3.774048	-1.568426
C	6.554821	1.756250	-1.397132
C	6.447847	3.153187	-1.414929
C	4.234148	-2.145804	-0.475847
C	4.422762	-2.512601	-1.816103

C	5.350363	-2.110393	0.378220
C	5.694431	-2.835806	-2.309482
C	6.625021	-2.441420	-0.091415
C	6.787358	-2.796915	-1.438613
C	-2.766636	-0.123464	3.094120
C	3.929537	0.512533	2.149270
C	3.516881	-0.355946	3.173466
C	5.291892	0.837424	2.045010
C	4.436834	-0.899734	4.077121
C	6.221102	0.337067	2.965943
C	5.785819	-0.538522	3.969156
C	-3.363329	1.923490	1.843570
C	-2.436796	2.971488	1.778269
C	-4.723398	2.231704	2.036383
C	-2.845578	4.307869	1.885357
C	-5.147375	3.557341	2.168730
C	-4.199755	4.588352	2.085606
C	1.750596	2.304221	3.124884
C	-2.044131	0.802771	4.104591
C	3.900702	0.436066	-4.206315
C	-3.981769	-3.610324	-2.386190
C	3.171916	-3.959122	1.475864
C	-3.410999	3.321954	-2.596114
C	3.668272	3.435668	1.930681
C	-4.141989	-0.536187	3.674406
C	1.914574	1.941703	-3.857333
C	-1.960637	-4.288723	-1.040169
C	1.825996	-4.027961	-0.661452
C	-2.041350	1.525756	-3.727092
C	1.488643	3.075996	0.753636
C	-1.887414	-1.375320	2.897115
C	-1.810167	-2.360870	-2.634161
C	1.672342	-0.541056	-3.653833
C	0.974361	-2.788242	1.354095
C	-1.208474	2.666330	-1.647232
H	-0.767594	3.456670	-2.266298
H	-3.123734	-3.982672	1.376676
H	-5.643809	-1.176648	-0.671125
H	-7.231512	-3.557122	2.531467
H	-4.099588	-0.482816	-3.478502
H	-5.264337	2.156912	-0.316535
H	-8.249728	0.421360	-2.877113
H	3.097141	3.457394	-1.834693
H	5.469464	-0.097503	-1.533180
H	7.342306	3.762097	-1.323857
H	3.569036	-2.537281	-2.479506
H	5.213004	-1.834331	1.413713
H	7.774749	-3.057500	-1.808504
H	2.463814	-0.597165	3.260464
H	5.614633	1.480814	1.236895
H	6.503115	-0.935446	4.681129
H	-1.389402	2.725928	1.656060
H	-5.443672	1.422849	2.067560
H	-4.523235	5.620152	2.185556
H	2.428339	1.924753	3.894397
H	1.377146	3.284958	3.442834
H	0.906053	1.620456	3.012754
H	-2.639797	1.689981	4.334495

H	-1.874081	0.244129	5.032257
H	-1.078537	1.116643	3.699507
H	3.604801	0.286569	-5.250589
H	4.570077	1.297293	-4.154551
H	4.441409	-0.449075	-3.860875
H	-3.660270	-4.262282	-3.206359
H	-4.631525	-4.182853	-1.717523
H	-4.555933	-2.774993	-2.796005
H	2.620052	-4.830237	1.846106
H	4.062424	-4.308213	0.949172
H	3.481739	-3.347188	2.328504
H	-2.867553	4.090023	-3.158041
H	-4.297042	3.033945	-3.166766
H	-3.727871	3.744611	-1.637279
H	3.271441	4.414582	2.223878
H	4.359569	3.097042	2.705807
H	4.208481	3.536792	0.985774
H	-3.988192	-1.099589	4.602667
H	-4.741867	0.347806	3.907990
H	-4.684156	-1.166302	2.965434
H	2.595284	2.795877	-3.824177
H	1.592992	1.802199	-4.896280
H	1.035571	2.150030	-3.244085
H	-2.617241	-4.925642	-0.441883
H	-1.551513	-4.895051	-1.857258
H	-1.134663	-3.930322	-0.421104
H	2.707782	-4.358575	-1.216839
H	1.290988	-4.914452	-0.302911
H	1.166438	-3.462814	-1.326169
H	-2.915760	1.199143	-4.296936
H	-1.515518	2.287810	-4.314653
H	-1.369140	0.676601	-3.574666
H	1.933160	3.127049	-0.241406
H	0.567932	2.497511	0.711174
H	1.250205	4.096248	1.075328
H	-2.346157	-2.062020	2.181182
H	-0.895734	-1.082067	2.547607
H	-1.791821	-1.908590	3.850313
H	-2.331555	-1.519680	-3.098516
H	-0.909408	-1.985971	-2.140834
H	-1.511426	-3.061295	-3.422600
H	2.092914	-1.474833	-3.272261
H	0.694167	-0.396472	-3.203005
H	1.560367	-0.630235	-4.740223
H	1.231707	-2.144662	2.199167
H	0.222711	-2.288472	0.741312
H	0.532009	-3.712274	1.743773
H	-1.485697	3.085140	-0.677304
H	-0.471478	1.879614	-1.493655
C	-6.615024	3.889222	2.384214
H	-6.732269	4.646714	3.167298
H	-7.064956	4.284106	1.464528
H	-7.178533	2.998930	2.680174
C	-1.817830	5.423817	1.794534
H	-1.035828	5.295225	2.552506
H	-1.334130	5.421899	0.810086
H	-2.285711	6.401521	1.945213
C	-7.972954	2.081886	-0.726184

H	-8.143019	1.591617	0.240642
H	-7.693394	3.122125	-0.529063
H	-8.917605	2.076896	-1.279324
C	-6.568845	-1.024132	-4.486294
H	-6.123921	-2.018349	-4.363911
H	-7.653247	-1.141723	-4.574763
H	-6.193120	-0.599947	-5.425554
C	-7.923809	-1.579658	0.774887
H	-7.936025	-0.629627	1.325562
H	-8.119679	-1.353740	-0.277738
H	-8.734994	-2.205299	1.161016
C	-4.965423	-4.951402	3.135166
H	-4.801054	-4.479452	4.112598
H	-5.849737	-5.592824	3.215737
H	-4.099492	-5.583677	2.915059
C	5.868008	-3.222628	-3.769332
H	5.570117	-2.395861	-4.425078
H	6.910882	-3.473189	-3.986095
H	5.247152	-4.090971	-4.019728
C	7.820898	-2.441785	0.846688
H	8.624957	-1.806876	0.456055
H	7.534648	-2.068085	1.832931
H	8.220446	-3.457040	0.962889
C	3.966518	-1.858690	5.159310
H	3.593174	-2.789307	4.714118
H	4.783959	-2.110819	5.841732
H	3.152658	-1.416614	5.745628
C	7.676992	0.769590	2.899786
H	7.807829	1.748071	3.379910
H	8.326529	0.051820	3.411229
H	8.010173	0.859606	1.861829
C	5.082206	5.289658	-1.575450
H	4.606005	5.641281	-0.651374
H	6.066873	5.761197	-1.651109
H	4.471558	5.630595	-2.419217
C	7.911448	1.088847	-1.240738
H	7.891591	0.073818	-1.648067
H	8.694198	1.662120	-1.749049
H	8.180646	1.016146	-0.179620

Gen-opt Structure 3Ta_T with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -3426.394683 a.u.
M06/GBS(2)//B3LYP/GBS(1) = a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	2.230771	-0.173557	0.028697
Ta	-2.549539	-0.095057	-0.091482
C	-0.380341	-0.112417	-0.109260
O	0.470610	0.760428	-0.646309
O	0.399512	-1.007337	0.528387
N	-3.032130	-2.076408	-0.123775
N	-3.338697	0.751582	-1.761793
N	-3.003565	1.022664	1.560849
N	3.081993	0.444359	-1.685247
N	2.870957	1.028290	1.511028

N	3.109744	-1.986916	0.371313
C	2.580922	0.101421	-3.073964
C	2.181818	2.133009	2.302551
C	2.741648	-3.157773	1.272940
C	-2.821116	0.645096	3.010678
C	-2.577476	-3.228378	-0.979520
C	-3.612276	2.306785	1.366269
C	-2.825668	3.421920	1.045802
C	-5.002798	2.490711	1.515510
C	-3.395478	4.690075	0.863453
C	-5.586102	3.751538	1.364549
C	-4.773138	4.845425	1.031180
C	-4.071736	-2.415566	0.809680
C	-3.799567	-3.125238	1.995582
C	-5.405184	-2.046007	0.546871
C	-4.817892	-3.450251	2.898334
C	-6.434446	-2.354586	1.443144
C	-6.131627	-3.060790	2.614167
C	4.287949	-2.270102	-0.418050
C	4.222141	-3.047302	-1.586250
C	5.545846	-1.813537	0.011674
C	5.375193	-3.366076	-2.315026
C	6.709393	-2.125155	-0.699546
C	6.614357	-2.901383	-1.862247
C	4.203890	0.766360	2.019573
C	4.420256	-0.128552	3.078116
C	5.303550	1.473227	1.501694
C	5.699357	-0.325514	3.614853
C	6.586209	1.301266	2.032327
C	6.774370	0.395313	3.085367
C	-2.728828	1.637932	-2.829879
C	4.053885	1.502218	-1.685443
C	3.651726	2.833417	-1.493931
C	5.411577	1.227824	-1.922019
C	4.579126	3.881554	-1.539024
C	6.346641	2.265676	-2.005171
C	5.921616	3.586637	-1.805088
C	-4.690626	0.349496	-2.048217
C	-4.971423	-0.675823	-2.973724
C	-5.766285	0.995929	-1.421619
C	-6.285228	-1.047885	-3.268255
C	-7.092661	0.639539	-1.705664
C	-7.341249	-0.380982	-2.628625
C	1.903962	1.331800	-3.726658
C	-1.994666	0.790751	-3.899007
C	4.011998	-3.729325	1.961336
C	-4.149415	0.165116	3.652194
C	3.115268	3.362715	2.469339
C	-3.791412	-3.933286	-1.638884
C	3.745447	-0.381910	-3.975787
C	-3.816301	2.498074	-3.527178
C	2.070459	-4.293006	0.457837
C	-2.280224	1.842963	3.834379
C	1.783074	1.610583	3.705784
C	-1.778081	-4.271972	-0.157706
C	1.537622	-1.034590	-2.974318
C	-1.724296	2.610021	-2.173285
C	-1.784919	-0.496807	3.088356

C	1.761813	-2.729655	2.393239
C	0.912393	2.622067	1.580254
C	-1.654150	-2.685246	-2.088298
H	-1.353302	-3.506122	-2.749901
H	-1.755521	3.288786	0.944460
H	-5.623061	1.630248	1.735456
H	-5.221340	5.826212	0.902633
H	-2.779767	-3.412551	2.218118
H	-5.631193	-1.536597	-0.380645
H	-6.927016	-3.313763	3.309054
H	3.261021	-3.404695	-1.932397
H	5.608681	-1.231010	0.920278
H	7.514983	-3.154962	-2.413329
H	3.583866	-0.679832	3.483592
H	5.143182	2.176141	0.697184
H	7.766733	0.261765	3.506247
H	2.602936	3.042098	-1.316218
H	5.726576	0.197549	-2.027793
H	6.644318	4.394848	-1.863299
H	-4.148704	-1.186564	-3.457462
H	-5.551296	1.787700	-0.715155
H	-8.365642	-0.655419	-2.862237
H	2.624060	2.141444	-3.873768
H	1.497976	1.043315	-4.703103
H	1.086142	1.684455	-3.093709
H	-2.693954	0.130741	-4.421340
H	-1.522786	1.448008	-4.639522
H	-1.218669	0.187425	-3.421592
H	3.705937	-4.522089	2.653057
H	4.709187	-4.150515	1.233754
H	4.523453	-2.943799	2.523860
H	-3.950985	-0.203124	4.666260
H	-4.862913	0.990368	3.726278
H	-4.586976	-0.643230	3.063301
H	2.559685	4.149913	2.990658
H	4.006608	3.120858	3.051500
H	3.424254	3.737929	1.489243
H	-3.434706	-4.719530	-2.314485
H	-4.435138	-4.387458	-0.880510
H	-4.381497	-3.210482	-2.208062
H	3.331579	-0.696131	-4.941028
H	4.465106	0.420625	-4.154635
H	4.257916	-1.227486	-3.510948
H	-3.321934	3.186478	-4.221917
H	-4.523596	1.881908	-4.088203
H	-4.368806	3.082739	-2.785120
H	2.779278	-4.751092	-0.236501
H	1.712362	-5.071100	1.142418
H	1.217288	-3.895284	-0.096972
H	-3.004062	2.661658	3.864602
H	-2.086660	1.508469	4.860181
H	-1.346278	2.212757	3.403547
H	2.668084	1.348063	4.290564
H	1.231667	2.390013	4.243829
H	1.138911	0.731937	3.606638
H	-2.425832	-4.793884	0.551102
H	-1.342480	-5.016490	-0.835291
H	-0.971997	-3.769898	0.384130

H	1.937987	-1.889785	-2.422148
H	0.624235	-0.678394	-2.498280
H	1.280951	-1.375607	-3.983547
H	-2.248072	3.237583	-1.447617
H	-0.919184	2.071034	-1.669146
H	-1.283864	3.249979	-2.948193
H	-2.127299	-1.369378	2.527250
H	-0.819106	-0.177003	2.691692
H	-1.655890	-0.801723	4.133409
H	2.172570	-1.897466	2.969077
H	0.798385	-2.431563	1.985739
H	1.620820	-3.579556	3.070542
H	1.143970	2.968641	0.570201
H	0.154293	1.842676	1.509165
H	0.493763	3.456273	2.154643
H	-2.170548	-1.926083	-2.682144
H	-0.756399	-2.244893	-1.648571
C	-2.510823	5.869858	0.494002
H	-1.734985	6.028342	1.252739
H	-2.011066	5.689282	-0.465566
H	-3.098665	6.788731	0.407380
C	-7.081145	3.948091	1.559538
H	-7.275815	4.626376	2.399380
H	-7.541135	4.382786	0.663838
H	-7.576040	2.995310	1.769202
C	-8.241566	1.360349	-1.019441
H	-8.278767	1.102623	0.046183
H	-8.122205	2.446575	-1.096850
H	-9.200558	1.085075	-1.469618
C	-6.565823	-2.182685	-4.239949
H	-6.557351	-3.147164	-3.715576
H	-7.546574	-2.062285	-4.711413
H	-5.806007	-2.222006	-5.027405
C	-7.863746	-1.929453	1.147704
H	-8.107964	-1.001324	1.681825
H	-7.998007	-1.746533	0.077737
H	-8.576621	-2.697388	1.467382
C	-4.489553	-4.175518	4.193442
H	-4.186904	-3.457807	4.967199
H	-5.359104	-4.726622	4.565969
H	-3.666446	-4.883434	4.050231
C	7.761186	2.104472	1.498911
H	8.565497	1.440995	1.159886
H	7.448867	2.725781	0.655996
H	8.169829	2.756766	2.280661
C	5.907715	-1.319010	4.746469
H	5.886651	-2.347153	4.363369
H	6.873029	-1.157797	5.236149
H	5.118361	-1.226175	5.500434
C	5.268738	-4.188092	-3.589681
H	4.884947	-3.572111	-4.413244
H	6.247093	-4.578712	-3.886191
H	4.585576	-5.034014	-3.455764
C	8.060408	-1.619379	-0.220011
H	8.321290	-0.685529	-0.733769
H	8.037485	-1.413058	0.854113
H	8.850796	-2.349406	-0.424666
C	7.799759	1.966147	-2.337751

H	7.927944	1.841021	-3.420611
H	8.455527	2.779426	-2.010704
H	8.126882	1.041838	-1.852416
C	4.123011	5.312614	-1.303030
H	3.793598	5.444854	-0.264886
H	4.935480	6.019740	-1.495838
H	3.281728	5.567526	-1.957546

Gen-opt Structure 4Ta_S with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -1694.228184 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1701.045562 a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	-0.017943	-0.091788	-1.482528
N	0.966842	1.599522	-0.999976
N	0.940007	-1.729015	-0.798673
N	-1.938421	-0.041602	-0.869464
C	1.975197	2.375440	-1.807051
C	2.640077	1.439579	-2.844233
C	1.289724	3.545912	-2.555493
C	3.088769	2.935396	-0.885015
H	3.122580	0.596842	-2.336064
H	1.907409	1.052244	-3.555350
H	3.406382	1.999755	-3.391396
H	0.844517	4.249474	-1.845730
H	2.026635	4.084727	-3.162154
H	0.508354	3.153526	-3.214858
H	3.832519	3.453876	-1.500072
H	2.685153	3.640020	-0.153410
H	3.581105	2.117089	-0.349287
C	-3.169977	0.366236	-1.636746
C	-2.776054	1.342842	-2.770481
C	-3.857395	-0.874320	-2.260654
C	-4.171603	1.094906	-0.704333
H	-2.284729	2.228186	-2.351186
H	-2.101272	0.866819	-3.484926
H	-3.682037	1.664838	-3.295727
H	-4.190502	-1.564254	-1.479681
H	-4.731711	-0.563747	-2.844296
H	-3.155262	-1.389830	-2.924285
H	-5.033789	1.421736	-1.295974
H	-4.523079	0.438892	0.096023
H	-3.698110	1.974187	-0.254872
C	1.133925	-3.066312	-1.464856
C	0.025576	-3.283578	-2.522406
C	2.514384	-3.133281	-2.164568
C	1.029998	-4.208673	-0.421471
H	-0.961943	-3.228662	-2.050153
H	0.081288	-2.533780	-3.314304
H	0.143438	-4.279040	-2.964604
H	3.321929	-3.026946	-1.434310
H	2.629956	-4.098184	-2.671567
H	2.590441	-2.332411	-2.907665
H	1.126730	-5.170727	-0.936530
H	1.817392	-4.133611	0.332938

H	0.057856	-4.173152	0.081263
C	1.678564	-1.535659	0.421319
C	1.073412	-1.787476	1.664733
C	3.004241	-1.071154	0.394739
C	1.781205	-1.605002	2.857905
H	0.043374	-2.119765	1.687140
C	3.725422	-0.872151	1.578248
H	3.460470	-0.841625	-0.560988
C	3.106049	-1.148794	2.802956
H	3.660577	-1.003941	3.725523
C	0.518150	2.243212	0.206319
C	-0.556202	3.147672	0.182724
C	1.137781	1.958782	1.435838
C	-1.002429	3.773410	1.353282
H	-1.059480	3.337897	-0.757805
C	0.714025	2.582401	2.614345
H	1.947933	1.240896	1.460087
C	-0.354832	3.488956	2.561238
H	-0.689441	3.975253	3.472956
C	-2.182984	-0.641643	0.415483
C	-2.433642	-2.019061	0.532273
C	-2.153323	0.143197	1.581428
C	-2.663187	-2.609812	1.780890
H	-2.421463	-2.631721	-0.361292
C	-2.391900	-0.426623	2.836821
H	-1.934434	1.199808	1.494834
C	-2.646276	-1.802857	2.924645
H	-2.829864	-2.251807	3.896446
O	-0.041219	-0.195214	-3.217423
C	-2.181902	4.731483	1.300158
H	-2.439282	5.092039	2.300741
H	-1.951842	5.600245	0.671619
H	-3.063582	4.234647	0.877179
C	1.416755	2.297107	3.931706
H	1.957837	1.348473	3.877858
H	2.137891	3.091905	4.163501
H	0.697999	2.243412	4.756871
C	-2.398086	0.438990	4.086177
H	-1.960495	-0.095096	4.936837
H	-1.827183	1.356261	3.917819
H	-3.425239	0.718048	4.355490
C	-2.910413	-4.106846	1.879777
H	-2.995742	-4.421371	2.924376
H	-3.836083	-4.385370	1.361621
H	-2.086282	-4.665401	1.419634
C	1.128689	-1.919611	4.194143
H	0.039507	-1.879236	4.105528
H	1.408525	-2.926304	4.531468
H	1.444651	-1.206427	4.963349
C	5.152762	-0.350853	1.520397
H	5.549018	-0.182097	2.526335
H	5.809456	-1.065161	1.009122
H	5.195531	0.597581	0.971238

Gen-opt Structure 5Ta_S with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -1732.223731 a.u.

M06/GBS(2)//B3LYP/GBS(1) = -1739.012951 a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	-0.123170	-0.491841	-0.786406
N	0.855816	-1.672247	0.512536
N	-2.139728	-0.186695	-1.036487
N	0.847629	1.236076	-1.218487
C	0.396657	-1.676965	-2.314841
O	0.696351	-2.418705	-3.182205
C	0.370345	-2.910168	1.220477
C	-0.930465	-3.391097	0.540187
C	1.423604	-4.040259	1.106112
C	0.083465	-2.614797	2.714283
C	1.832690	1.750654	-2.234221
C	2.174104	0.659627	-3.268329
C	1.261374	2.973336	-3.002902
C	3.149805	2.173550	-1.527899
C	-2.977396	-0.130693	-2.269947
C	-2.127362	0.555935	-3.367904
C	-3.368567	-1.539350	-2.797969
C	-4.242772	0.729452	-2.030240
C	-2.732971	-0.324732	0.238664
C	-2.215180	0.466813	1.292258
C	-3.739582	-1.268129	0.563711
C	-2.627735	0.284886	2.620348
C	-4.189415	-1.425225	1.874585
C	-3.616664	-0.659826	2.903433
C	2.231701	-1.322068	0.750170
C	3.206481	-1.654405	-0.203407
C	2.623804	-0.649921	1.919946
C	4.550074	-1.314809	-0.008895
C	3.966969	-0.319552	2.140088
C	4.918616	-0.652983	1.168555
C	0.443146	2.231216	-0.254112
C	-0.670976	3.056016	-0.488004
C	1.124648	2.361863	0.973492
C	-1.106678	3.983675	0.465836
C	0.711357	3.288223	1.936122
C	-0.406636	4.094355	1.671989
H	-1.718892	-2.636213	0.606447
H	-0.745335	-3.639134	-0.509599
H	-1.291730	-4.288785	1.054520
H	2.355301	-3.771112	1.609883
H	1.019741	-4.945555	1.572165
H	1.636975	-4.252663	0.053474
H	-0.316547	-3.517052	3.190898
H	1.000559	-2.329707	3.236822
H	-0.655301	-1.812583	2.802507
H	1.285012	0.350715	-3.824833
H	2.902577	1.069169	-3.977785
H	2.603687	-0.218951	-2.783578
H	1.048329	3.802691	-2.323189
H	1.993393	3.311608	-3.744954
H	0.339791	2.692183	-3.523801
H	3.876153	2.511094	-2.276423
H	2.969656	2.992685	-0.825783
H	3.568464	1.322290	-0.982505

H	-1.821848	1.553753	-3.043448
H	-1.228294	-0.030959	-3.589697
H	-2.711480	0.640183	-4.290897
H	-4.080770	-2.038719	-2.136997
H	-3.830857	-1.448284	-3.787884
H	-2.469112	-2.157160	-2.881230
H	-4.810458	0.819532	-2.962852
H	-4.887141	0.281896	-1.268801
H	-3.951039	1.730042	-1.693236
H	-1.548572	1.285119	1.048596
H	-4.154236	-1.897395	-0.211019
H	-3.959695	-0.792226	3.924879
H	2.900544	-2.177429	-1.101554
H	1.870131	-0.369160	2.645953
H	5.959341	-0.391097	1.330298
H	-1.216164	2.939332	-1.416335
H	1.973542	1.716478	1.161462
H	-0.733861	4.815351	2.415443
C	-2.340319	4.829083	0.195628
H	-3.234808	4.195684	0.146207
H	-2.490088	5.569549	0.987306
H	-2.249291	5.359904	-0.759024
C	1.451985	3.432367	3.255829
H	2.277845	2.718593	3.318874
H	1.866883	4.442190	3.360842
H	0.779595	3.253195	4.103634
C	-5.290365	-2.423053	2.196495
H	-5.018053	-3.041468	3.059291
H	-6.224116	-1.900107	2.439318
H	-5.482680	-3.083933	1.345826
C	-2.016636	1.127885	3.727455
H	-1.127014	0.632015	4.138444
H	-1.706294	2.103321	3.340923
H	-2.728678	1.277917	4.545513
C	4.377874	0.388600	3.420550
H	5.429286	0.688700	3.382470
H	3.771147	1.287202	3.577083
H	4.239070	-0.265577	4.290117
C	5.580556	-1.655733	-1.072345
H	5.384282	-1.089819	-1.991152
H	6.591176	-1.413175	-0.730341
H	5.547205	-2.722664	-1.321102

Gen-opt Structure 5Ta_T with Ar=3,5-$C_6H_3Me_2$
B3LYP/GBS(1) = -1732.228648 a.u.
M06/GBS(2)//B3LYP/GBS(1) = -1739.028538 a.u.

Atomic No	x-coord	y-coord	z-coord
Ta	-0.088066	0.064545	-1.321356
N	-1.594830	1.262607	-0.684401
N	1.772197	0.768946	-0.927862
N	-0.349175	-1.904218	-0.912860
C	-0.220116	0.155762	-3.322687
O	-0.298965	0.209879	-4.499642
C	-2.273116	2.477534	-1.251868

C	-1.433022	3.050114	-2.415839
C	-3.681236	2.113620	-1.789037
C	-2.411034	3.585659	-0.174537
C	-1.105551	-3.019169	-1.579916
C	-2.080619	-2.438494	-2.628727
C	-0.128461	-3.988193	-2.294668
C	-1.941951	-3.815770	-0.543632
C	3.071907	0.765765	-1.683123
C	2.986636	-0.219498	-2.870686
C	3.383972	2.180814	-2.234832
C	4.240124	0.310128	-0.768946
C	1.810805	1.461877	0.333768
C	2.095838	0.759292	1.520332
C	1.548616	2.840116	0.412839
C	2.138904	1.416620	2.753811
C	1.573752	3.513798	1.640713
C	1.874995	2.793316	2.802467
C	-2.146863	0.787285	0.557935
C	-3.212075	-0.129476	0.574279
C	-1.609375	1.220726	1.784940
C	-3.740952	-0.604495	1.781146
C	-2.132780	0.768034	3.000386
C	-3.196867	-0.145261	2.986594
C	0.410390	-2.300535	0.244776
C	1.733787	-2.756206	0.121188
C	-0.159062	-2.219012	1.530093
C	2.479322	-3.132501	1.245850
C	0.564514	-2.602628	2.663657
C	1.882965	-3.056419	2.509934
H	-0.410189	3.256904	-2.083524
H	-1.399450	2.359452	-3.260869
H	-1.886162	3.988195	-2.755889
H	-4.320856	1.749949	-0.979615
H	-4.152059	2.997912	-2.233858
H	-3.593876	1.336074	-2.555628
H	-2.878605	4.468588	-0.624113
H	-3.028905	3.249399	0.661948
H	-1.423627	3.863193	0.208362
H	-2.745997	-1.701898	-2.165967
H	-1.544379	-1.965180	-3.453705
H	-2.690415	-3.252395	-3.037252
H	0.545597	-4.459542	-1.573484
H	-0.692181	-4.774803	-2.809476
H	0.463603	-3.437017	-3.033159
H	-2.502579	-4.602011	-1.061362
H	-1.300864	-4.280514	0.209655
H	-2.649322	-3.149588	-0.039423
H	2.703273	-1.218187	-2.521382
H	2.262023	0.115546	-3.615613
H	3.969283	-0.283885	-3.351683
H	3.500756	2.896731	-1.416071
H	4.314632	2.159236	-2.813674
H	2.568991	2.510655	-2.887979
H	5.166985	0.288569	-1.352772
H	4.372620	0.993374	0.073701
H	4.043463	-0.693607	-0.378819
H	2.286051	-0.305174	1.464575
H	1.305027	3.377839	-0.495953

```
H      1.905847    3.310610    3.757097
H     -3.611142   -0.483322   -0.369191
H     -0.780272    1.917131    1.775091
H     -3.608002   -0.501626    3.926651
H      2.181324   -2.796428   -0.864963
H     -1.174361   -1.856100    1.630059
H      2.451037   -3.356268    3.385853
C      3.914536   -3.607472    1.083615
H      4.521231   -2.838794    0.589952
H      4.366413   -3.828259    2.055436
H      3.958582   -4.515827    0.470877
C     -0.074123   -2.552711    4.042110
H      0.598085   -2.083335    4.769466
H     -1.005432   -1.980669    4.011376
H     -0.302552   -3.565429    4.398334
C     -4.882546   -1.608719    1.769109
H     -4.593669   -2.513344    1.220577
H     -5.159311   -1.899458    2.787020
H     -5.768872   -1.187219    1.279965
C     -1.573590    1.277107    4.318925
H     -2.253813    2.012468    4.767694
H     -1.444470    0.456900    5.034114
H     -0.603959    1.757519    4.161986
C      2.484394    0.656294    4.023995
H      2.479199   -0.420882    3.836932
H      3.480662    0.940344    4.386151
H      1.761930    0.873302    4.819262
C      1.269653    5.002473    1.698533
H      0.279364    5.210161    1.275733
H      1.284082    5.365223    2.730762
H      2.007822    5.574705    1.123820
```

7.2 The effect of the extra methyl groups in Ar=3,5-$C_6H_3Me_2$

Comparison of relative energies of the intermediates for the tantalum reaction (kJ mol^{-1}).
(These relative energies are based on uncorrected electronic energies at the M06/GBS2//B3LYP/GBS1 level of theory.)

	Ar=C_6H_5 (shown in Figure 5 in manuscript)	Ar=3,5-$C_6H_3Me_2$
1_T + CO_2	0.0	0.0
1_S + CO_2	22.4	23.1
2_S	-181.6	-189.9
3_S	-395.3	[a]
3_T	-345.1	[a]
4_S + CO	-268.6	-274.3
4_S + 5_S	-411.6	-424.3
4_S + 5_T	-452.7	-465.2

[a] Calculations had not completed as at time of submission of manuscript.