Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Theoretical mechanism studies on the competitive CO-induced N-N bond cleavage of N_2O with N-O bond cleavage mediated by (η^5-C_5Me_5)Mo[N(^{i}Pr)C(Me)N(^{i}Pr)](CO)$_2$

Nan Lu* and Huatian Wang*

College of Chemistry and Material Science, Shandong Agricultural University, Taian City 271018, Shandong Prov. P. R. China

Full Gaussian 09 Reference

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

Theoretical Calculations.

All calculations were carried out using DFT as implemented in Gaussian 09. We chose to use the popular B3LYP functional, which includes Becke's three-parameter hybrid functional combined with the Lee−Yang−Parr correction for correlation. The standard 6-31G(d,p) basis set was used for H, C, N, and O atoms, while the effective core potentials (ECPs) of Hay and Wadt were combined with double-ζvalence basis sets (LanL2DZ) for Molybdenum. All structures studied in this paper were optimized. Frequencies were analyzed at the same level to characterize the nature of stationary points (energy minima or first-order saddle-points) and to provide free energies at 298.15 K and 1 atm pressure, which include entropic contributions by considering the vibrations, rotations, and translations of the structures. When necessary, the intrinsic reaction coordinate (IRC) calculations were performed to verify the right connections among a transition state and its forward, backward minima.

To consider the solvent effect on reaction, single-point calculations with self-consistent reaction field based on the integral equation formalism polarizable continuum model (IEFPCM) with UAKS radii and cavity-dispersion-solvent-structure terms in Truhlar and co-workers' SMD solvation model for benzene were applied for all gas-phase optimized structures at B3LYP/6-311++G(d,p) level. For all cited energies, ZPE corrections were taken into account. In order to evaluate the direction and magnitude of the donor–acceptor interactions for some stationary points, natural bond orbital (NBO) analysis was also performed. The Los Alamos National Laboratory 2-Double-Zeta (LanL2DZ) basis set was used for the Mo atom, and the other atoms were computed with 6-311++G(d,p) basis sets.

Table S1 Calculated relative energies (all in kcal mol^{-1}, relative to **Cat-B**+N_2O) for the ZPE-corrected Gibbs free energies (ΔGgas), relative solvation energies (ΔGsolv) and Gibbs free energies (ΔGsol) for all species in benzene at 298 K by B3LYP/6-311++G(d,p)//B3LYP/6-31G(d,p) method.

Species	ΔGgas	ΔGsol	ΔGsolv
1/2**Cat-A** + 2CO – 1/2N_2 + N_2O	-274.9	-289.4	4.5
Cat-B + N_2O	0.0	-19.0	0.0
Int0 + N_2O	37.2	17.9	-0.2
Int1 + CO	39.1	21.1	0.9
TS1 + CO	49.5	34.2	3.7
Int2 + CO	-33.7	-48.4	4.3
TS2 + CO	-23.0	-37.4	4.6
Int3 + CO	-40.0	-54.0	4.9
Int4 + CO + N_2	-48.2	-62.2	5.0
TS3 + CO + N_2	-36.2	-50.8	4.4
Int5 + CO + N_2	-43.1	-59.9	2.2
TS4 + CO + N_2	-22.4	-39.4	1.9
Int6 + CO + N_2	-39.7	-59.3	0.6
Int7+ N_2	-32.6	-51.9	-0.3
TS5 + N_2	-20.7	-40.6	-0.9
Int8 + N_2	-48.0	-66.5	0.4
TS6 + N_2	-47.1	-63.6	2.5
Int9 + N_2	-18.5	-65.1	2.4
TS7 + CO	46.2	29.0	1.7
Int10 + CO	27.7	10.4	1.7
TS8 + CO	58.2	36.9	-2.2
Int11 + CO	54.6	33.1	-2.5
TS9 + CO	85.5	66.9	0.5
TS10 + CO	66.7	50.2	2.5
Int12 + CO	19.2	1.5	1.2
Int13 + CO	-14.4	-34.9	-1.6

Table S2 The donor–acceptor orbital interactions and their second-order perturbation stabilization energies ($\Delta E_{i\text{-}j^*}^{(2)}$)

	Bond	Donor	Acceptor	Interaction	$\Delta E_{i\text{-}j^*}^{(2)}$ (kcal mol^{-1})
TS1	N1-N2⋯O1	BD(1)N1-N2	RY*(3)O1	σ→n*	1.3
	O1⋯Mo	LP(1)O1	LP*(2)Mo	n→n*	6.8
	N1⋯N2-O1	LP(1)N1	BD*(1)N2-O1	n→σ*	11.0
TS7	N2-N1⋯Mo	BD(1)N2-N1	LP*(3)Mo	σ→n*	3.6
	O1-N2⋯N2-N1	BD(1)O1-N2	BD*(1)N2-N1	σ→σ*	2.8
TS10	C1-N1⋯N2	BD (3)C1-N1	RY*(3)N2	σ→n*	2.2
	O1-N2⋯N1	BD(1)O1-N2	RY*(1)N1	σ→n*	2.0
	O2-C1⋯C1-N1	BD(1)O2-C1	BD*(1)C1-N1	σ→σ*	139.8

Fig. S1 Evolution of the energy changes along the IRC for (a) **TS1** (b) **TS7** (c) **TS8** (d) **TS10** and with Scan calculation along (e) Mo-C bond in **Cat-B** (f) Mo-N2 bond in **Int13** at B3LYP/6-31G(d,p) level.

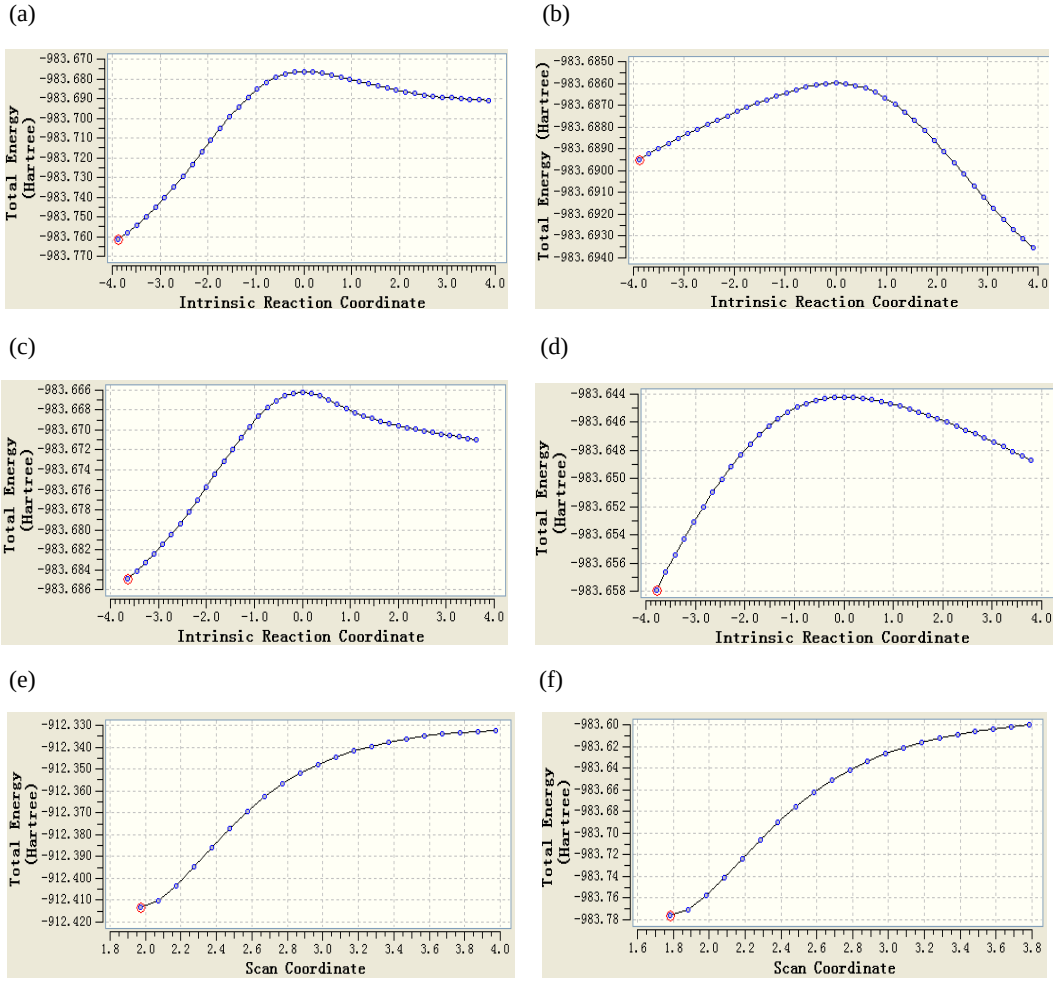
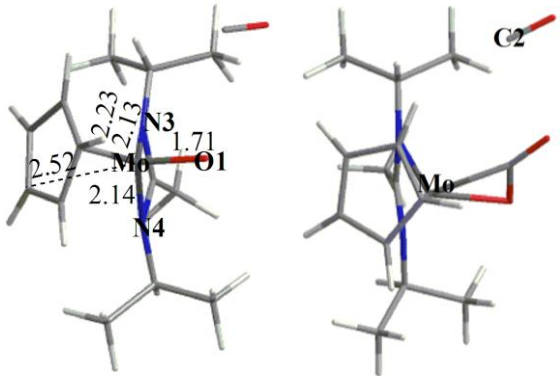


Fig. S2 Optimized structures and selected geometric parameters of **Int4** and **Int7**.



Int4 **Int7**

Optimized Cartesian coordinates (in Å)

Optimized Cartesian coordinates for **Cat-A**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.320539	1.080442	-2.084450
2	6	0	-4.161551	2.197727	-1.244150
3	6	0	-2.850283	2.734718	-1.425599
4	6	0	-2.205991	1.919903	-2.421687
5	6	0	-3.113204	0.877787	-2.824072
6	1	0	-5.190635	0.436912	-2.115894
7	1	0	-4.889099	2.549050	-0.524128
8	1	0	-2.460923	3.638174	-0.977167
9	1	0	-1.218603	2.088848	-2.832756
10	1	0	-2.957798	0.149723	-3.608339
11	42	0	-2.363764	0.564386	-0.625069
12	7	0	-3.400049	-1.214993	0.007978
13	7	0	-3.176888	0.463693	1.380443
14	6	0	-3.656430	-2.523662	-0.585620
15	6	0	-5.147660	-2.911367	-0.608719
16	6	0	-3.126676	1.220513	2.623702
17	6	0	-3.865963	2.558140	2.475338
18	6	0	-3.580850	-0.802994	1.264212
19	6	0	-4.124581	-1.619687	2.418744
20	6	0	-2.764205	-3.639604	-0.009940
21	6	0	-1.670704	1.439914	3.064144
22	7	0	-0.612273	0.131109	-0.450469
23	7	0	0.610767	-0.125484	-0.447970
24	1	0	-3.355029	-2.397555	-1.631764
25	1	0	-5.295104	-3.806397	-1.224995
26	1	0	-5.745930	-2.099661	-1.036851
27	1	0	-5.544332	-3.131035	0.388399
28	1	0	-3.635742	0.648058	3.412426
29	1	0	-3.841460	3.121122	3.415963
30	1	0	-4.913762	2.396636	2.197927
31	1	0	-3.395010	3.168544	1.697267
32	1	0	-4.983355	-1.116023	2.876256
33	1	0	-3.359609	-1.736619	3.194942
34	1	0	-4.439827	-2.611510	2.100991
35	1	0	-2.876442	-4.558138	-0.598932
36	1	0	-1.713097	-3.334850	-0.043260
37	1	0	-3.015301	-3.880510	1.029019

38	1	0	-1.160462	0.481649	3.208940
39	1	0	-1.124657	1.994001	2.292926
40	1	0	-1.626684	2.004818	4.003733
41	6	0	4.318264	-1.085543	-2.073200
42	6	0	4.156221	-2.200303	-1.230112
43	6	0	2.844237	-2.735515	-1.411869
44	6	0	2.202694	-1.922145	-2.410884
45	6	0	3.112332	-0.882869	-2.815058
46	1	0	5.189497	-0.443571	-2.105159
47	1	0	4.882106	-2.550895	-0.508058
48	1	0	2.452639	-3.637056	-0.961587
49	1	0	1.215310	-2.090054	-2.822397
50	1	0	2.959167	-0.156554	-3.601379
51	42	0	2.361876	-0.562302	-0.617519
52	7	0	3.401644	1.216283	0.013003
53	7	0	3.172007	-0.458648	1.388974
54	6	0	3.663232	2.522680	-0.583367
55	6	0	5.155762	2.905418	-0.605183
56	6	0	3.116123	-1.211417	2.634473
57	6	0	3.838645	-2.558192	2.487415
58	6	0	3.579472	0.806739	1.270439
59	6	0	4.123889	1.624390	2.423942
60	6	0	2.773741	3.642984	-0.011941
61	6	0	1.658894	-1.412292	3.079835
62	1	0	3.363015	2.394970	-1.629658
63	1	0	5.307079	3.798557	-1.223267
64	1	0	5.751972	2.090777	-1.030610
65	1	0	5.551717	3.126023	0.392016
66	1	0	3.634352	-0.643038	3.420191
67	1	0	3.809016	-3.118876	3.429252
68	1	0	4.887803	-2.410232	2.207653
69	1	0	3.358547	-3.164125	1.711452
70	1	0	4.980645	1.119292	2.883657
71	1	0	3.358202	1.745002	3.198873
72	1	0	4.442343	2.614648	2.104547
73	1	0	2.889933	4.559627	-0.603112
74	1	0	1.721692	3.341604	-0.046249
75	1	0	3.023884	3.885769	1.026800
76	1	0	1.160470	-0.447613	3.223412
77	1	0	1.104054	-1.962152	2.311872
78	1	0	1.611005	-1.973932	4.021194

Optimized Cartesian coordinates for **Cat-B**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.087702	-1.654026	-2.270085
2	6	0	1.248535	-0.856525	-2.389602
3	6	0	2.236062	-1.368710	-1.497065
4	6	0	1.680798	-2.508363	-0.834031
5	6	0	0.340392	-2.671799	-1.302706
6	1	0	-0.842968	-1.500756	-2.799033
7	1	0	1.356946	0.012010	-3.024176
8	1	0	3.245290	-0.997300	-1.385876
9	1	0	2.199902	-3.162426	-0.147525
10	1	0	-0.340830	-3.462219	-1.018993
11	42	0	0.495779	-0.664809	-0.027065
12	7	0	-1.500602	0.227121	-0.131654
13	7	0	0.244201	1.517381	-0.264064
14	6	0	-2.859929	-0.292609	-0.001643
15	6	0	-3.721865	-0.078425	-1.260710
16	6	0	1.027889	2.748643	-0.264349
17	6	0	2.351417	2.546953	-1.010392
18	6	0	-1.086906	1.487959	-0.248369
19	6	0	-1.954918	2.722749	-0.354782
20	1	0	-4.656701	-0.643279	-1.176514
21	1	0	-3.192379	-0.427180	-2.152717
22	1	0	-3.986311	0.971511	-1.417684
23	1	0	2.925265	3.479154	-1.031801
24	1	0	2.175477	2.230280	-2.042807
25	1	0	2.961425	1.784586	-0.516028
26	1	0	-1.755648	3.250521	-1.293714
27	1	0	-1.740968	3.418068	0.462911
28	1	0	-3.013828	2.477934	-0.322781
29	6	0	-3.571070	0.165703	1.285274
30	1	0	-2.951125	-0.053191	2.158687
31	1	0	-3.788819	1.238166	1.281639
32	1	0	-4.522638	-0.364771	1.400813
33	1	0	-2.724959	-1.376314	0.092341
34	1	0	0.462019	3.517547	-0.812196
35	6	0	1.275152	3.277306	1.160695
36	1	0	0.332547	3.432099	1.695039
37	1	0	1.874487	2.569251	1.738566
38	1	0	1.808868	4.234041	1.130096
39	6	0	1.798628	-0.193915	1.384266
40	8	0	2.582094	0.054618	2.209696
41	6	0	-0.273019	-1.519506	1.576581

42	8	0	-0.739795	-2.038590	2.509276

Optimized Cartesian coordinates for **Int0**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.078791	0.182572	2.537215
2	6	0	0.008170	-1.236330	2.528204
3	6	0	1.258150	-1.727220	2.075170
4	6	0	2.126054	-0.608042	1.838234
5	6	0	1.390564	0.582398	2.140162
6	1	0	-0.727070	0.850125	2.812352
7	1	0	-0.858404	-1.830409	2.785149
8	1	0	1.521526	-2.771339	1.958847
9	1	0	3.174231	-0.657192	1.577364
10	1	0	1.771134	1.593220	2.110667
11	42	0	0.466822	-0.390298	0.223504
12	7	0	-1.160402	0.925090	-0.336503
13	7	0	-1.228167	-1.188731	-0.836609
14	6	0	-1.379801	2.369203	-0.304880
15	6	0	-2.610625	2.788552	0.519980
16	6	0	-1.823946	-2.479183	-1.174254
17	6	0	-1.363634	-3.566980	-0.197346
18	6	0	-1.908248	-0.027286	-0.879706
19	6	0	-3.315088	0.108289	-1.417255
20	1	0	-2.615772	3.875004	0.660090
21	1	0	-2.590972	2.318521	1.508226
22	1	0	-3.552893	2.515076	0.036291
23	1	0	-1.797630	-4.534752	-0.469562
24	1	0	-1.664922	-3.329475	0.826626
25	1	0	-0.272394	-3.669457	-0.214759
26	1	0	-4.049699	-0.258416	-0.689699
27	1	0	-3.437226	-0.476239	-2.333034
28	1	0	-3.559880	1.144668	-1.643087
29	6	0	-1.359679	3.004598	-1.706948
30	1	0	-0.449406	2.716396	-2.238284
31	1	0	-2.220470	2.701605	-2.311459
32	1	0	-1.380338	4.096932	-1.626063
33	1	0	-0.504261	2.759978	0.225350
34	1	0	-2.918896	-2.412248	-1.096663
35	6	0	-1.471646	-2.862987	-2.622680
36	1	0	-1.805995	-2.095823	-3.327690
37	1	0	-0.386359	-2.963446	-2.732943

38	1	0	-1.938191	-3.814543	-2.901587
39	6	0	2.336091	3.900791	0.443400
40	8	0	2.171333	4.641305	-0.403504
41	6	0	1.434876	0.704119	-1.050212
42	8	0	2.023902	1.405628	-1.786267

Optimized Cartesian coordinates for **Int1**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.238262	-0.939109	2.563651
2	6	0	-0.957359	-1.552277	2.101065
3	6	0	-0.612411	-2.619283	1.215479
4	6	0	0.814894	-2.633103	1.098163
5	6	0	1.329082	-1.586678	1.932364
6	1	0	0.300485	-0.104310	3.249151
7	1	0	-1.959481	-1.272851	2.396685
8	1	0	-1.299942	-3.323653	0.768759
9	1	0	1.402584	-3.360797	0.555965
10	1	0	2.375536	-1.350266	2.082075
11	42	0	0.047919	-0.673711	0.091632
12	7	0	0.127731	1.434125	-0.025001
13	7	0	-1.763653	0.460800	-0.465506
14	6	0	1.084595	2.413824	0.498362
15	6	0	0.587463	3.210539	1.717332
16	6	0	-3.166870	0.269680	-0.819469
17	6	0	-4.060320	0.231718	0.433345
18	6	0	-1.181034	1.637823	-0.313854
19	6	0	-1.879379	2.973342	-0.426507
20	1	0	1.418156	3.766087	2.165850
21	1	0	0.179937	2.537330	2.478217
22	1	0	-0.186964	3.937046	1.455816
23	1	0	-5.115671	0.148905	0.151540
24	1	0	-3.939249	1.135420	1.038871
25	1	0	-3.808392	-0.631888	1.056948
26	1	0	-2.420439	3.219120	0.494557
27	1	0	-2.610268	2.958597	-1.239584
28	1	0	-1.170505	3.775314	-0.628270
29	6	0	1.649611	3.326062	-0.606411
30	1	0	2.032686	2.724089	-1.434459
31	1	0	0.895093	4.011897	-1.004736
32	1	0	2.473283	3.931127	-0.212040
33	1	0	1.929092	1.803961	0.844723

34	1	0	-3.490711	1.124322	-1.431460
35	6	0	-3.354012	-0.993065	-1.665898
36	1	0	-2.754169	-0.950717	-2.577339
37	1	0	-3.051305	-1.883593	-1.106197
38	1	0	-4.406908	-1.104564	-1.946002
39	6	0	-0.091165	-1.342495	-1.731888
40	8	0	-0.161013	-1.744938	-2.830638
41	7	0	4.155495	-0.366753	-0.964448
42	7	0	4.084928	-1.481842	-1.155772
43	8	0	4.230377	0.807326	-0.757727

Optimized Cartesian coordinates for **TS1**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.876947	-1.159488	-2.258310
2	6	0	0.501621	-1.413482	-2.027714
3	6	0	0.620339	-2.488765	-1.085358
4	6	0	-0.699795	-2.870420	-0.712734
5	6	0	-1.611259	-2.042444	-1.433275
6	1	0	-1.287371	-0.413384	-2.924740
7	1	0	1.322748	-0.899623	-2.505315
8	1	0	1.536672	-2.965175	-0.768048
9	1	0	-0.967533	-3.661725	-0.026486
10	1	0	-2.689739	-2.076415	-1.344997
11	42	0	-0.235656	-0.660912	0.116917
12	7	0	-0.255605	1.502543	-0.032976
13	7	0	1.656823	0.480385	0.097003
14	6	0	-1.316930	2.485755	-0.213790
15	6	0	-1.320280	3.150612	-1.603108
16	6	0	3.106562	0.312873	0.195219
17	6	0	3.739944	-0.026489	-1.167244
18	6	0	1.063403	1.669397	-0.037110
19	6	0	1.814566	2.977900	-0.143463
20	1	0	-2.228785	3.748070	-1.736233
21	1	0	-1.294167	2.389909	-2.389328
22	1	0	-0.464384	3.816106	-1.751819
23	1	0	4.833239	-0.026061	-1.094147
24	1	0	3.450630	0.700217	-1.933639
25	1	0	3.430640	-1.020368	-1.506099
26	1	0	2.595128	2.923232	-0.908011
27	1	0	2.302462	3.215607	0.808754
28	1	0	1.150197	3.802062	-0.393113

29	6	0	-1.393409	3.509249	0.934525
30	1	0	-1.405708	2.993367	1.898760
31	1	0	-0.546563	4.202420	0.931738
32	1	0	-2.308745	4.105467	0.850534
33	1	0	-2.244059	1.900460	-0.154966
34	1	0	3.536708	1.269147	0.524489
35	6	0	3.494552	-0.732835	1.246375
36	1	0	3.121127	-0.460181	2.235241
37	1	0	3.086156	-1.716092	0.992391
38	1	0	4.584789	-0.822529	1.299424
39	6	0	0.360494	-1.015155	1.953607
40	8	0	0.719502	-1.263415	3.035275
41	7	0	-3.285757	-0.250130	0.758616
42	7	0	-4.368068	-0.578816	0.584787
43	8	0	-2.060144	-0.667056	1.129575

Optimized Cartesian coordinates for **Int2**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.829729	-1.182843	-2.217490
2	6	0	0.555331	-1.380503	-1.944243
3	6	0	0.678868	-2.505082	-1.084059
4	6	0	-0.635782	-3.020278	-0.862144
5	6	0	-1.552928	-2.216822	-1.575092
6	1	0	-1.247712	-0.400336	-2.836830
7	1	0	1.365422	-0.765889	-2.306318
8	1	0	1.600404	-2.936884	-0.719637
9	1	0	-0.885716	-3.863792	-0.232139
10	1	0	-2.630011	-2.308347	-1.538602
11	42	0	-0.341096	-0.737383	0.233531
12	7	0	-0.132369	1.350070	-0.095856
13	7	0	1.849478	0.427337	0.228585
14	6	0	-1.197193	2.306095	-0.420106
15	6	0	-1.036079	3.004787	-1.782566
16	6	0	3.306897	0.330116	0.286465
17	6	0	3.924480	0.152686	-1.114023
18	6	0	1.194551	1.545626	-0.050923
19	6	0	1.866551	2.875634	-0.320875
20	1	0	-1.965024	3.522235	-2.044805
21	1	0	-0.823487	2.273453	-2.568678
22	1	0	-0.236180	3.750004	-1.785891
23	1	0	5.018671	0.147823	-1.055888

24	1	0	3.627823	0.959074	-1.792107
25	1	0	3.607992	-0.797428	-1.556694
26	1	0	2.147440	2.961919	-1.375866
27	1	0	2.779136	2.971040	0.271108
28	1	0	1.214438	3.712601	-0.076355
29	6	0	-1.467355	3.297425	0.726034
30	1	0	-1.624132	2.756532	1.663399
31	1	0	-0.641027	4.000006	0.874461
32	1	0	-2.366736	3.885421	0.513044
33	1	0	-2.094400	1.683529	-0.500663
34	1	0	3.724218	1.253779	0.717589
35	6	0	3.735813	-0.821948	1.203539
36	1	0	3.396473	-0.666142	2.229389
37	1	0	3.323516	-1.772933	0.849430
38	1	0	4.827026	-0.909489	1.213874
39	6	0	0.541015	-0.618020	2.071462
40	8	0	0.977191	-0.572099	3.138710
41	7	0	-4.641304	0.405281	0.289402
42	7	0	-5.049132	-0.246465	1.082868
43	8	0	-1.799101	-1.014480	1.100855

Optimized Cartesian coordinates for **TS2**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.317049	-1.042947	-2.043674
2	6	0	0.009401	-0.655847	-2.450670
3	6	0	0.909018	-1.646633	-2.039200
4	6	0	0.182531	-2.679950	-1.366492
5	6	0	-1.194979	-2.324991	-1.425181
6	1	0	-2.236998	-0.532683	-2.292381
7	1	0	0.271100	0.277850	-2.929408
8	1	0	1.983468	-1.605609	-2.143399
9	1	0	0.595193	-3.596176	-0.968487
10	1	0	-2.010152	-2.896840	-1.004468
11	42	0	-0.294195	-0.715903	0.035424
12	7	0	-0.206494	1.390913	0.006574
13	7	0	1.728263	0.391422	0.230302
14	6	0	-1.254601	2.387855	-0.213939
15	6	0	-0.967696	3.380600	-1.355140
16	6	0	3.171223	0.233016	0.403778
17	6	0	3.945297	0.532885	-0.894890
18	6	0	1.117636	1.563480	0.167479

19	6	0	1.806627	2.907082	0.260383
20	1	0	-1.876528	3.942869	-1.594721
21	1	0	-0.650954	2.851360	-2.259478
22	1	0	-0.194413	4.108975	-1.095521
23	1	0	5.025010	0.449158	-0.728028
24	1	0	3.739772	1.541021	-1.265735
25	1	0	3.670000	-0.175487	-1.682640
26	1	0	2.060082	3.283406	-0.736094
27	1	0	2.733669	2.830161	0.831916
28	1	0	1.164371	3.643563	0.743816
29	6	0	-1.666148	3.098246	1.088478
30	1	0	-1.901704	2.361356	1.861328
31	1	0	-0.873819	3.750416	1.471286
32	1	0	-2.553194	3.719205	0.921175
33	1	0	-2.118774	1.792396	-0.528901
34	1	0	3.527568	0.940634	1.170006
35	6	0	3.507873	-1.175472	0.905705
36	1	0	3.049505	-1.376382	1.876136
37	1	0	3.152782	-1.935487	0.203217
38	1	0	4.591718	-1.287768	1.013217
39	6	0	0.594021	-0.974025	2.569831
40	8	0	0.600954	-1.475865	3.595057
41	7	0	-4.496817	-0.066854	0.022751
42	7	0	-4.759111	-0.523880	0.993896
43	8	0	-1.517981	-1.223078	1.128793

Optimized Cartesian coordinates for **Int3**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.177145	-2.122273	-2.114138
2	6	0	-0.824424	-1.313638	-2.647350
3	6	0	-0.263622	-0.033557	-2.984433
4	6	0	1.143142	-0.111456	-2.701085
5	6	0	1.411718	-1.384156	-2.089660
6	1	0	0.036338	-3.112159	-1.700355
7	1	0	-1.873071	-1.569989	-2.715385
8	1	0	-0.767853	0.765817	-3.508434
9	1	0	1.876604	0.655251	-2.917839
10	1	0	2.383141	-1.773997	-1.819939
11	42	0	0.224026	0.074272	-0.673249
12	7	0	-0.140186	-1.267038	0.935146
13	7	0	-1.746200	0.000583	0.170427

14	6	0	0.710984	-2.118917	1.766479
15	6	0	0.116723	-3.518277	2.007167
16	6	0	-2.956308	0.818925	0.161968
17	6	0	-3.594562	0.803969	-1.231303
18	6	0	-1.358271	-0.777496	1.185275
19	6	0	-2.197210	-1.016641	2.420234
20	1	0	0.865885	-4.168004	2.471948
21	1	0	-0.188100	-3.972537	1.059518
22	1	0	-0.755258	-3.499972	2.667749
23	1	0	-4.517060	1.393843	-1.237188
24	1	0	-3.837100	-0.218074	-1.537637
25	1	0	-2.909972	1.230303	-1.970786
26	1	0	-3.157073	-1.463565	2.141970
27	1	0	-2.408624	-0.067238	2.921600
28	1	0	-1.702629	-1.676075	3.128980
29	6	0	1.173280	-1.431963	3.063484
30	1	0	1.602557	-0.451657	2.837511
31	1	0	0.352702	-1.287677	3.773399
32	1	0	1.938454	-2.037529	3.561289
33	1	0	1.607762	-2.263878	1.154641
34	1	0	-3.680366	0.375579	0.860610
35	6	0	-2.660642	2.253807	0.627625
36	1	0	-2.249213	2.264152	1.642051
37	1	0	-1.924545	2.722111	-0.032994
38	1	0	-3.572709	2.860787	0.621206
39	6	0	0.848220	4.311988	0.911798
40	8	0	0.815312	4.029426	2.013914
41	7	0	4.341113	0.216225	0.080573
42	7	0	4.479036	1.298851	0.253304
43	8	0	0.961613	1.430266	0.060528

Optimized Cartesian coordinates for **Int4**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.377452	0.050378	2.832879
2	6	0	-0.359211	-1.320626	2.585067
3	6	0	0.919095	-1.679628	2.033100
4	6	0	1.713811	-0.482440	2.017504
5	6	0	0.888427	0.613244	2.445411
6	1	0	-1.232335	0.618920	3.174823
7	1	0	-1.197906	-1.994192	2.699037
8	1	0	1.267642	-2.682788	1.832890

9	1	0	2.758120	-0.416997	1.738746
10	1	0	1.210383	1.632330	2.607094
11	42	0	0.308938	-0.183956	0.304978
12	7	0	-1.428574	0.998394	-0.021844
13	7	0	-1.449460	-1.140350	-0.465488
14	6	0	-1.715275	2.432670	0.024038
15	6	0	-3.054331	2.762977	0.707817
16	6	0	-1.787980	-2.395527	-1.131632
17	6	0	-1.649597	-3.567062	-0.153075
18	6	0	-2.081598	0.020881	-0.657946
19	6	0	-3.330424	0.160284	-1.498624
20	1	0	-3.129412	3.841790	0.880912
21	1	0	-3.125239	2.256583	1.675188
22	1	0	-3.920707	2.467498	0.108473
23	1	0	-1.931019	-4.507522	-0.638089
24	1	0	-2.293151	-3.423043	0.720106
25	1	0	-0.615792	-3.656265	0.193899
26	1	0	-4.131784	-0.462686	-1.088243
27	1	0	-3.137004	-0.182420	-2.519667
28	1	0	-3.680842	1.188262	-1.542129
29	6	0	-1.549948	3.127945	-1.338656
30	1	0	-0.573696	2.887493	-1.768498
31	1	0	-2.320936	2.827377	-2.055271
32	1	0	-1.615691	4.215007	-1.219785
33	1	0	-0.929405	2.831924	0.674447
34	1	0	-2.841160	-2.350509	-1.444057
35	6	0	-0.925642	-2.608265	-2.386311
36	1	0	-1.064885	-1.794799	-3.105594
37	1	0	0.134838	-2.632429	-2.117240
38	1	0	-1.183714	-3.551585	-2.880264
39	6	0	2.804032	2.800351	-0.595810
40	8	0	2.461772	3.226176	-1.593854
41	8	0	1.285343	0.093312	-1.069435

Optimized Cartesian coordinates for **TS3**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.425650	-1.560850	2.140223
2	6	0	-0.952651	-1.623268	1.916329
3	6	0	-1.193076	-2.456003	0.772315
4	6	0	0.077565	-2.941297	0.327825
5	6	0	1.087071	-2.342095	1.151867

6	1	0	0.916075	-0.953613	2.889670
7	1	0	-1.706173	-1.065471	2.453223
8	1	0	-2.159419	-2.769655	0.402938
9	1	0	0.241315	-3.668905	-0.455583
10	1	0	2.150718	-2.522142	1.085822
11	42	0	-0.021264	-0.768525	-0.407137
12	7	0	0.780906	1.035677	0.361913
13	7	0	-1.389365	0.803723	0.180123
14	6	0	2.129570	1.581707	0.530114
15	6	0	2.386420	2.149990	1.937652
16	6	0	-2.760056	1.195377	-0.147446
17	6	0	-3.748868	0.119232	0.310687
18	6	0	-0.397194	1.671947	0.378505
19	6	0	-0.614173	3.156097	0.562623
20	1	0	3.452174	2.369694	2.061998
21	1	0	2.096870	1.423690	2.702879
22	1	0	1.837814	3.077218	2.129186
23	1	0	-4.775934	0.433865	0.099816
24	1	0	-3.662240	-0.067432	1.384856
25	1	0	-3.565656	-0.820556	-0.218815
26	1	0	0.290468	3.663526	0.888038
27	1	0	-1.397654	3.334236	1.304881
28	1	0	-0.941925	3.609247	-0.378542
29	6	0	2.536396	2.554686	-0.590450
30	1	0	2.359729	2.099472	-1.568939
31	1	0	1.980256	3.496204	-0.547313
32	1	0	3.601971	2.796114	-0.511902
33	1	0	2.779516	0.706502	0.431387
34	1	0	-2.995949	2.114538	0.409766
35	6	0	-2.926075	1.490157	-1.648690
36	1	0	-2.262554	2.297994	-1.972636
37	1	0	-2.677081	0.605587	-2.240736
38	1	0	-3.957451	1.787244	-1.869406
39	6	0	2.206143	-1.488832	-1.507222
40	8	0	3.174510	-1.041902	-1.924548
41	8	0	-0.167914	-0.402948	-2.076593

Optimized Cartesian coordinates for **Int5**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.751210	-0.999949	-1.808368
2	6	0	0.916467	0.359824	-2.112757

3	6	0	2.199062	0.780592	-1.624437
4	6	0	2.825385	-0.357975	-1.040351
5	6	0	1.907229	-1.459592	-1.137058
6	1	0	-0.140322	-1.583178	-1.995668
7	1	0	0.184811	1.000228	-2.579141
8	1	0	2.656035	1.748772	-1.778571
9	1	0	3.838389	-0.404103	-0.663679
10	1	0	2.089536	-2.467909	-0.791001
11	42	0	1.151829	0.463960	0.472756
12	7	0	-0.843682	-0.066096	0.762416
13	7	0	-0.581474	1.948849	-0.123503
14	6	0	-1.443284	-1.216553	1.448842
15	6	0	-2.522085	-1.937618	0.618987
16	6	0	-0.862106	3.361344	-0.349457
17	6	0	-0.250992	3.817542	-1.680544
18	6	0	-1.429532	1.120016	0.444062
19	6	0	-2.873509	1.467336	0.744618
20	1	0	-2.785528	-2.887594	1.096571
21	1	0	-2.148729	-2.154482	-0.386389
22	1	0	-3.444209	-1.358327	0.516725
23	1	0	-0.455239	4.879224	-1.854486
24	1	0	-0.664056	3.251161	-2.521273
25	1	0	0.835311	3.679631	-1.673343
26	1	0	-3.341991	1.931624	-0.127502
27	1	0	-2.922828	2.187899	1.567889
28	1	0	-3.461306	0.596783	1.022447
29	6	0	-1.899959	-0.907605	2.886335
30	1	0	-1.094110	-0.416036	3.439248
31	1	0	-2.778303	-0.256365	2.917875
32	1	0	-2.158662	-1.835726	3.407868
33	1	0	-0.613789	-1.924983	1.538413
34	1	0	-1.948306	3.525316	-0.416683
35	6	0	-0.329146	4.213011	0.816783
36	1	0	-0.797904	3.924200	1.762185
37	1	0	0.748968	4.069321	0.930405
38	1	0	-0.528096	5.276534	0.642200
39	6	0	2.122848	-0.973849	1.578300
40	8	0	2.608990	-1.772939	2.253494
41	8	0	1.392617	1.476480	1.844730

Optimized Cartesian coordinates for **TS4**.

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	0.804038	-1.431513	-1.864954
2	6	0	1.967171	-0.625079	-1.813645
3	6	0	2.815442	-1.134559	-0.802175
4	6	0	2.173550	-2.265647	-0.230002
5	6	0	0.917339	-2.466663	-0.878887
6	1	0	-0.034150	-1.287535	-2.531424
7	1	0	2.155794	0.244604	-2.426634
8	1	0	3.761975	-0.717079	-0.487276
9	1	0	2.554984	-2.850205	0.595986
10	1	0	0.241753	-3.297606	-0.734517
11	42	0	0.631165	-0.484743	0.357664
12	7	0	-1.421019	-0.145521	-0.337596
13	7	0	-0.020958	1.490662	-0.091422
14	6	0	-2.642689	-0.951151	-0.327456
15	6	0	-3.305542	-1.072328	-1.712410
16	6	0	0.569834	2.824861	-0.169218
17	6	0	1.564565	2.955089	-1.332645
18	6	0	-1.274167	1.166197	-0.443637
19	6	0	-2.305836	2.171259	-0.898242
20	1	0	-4.108631	-1.816225	-1.678056
21	1	0	-2.579230	-1.393545	-2.465138
22	1	0	-3.746598	-0.129905	-2.051378
23	1	0	1.938788	3.981952	-1.403600
24	1	0	1.094122	2.696031	-2.286922
25	1	0	2.421881	2.292674	-1.179391
26	1	0	-1.960144	2.694382	-1.795802
27	1	0	-2.471873	2.923789	-0.120703
28	1	0	-3.257007	1.695347	-1.124626
29	6	0	-3.634942	-0.524931	0.768415
30	1	0	-3.134602	-0.489251	1.739570
31	1	0	-4.073205	0.458355	0.568567
32	1	0	-4.457737	-1.245231	0.831691
33	1	0	-2.293536	-1.954794	-0.060810
34	1	0	-0.240451	3.546255	-0.341309
35	6	0	1.231489	3.173748	1.170878
36	1	0	0.501024	3.139846	1.984237
37	1	0	2.024749	2.455989	1.404021
38	1	0	1.670182	4.176720	1.137581
39	6	0	-0.243841	-0.672167	2.147489
40	8	0	-0.805540	-0.737596	3.179425
41	8	0	1.440014	-0.676445	2.019951

Optimized Cartesian coordinates for **Int6**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.840628	-1.586225	-1.896839
2	6	0	1.067753	-0.385565	-2.598983
3	6	0	2.284955	0.196428	-2.121775
4	6	0	2.800422	-0.678813	-1.100171
5	6	0	1.885093	-1.774156	-0.948209
6	1	0	-0.035321	-2.212347	-1.997412
7	1	0	0.407477	0.052134	-3.334760
8	1	0	2.758220	1.086889	-2.511516
9	1	0	3.730222	-0.562666	-0.559856
10	1	0	2.000012	-2.606649	-0.269592
11	42	0	0.937660	0.274789	-0.264952
12	7	0	-1.008309	-0.329915	0.113169
13	7	0	-0.699307	1.702705	-0.647117
14	6	0	-1.558694	-1.513105	0.780496
15	6	0	-2.740834	-2.143779	0.022078
16	6	0	-0.935533	3.111739	-0.935940
17	6	0	-0.271502	3.477242	-2.268999
18	6	0	-1.574274	0.884175	-0.092073
19	6	0	-2.982003	1.278521	0.292905
20	1	0	-2.982299	-3.120543	0.454269
21	1	0	-2.489997	-2.290843	-1.033122
22	1	0	-3.647629	-1.533613	0.068036
23	1	0	-0.445391	4.530058	-2.514016
24	1	0	-0.667064	2.862940	-3.083874
25	1	0	0.809834	3.313376	-2.211056
26	1	0	-3.523822	1.637047	-0.588077
27	1	0	-2.957807	2.095450	1.020474
28	1	0	-3.539343	0.450957	0.723526
29	6	0	-1.856175	-1.289170	2.273617
30	1	0	-0.977445	-0.878113	2.777776
31	1	0	-2.694602	-0.604826	2.435125
32	1	0	-2.110548	-2.241574	2.751075
33	1	0	-0.737144	-2.236061	0.737552
34	1	0	-2.017218	3.280670	-1.045506
35	6	0	-0.423497	4.007510	0.204238
36	1	0	-0.920817	3.770839	1.149473
37	1	0	0.649570	3.857220	0.352814
38	1	0	-0.602743	5.063763	-0.025620
39	6	0	1.834488	0.133690	1.569761
40	8	0	2.533736	-0.380726	2.408543

41	8	0	1.212442	1.296407	1.474466

Optimized Cartesian coordinates for **Int7**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.592885	-1.311616	-2.170220
2	6	0	0.847994	-0.133735	-2.902263
3	6	0	2.057260	0.453616	-2.409199
4	6	0	2.534653	-0.394917	-1.347600
5	6	0	1.608726	-1.479893	-1.188986
6	1	0	-0.286172	-1.933099	-2.274802
7	1	0	0.212849	0.284510	-3.670765
8	1	0	2.550032	1.326856	-2.813356
9	1	0	3.448214	-0.266762	-0.782631
10	1	0	1.694264	-2.278851	-0.467142
11	42	0	0.657468	0.605449	-0.602107
12	7	0	-1.316395	0.053754	-0.303260
13	7	0	-0.924695	2.059621	-1.092918
14	6	0	-1.925213	-1.097656	0.368664
15	6	0	-3.202657	-1.607770	-0.321902
16	6	0	-1.107018	3.459262	-1.458280
17	6	0	-0.260722	3.776009	-2.696996
18	6	0	-1.846184	1.273767	-0.568305
19	6	0	-3.277473	1.674030	-0.290972
20	1	0	-3.477935	-2.585922	0.086044
21	1	0	-3.043232	-1.721821	-1.398960
22	1	0	-4.056970	-0.941549	-0.173217
23	1	0	-0.396378	4.818823	-3.001188
24	1	0	-0.540398	3.132405	-3.536759
25	1	0	0.801267	3.616604	-2.482297
26	1	0	-3.920437	1.380703	-1.128212
27	1	0	-3.362669	2.753122	-0.158888
28	1	0	-3.655735	1.187981	0.607880
29	6	0	-2.112956	-0.885171	1.881312
30	1	0	-1.170069	-0.581015	2.343429
31	1	0	-2.864161	-0.120627	2.104238
32	1	0	-2.441210	-1.817736	2.353217
33	1	0	-1.173699	-1.887280	0.260233
34	1	0	-2.160161	3.627053	-1.728558
35	6	0	-0.748745	4.389498	-0.287540
36	1	0	-1.379827	4.190447	0.584095
37	1	0	0.289681	4.231286	0.017235

38	1	0	-0.876667	5.439466	-0.573648
39	6	0	1.456229	0.486431	1.275339
40	8	0	2.087575	-0.024542	2.172307
41	8	0	0.883194	1.666982	1.120382
42	6	0	2.293351	-2.994195	2.095663
43	8	0	2.571038	-3.110327	3.192189

Optimized Cartesian coordinates for **TS5**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.692042	-0.320521	-2.394625
2	6	0	1.942539	0.250548	-1.971714
3	6	0	2.631285	-0.784659	-1.271541
4	6	0	1.848228	-1.981972	-1.297696
5	6	0	0.661194	-1.696226	-1.995229
6	1	0	-0.075522	0.191647	-2.958717
7	1	0	2.317132	1.235188	-2.209602
8	1	0	3.595126	-0.691161	-0.789107
9	1	0	2.108558	-2.915355	-0.818671
10	1	0	-0.153650	-2.386876	-2.161512
11	42	0	0.668334	-0.136717	-0.123714
12	7	0	-1.450031	-0.302381	-0.115725
13	7	0	-0.543878	1.676151	-0.012057
14	6	0	-2.425641	-1.383682	-0.271635
15	6	0	-3.070582	-1.433712	-1.670675
16	6	0	-0.353690	3.110612	0.162418
17	6	0	0.888101	3.574997	-0.606343
18	6	0	-1.691154	1.031876	-0.063603
19	6	0	-3.053976	1.682794	-0.032546
20	1	0	-3.662804	-2.348578	-1.782359
21	1	0	-2.308858	-1.424326	-2.455264
22	1	0	-3.741140	-0.587149	-1.848592
23	1	0	1.020858	4.655907	-0.494022
24	1	0	0.792803	3.350931	-1.673577
25	1	0	1.782680	3.074630	-0.224871
26	1	0	-2.997384	2.723227	-0.355835
27	1	0	-3.452032	1.670235	0.987664
28	1	0	-3.763428	1.160806	-0.674711
29	6	0	-3.489615	-1.433014	0.841868
30	1	0	-3.024123	-1.360012	1.828129
31	1	0	-4.228172	-0.631717	0.752565
32	1	0	-4.032380	-2.382944	0.792379

33	1	0	-1.829698	-2.296762	-0.167286
34	1	0	-1.219121	3.645935	-0.256684
35	6	0	-0.248591	3.461813	1.656767
36	1	0	-1.155958	3.165371	2.193251
37	1	0	0.598513	2.936744	2.105951
38	1	0	-0.110305	4.540452	1.791405
39	6	0	2.052980	-0.557269	1.417622
40	8	0	2.771484	-1.356129	1.967503
41	8	0	1.787570	0.692628	1.483336
42	6	0	-0.260512	-1.862138	2.228973
43	8	0	-0.471171	-2.980395	2.314065

Optimized Cartesian coordinates for **Int8**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.429564	-2.586381	-1.488867
2	6	0	1.495618	-1.769974	-1.960969
3	6	0	2.592100	-1.968254	-1.097286
4	6	0	2.222289	-2.928453	-0.099070
5	6	0	0.877660	-3.324588	-0.350650
6	1	0	-0.553706	-2.648392	-1.930882
7	1	0	1.455139	-1.093015	-2.802610
8	1	0	3.541021	-1.450882	-1.146290
9	1	0	2.865116	-3.322932	0.675234
10	1	0	0.323070	-4.082596	0.183972
11	42	0	0.784083	-1.067006	0.339740
12	7	0	-1.372707	-0.811483	0.055436
13	7	0	-0.034254	0.873948	-0.240059
14	6	0	-2.561811	-1.603276	0.384051
15	6	0	-3.385769	-2.007929	-0.854448
16	6	0	0.455109	2.197153	-0.612884
17	6	0	1.660435	2.090283	-1.556759
18	6	0	-1.295019	0.478125	-0.304085
19	6	0	-2.443316	1.356480	-0.747109
20	1	0	-4.167795	-2.718703	-0.566320
21	1	0	-2.756604	-2.488431	-1.609040
22	1	0	-3.877320	-1.152004	-1.326608
23	1	0	2.012626	3.087782	-1.839879
24	1	0	1.393332	1.551280	-2.471382
25	1	0	2.484633	1.562094	-1.069355
26	1	0	-2.262934	1.738913	-1.756940
27	1	0	-2.547581	2.219673	-0.081982

28	1	0	-3.386595	0.816018	-0.756699
29	6	0	-3.445416	-0.976649	1.479509
30	1	0	-2.849072	-0.732082	2.360954
31	1	0	-3.948908	-0.066892	1.139091
32	1	0	-4.222375	-1.687259	1.781468
33	1	0	-2.159922	-2.531956	0.804452
34	1	0	-0.340803	2.729339	-1.152932
35	6	0	0.800337	3.011086	0.645543
36	1	0	-0.071711	3.102061	1.300885
37	1	0	1.598067	2.518691	1.207841
38	1	0	1.132747	4.019425	0.374365
39	6	0	0.020386	-1.283262	2.128578
40	8	0	-0.474396	-1.504784	3.160659
41	6	0	2.429758	-0.899923	1.875927
42	8	0	2.918871	-1.438894	2.823074
43	8	0	2.527278	0.075377	1.104189

Optimized Cartesian coordinates for **TS6**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.042975	-1.556633	-2.199689
2	6	0	0.914258	-0.587112	-2.595192
3	6	0	2.108927	-0.856036	-1.885537
4	6	0	1.909253	-2.020107	-1.069421
5	6	0	0.563716	-2.459871	-1.273914
6	1	0	-1.066710	-1.605244	-2.543949
7	1	0	0.746380	0.233333	-3.278885
8	1	0	3.022267	-0.277808	-1.949199
9	1	0	2.663391	-2.537933	-0.492237
10	1	0	0.113478	-3.351110	-0.860035
11	42	0	0.483712	-0.425410	-0.122659
12	7	0	-1.657907	-0.182991	-0.010535
13	7	0	-0.399261	1.589143	-0.081602
14	6	0	-2.764032	-1.092477	0.288584
15	6	0	-3.841802	-1.129604	-0.812535
16	6	0	-0.027354	2.984499	-0.285807
17	6	0	1.037631	3.117934	-1.383548
18	6	0	-1.655831	1.153267	-0.046400
19	6	0	-2.872270	2.053640	-0.074636
20	1	0	-4.541330	-1.951642	-0.625203
21	1	0	-3.387950	-1.288027	-1.795697
22	1	0	-4.425978	-0.205867	-0.860263

23	1	0	1.304300	4.169769	-1.533638
24	1	0	0.670292	2.718925	-2.333908
25	1	0	1.946788	2.572760	-1.111719
26	1	0	-3.025867	2.468303	-1.077969
27	1	0	-2.749753	2.893393	0.615233
28	1	0	-3.776086	1.516481	0.204576
29	6	0	-3.365661	-0.883418	1.690612
30	1	0	-2.580210	-0.922850	2.448642
31	1	0	-3.883975	0.076264	1.781067
32	1	0	-4.093041	-1.673103	1.909443
33	1	0	-2.299929	-2.084994	0.297288
34	1	0	-0.908917	3.549203	-0.620999
35	6	0	0.456347	3.611144	1.033845
36	1	0	-0.314922	3.535461	1.806715
37	1	0	1.347574	3.091385	1.397897
38	1	0	0.704577	4.669842	0.896926
39	6	0	0.202540	-1.199105	1.623620
40	8	0	-0.001288	-1.749521	2.643044
41	6	0	2.832978	-0.131602	1.513955
42	8	0	3.342014	-0.850624	2.277033
43	8	0	2.461992	0.719778	0.772691

Optimized Cartesian coordinates for **Int9**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.177002	-1.534937	-2.416056
2	6	0	1.145611	-0.525994	-2.640015
3	6	0	2.258260	-0.806993	-1.806852
4	6	0	2.004495	-2.022336	-1.091754
5	6	0	0.699505	-2.475471	-1.472005
6	1	0	-0.797817	-1.586450	-2.881453
7	1	0	1.036674	0.326976	-3.295529
8	1	0	3.154000	-0.203673	-1.727036
9	1	0	2.700703	-2.545532	-0.451085
10	1	0	0.231702	-3.401156	-1.167602
11	42	0	0.446985	-0.538074	-0.225143
12	7	0	-1.697081	-0.406184	-0.243202
13	7	0	-0.555814	1.452414	-0.206526
14	6	0	-2.765439	-1.387586	-0.054596
15	6	0	-3.768507	-1.445707	-1.222794
16	6	0	-0.300873	2.869405	-0.473267
17	6	0	1.016258	3.059608	-1.235274

18	6	0	-1.780906	0.923884	-0.285414
19	6	0	-3.049245	1.732231	-0.455625
20	1	0	-4.420711	-2.319036	-1.112730
21	1	0	-3.244468	-1.534010	-2.179675
22	1	0	-4.410193	-0.561395	-1.272055
23	1	0	1.190536	4.121944	-1.436940
24	1	0	0.995854	2.528283	-2.190374
25	1	0	1.863660	2.681287	-0.654704
26	1	0	-3.216854	1.972919	-1.512734
27	1	0	-2.993918	2.674109	0.094763
28	1	0	-3.921039	1.185782	-0.099650
29	6	0	-3.460555	-1.262774	1.313454
30	1	0	-2.719188	-1.288073	2.115758
31	1	0	-4.034251	-0.334993	1.405143
32	1	0	-4.155247	-2.096926	1.461941
33	1	0	-2.245773	-2.351765	-0.048363
34	1	0	-1.100767	3.269745	-1.113862
35	6	0	-0.299144	3.692433	0.828590
36	1	0	-1.231644	3.559233	1.384950
37	1	0	0.520947	3.386888	1.486730
38	1	0	-0.177208	4.760188	0.613889
39	6	0	0.163297	-1.501512	1.424402
40	8	0	-0.006650	-2.171060	2.377014
41	6	0	1.682212	0.910730	2.084943
42	8	0	1.311291	1.214022	3.145335
43	8	0	2.173470	0.658797	1.037933

Optimized Cartesian coordinates for **TS7**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.794403	-1.400688	2.358212
2	6	0	-0.554095	-1.375585	1.937721
3	6	0	-0.745806	-2.390770	0.940390
4	6	0	0.508969	-3.048688	0.749667
5	6	0	1.454383	-2.415031	1.611985
6	1	0	1.250438	-0.750779	3.092486
7	1	0	-1.311848	-0.697780	2.302695
8	1	0	-1.687121	-2.670230	0.489203
9	1	0	0.693002	-3.907514	0.119400
10	1	0	2.499539	-2.679308	1.712071
11	42	0	0.655936	-0.862637	-0.100633
12	7	0	1.236453	1.269523	-0.047824

13	7	0	-0.843399	0.692291	-0.358455
14	6	0	2.408578	2.051591	0.355254
15	6	0	2.257701	2.764738	1.712963
16	6	0	-2.264662	0.853816	-0.665536
17	6	0	-3.143894	0.740378	0.593995
18	6	0	-0.007736	1.721430	-0.198367
19	6	0	-0.458156	3.166826	-0.237284
20	1	0	3.221447	3.178618	2.029343
21	1	0	1.926528	2.055018	2.477540
22	1	0	1.539700	3.589072	1.685975
23	1	0	-4.183233	0.996822	0.360565
24	1	0	-2.796752	1.413677	1.384577
25	1	0	-3.135393	-0.281335	0.986336
26	1	0	-1.274340	3.346563	0.469523
27	1	0	-0.826854	3.422855	-1.237009
28	1	0	0.352979	3.850536	-0.001543
29	6	0	2.915992	2.988189	-0.758279
30	1	0	3.027298	2.433771	-1.694812
31	1	0	2.237582	3.825808	-0.944518
32	1	0	3.891784	3.406275	-0.486914
33	1	0	3.199936	1.312438	0.506339
34	1	0	-2.408134	1.865190	-1.068934
35	6	0	-2.742449	-0.122863	-1.745855
36	1	0	-2.170758	-0.006739	-2.668709
37	1	0	-2.639482	-1.160633	-1.414571
38	1	0	-3.799870	0.057238	-1.967911
39	6	0	0.205214	-1.328324	-1.934244
40	8	0	-0.050976	-1.684768	-3.017641
41	7	0	2.787895	-1.351687	-1.257743
42	7	0	3.355692	-1.098624	-0.285194
43	8	0	4.176176	-0.904774	0.570646

Optimized Cartesian coordinates for **Int10**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.883076	-1.046134	-2.672556
2	6	0	1.842225	-0.017265	-2.525934
3	6	0	2.851292	-0.456725	-1.609658
4	6	0	2.499210	-1.774817	-1.181488
5	6	0	1.269401	-2.120433	-1.827849
6	1	0	-0.006540	-1.005531	-3.286158
7	1	0	1.813180	0.942191	-3.021245

8	1	0	3.754996	0.077913	-1.352222
9	1	0	3.089107	-2.419159	-0.544568
10	1	0	0.738970	-3.057698	-1.717368
11	42	0	0.932073	-0.299599	-0.274955
12	7	0	-1.108614	0.511340	-0.312830
13	7	0	0.590262	1.870533	-0.324449
14	6	0	-2.447548	-0.060074	-0.410668
15	6	0	-3.135852	0.180745	-1.768009
16	6	0	1.313967	3.140294	-0.301176
17	6	0	1.743956	3.586543	-1.711478
18	6	0	-0.740922	1.788909	-0.377322
19	6	0	-1.650651	2.996784	-0.452723
20	1	0	-4.057745	-0.407503	-1.835874
21	1	0	-2.477624	-0.122298	-2.588015
22	1	0	-3.403721	1.229793	-1.924073
23	1	0	2.177790	4.592450	-1.682724
24	1	0	0.895044	3.601617	-2.402744
25	1	0	2.502178	2.909156	-2.117506
26	1	0	-1.343842	3.671935	-1.257099
27	1	0	-1.610761	3.563698	0.484531
28	1	0	-2.686317	2.712707	-0.624982
29	6	0	-3.352311	0.308122	0.781076
30	1	0	-2.834201	0.110606	1.724172
31	1	0	-3.641404	1.363194	0.772648
32	1	0	-4.271907	-0.287276	0.761386
33	1	0	-2.285948	-1.143370	-0.346790
34	1	0	0.638285	3.912270	0.093906
35	6	0	2.524667	3.086535	0.635766
36	1	0	2.227617	2.828794	1.654271
37	1	0	3.247227	2.337599	0.296683
38	1	0	3.027907	4.059242	0.655343
39	6	0	1.881501	0.042055	1.394100
40	8	0	2.490694	0.193042	2.381917
41	7	0	0.024084	-1.782017	0.948750
42	7	0	-0.455892	-2.604772	1.572309
43	8	0	-0.961821	-3.475912	2.230792

Optimized Cartesian coordinates for **TS8**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.980081	-2.449880	-1.018949
2	6	0	1.944855	-1.585648	-1.580009

3	6	0	2.838414	-1.177634	-0.553505
4	6	0	2.439010	-1.839002	0.661106
5	6	0	1.275299	-2.622372	0.368919
6	1	0	0.136213	-2.878627	-1.541055
7	1	0	1.948014	-1.225345	-2.598633
8	1	0	3.692290	-0.526169	-0.667857
9	1	0	2.958835	-1.791332	1.607663
10	1	0	0.735656	-3.253970	1.060878
11	42	0	0.770278	-0.352088	0.223773
12	7	0	-1.320240	-0.348967	-0.413537
13	7	0	0.166153	0.997188	-1.291892
14	6	0	-2.556189	-1.042760	-0.039633
15	6	0	-3.221177	-1.755548	-1.231530
16	6	0	0.682750	2.218386	-1.914741
17	6	0	2.048341	1.959676	-2.558508
18	6	0	-1.146103	0.689248	-1.217020
19	6	0	-2.213345	1.473622	-1.943206
20	1	0	-4.032936	-2.399919	-0.877887
21	1	0	-2.497889	-2.381484	-1.763782
22	1	0	-3.650701	-1.052885	-1.952207
23	1	0	2.417362	2.869130	-3.043048
24	1	0	1.985952	1.172020	-3.315711
25	1	0	2.779323	1.659520	-1.801678
26	1	0	-1.994796	1.512206	-3.015054
27	1	0	-2.242733	2.503603	-1.574072
28	1	0	-3.198205	1.034468	-1.806628
29	6	0	-3.547684	-0.175726	0.755883
30	1	0	-3.055984	0.286302	1.614756
31	1	0	-3.989997	0.618173	0.146198
32	1	0	-4.367674	-0.799989	1.127368
33	1	0	-2.218147	-1.829244	0.644871
34	1	0	-0.008483	2.500865	-2.721192
35	6	0	0.754020	3.389693	-0.920106
36	1	0	-0.212265	3.564143	-0.437951
37	1	0	1.485752	3.187530	-0.132767
38	1	0	1.053784	4.309238	-1.435112
39	7	0	-0.651266	1.613298	2.212955
40	8	0	-1.371469	1.364111	3.172827
41	7	0	0.178265	0.663662	1.799381
42	6	0	1.742120	0.939820	1.407198
43	8	0	2.511519	1.614567	2.003585

Optimized Cartesian coordinates for **Int11**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470650	-1.457017	2.464215
2	6	0	-1.600802	-2.018178	1.834740
3	6	0	-1.175145	-3.070166	0.978006
4	6	0	0.249048	-3.192699	1.121852
5	6	0	0.690722	-2.177737	2.038594
6	1	0	-0.473269	-0.602882	3.127357
7	1	0	-2.611339	-1.645643	1.917670
8	1	0	-1.801960	-3.696887	0.360980
9	1	0	0.863821	-3.946891	0.650080
10	1	0	1.701205	-2.016620	2.388247
11	42	0	-0.043228	-1.197029	0.089465
12	7	0	0.251672	0.963759	0.319863
13	7	0	-1.601323	0.090681	-0.455486
14	6	0	1.273482	1.873219	0.845400
15	6	0	0.766440	2.716252	2.029202
16	6	0	-2.821526	0.014463	-1.266806
17	6	0	-3.843982	-0.940333	-0.641718
18	6	0	-0.914833	1.240582	-0.229139
19	6	0	-1.450580	2.600280	-0.613226
20	1	0	1.600483	3.255775	2.490160
21	1	0	0.310417	2.078451	2.793035
22	1	0	0.023279	3.459391	1.723918
23	1	0	-4.754775	-0.965065	-1.248351
24	1	0	-4.117594	-0.618218	0.367876
25	1	0	-3.446662	-1.958091	-0.589396
26	1	0	-2.438916	2.761911	-0.171645
27	1	0	-1.557841	2.673449	-1.700468
28	1	0	-0.788527	3.397286	-0.284377
29	6	0	1.965538	2.721746	-0.234542
30	1	0	2.313939	2.082076	-1.048080
31	1	0	1.305133	3.487573	-0.653208
32	1	0	2.831069	3.235741	0.197627
33	1	0	2.041133	1.201199	1.245624
34	1	0	-3.278512	1.013057	-1.274935
35	6	0	-2.513507	-0.374430	-2.722104
36	1	0	-1.791469	0.314870	-3.171412
37	1	0	-2.095694	-1.383884	-2.776646
38	1	0	-3.427532	-0.349352	-3.325710
39	6	0	0.213972	-2.303581	-1.643129
40	8	0	-0.015663	-3.250094	-2.361533
41	7	0	1.049700	-1.216039	-1.647791

42	7	0	1.519568	-0.591079	-2.800225
43	8	0	2.354036	0.258278	-2.599075

Optimized Cartesian coordinates for **TS9**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.683115	-1.382670	-2.336307
2	6	0	0.374058	-0.446469	-2.469497
3	6	0	1.549290	-0.987965	-1.850431
4	6	0	1.211412	-2.302136	-1.355982
5	6	0	-0.185760	-2.537339	-1.640823
6	1	0	-1.698876	-1.240229	-2.671442
7	1	0	0.291055	0.532003	-2.915539
8	1	0	2.526032	-0.532659	-1.826664
9	1	0	1.895185	-3.003533	-0.902990
10	1	0	-0.740603	-3.439434	-1.435058
11	42	0	0.031346	-0.824679	-0.044270
12	7	0	-2.003944	-0.133298	0.343843
13	7	0	-0.268099	1.172297	0.206979
14	6	0	-3.348070	-0.744025	0.465292
15	6	0	-4.338478	-0.188715	-0.584720
16	6	0	0.516608	2.437205	0.259068
17	6	0	1.728872	2.369089	-0.687834
18	6	0	-1.637086	1.128445	0.459208
19	6	0	-2.457361	2.350219	0.793857
20	1	0	-5.264042	-0.774312	-0.565800
21	1	0	-3.900973	-0.254365	-1.586230
22	1	0	-4.589153	0.856700	-0.382110
23	1	0	2.256106	3.329357	-0.667920
24	1	0	1.414412	2.165403	-1.715016
25	1	0	2.413957	1.587022	-0.351269
26	1	0	-2.478020	3.039130	-0.059873
27	1	0	-2.007443	2.873697	1.642911
28	1	0	-3.480004	2.081511	1.053234
29	6	0	-3.909088	-0.658963	1.903479
30	1	0	-3.173325	-1.054270	2.607023
31	1	0	-4.141691	0.374084	2.178993
32	1	0	-4.828147	-1.251087	1.974393
33	1	0	-3.178290	-1.801478	0.240284
34	1	0	-0.138358	3.255131	-0.072226
35	6	0	0.999917	2.735504	1.699308
36	1	0	0.171440	2.722088	2.410430

37	1	0	1.722276	1.974177	2.002560
38	1	0	1.485790	3.717587	1.727258
39	7	0	-0.559749	-0.818183	2.593584
40	8	0	-0.548274	0.338663	3.004739
41	7	0	0.865026	-1.413904	1.779975
42	6	0	1.855001	-0.701311	1.274920
43	8	0	2.958580	-0.201252	1.363641

Optimized Cartesian coordinates for **TS10**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.902965	0.485933	-1.579315
2	6	0	1.751768	1.297994	-0.804291
3	6	0	2.640452	0.458283	-0.061987
4	6	0	2.329806	-0.903675	-0.415182
5	6	0	1.224208	-0.884288	-1.337634
6	1	0	0.094461	0.840113	-2.204757
7	1	0	1.709206	2.376758	-0.746297
8	1	0	3.459608	0.795903	0.557911
9	1	0	2.877542	-1.786748	-0.111765
10	1	0	0.793371	-1.738486	-1.841420
11	42	0	0.566848	-0.165159	0.781789
12	7	0	-1.449831	0.322636	0.476964
13	7	0	-0.278242	1.613828	1.768097
14	6	0	-2.520733	-0.262588	-0.329247
15	6	0	-3.143199	0.685322	-1.371249
16	6	0	0.123455	2.754260	2.584526
17	6	0	0.525832	3.971322	1.732992
18	6	0	-1.464495	1.465661	1.198377
19	6	0	-2.628765	2.417497	1.339189
20	1	0	-3.761828	0.113126	-2.070872
21	1	0	-2.366469	1.196013	-1.949039
22	1	0	-3.785070	1.446039	-0.918302
23	1	0	0.762679	4.829339	2.371784
24	1	0	-0.278406	4.267749	1.052292
25	1	0	1.412573	3.743069	1.133189
26	1	0	-2.663970	3.119962	0.498971
27	1	0	-2.545611	3.002154	2.257598
28	1	0	-3.577396	1.879253	1.363263
29	6	0	-3.591974	-0.943781	0.542104
30	1	0	-3.124441	-1.646213	1.237502
31	1	0	-4.166034	-0.218188	1.128033

32	1	0	-4.299582	-1.497198	-0.084975
33	1	0	-2.019767	-1.060775	-0.889158
34	1	0	-0.729579	3.054652	3.212777
35	6	0	1.260357	2.343581	3.525526
36	1	0	0.959131	1.501236	4.153007
37	1	0	2.141012	2.037244	2.952272
38	1	0	1.542724	3.179349	4.174436
39	7	0	-0.611493	-1.446748	4.068038
40	8	0	-1.108636	-0.411456	3.968706
41	7	0	0.521165	-1.501897	2.333822
42	6	0	0.995371	-2.508663	1.785684
43	8	0	1.439290	-3.559374	1.454248

Optimized Cartesian coordinates for **Int12**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.179751	-0.103617	-2.636401
2	6	0	0.986672	0.819145	-1.943386
3	6	0	2.026010	0.101771	-1.266988
4	6	0	1.845914	-1.295417	-1.575693
5	6	0	0.685659	-1.419034	-2.412804
6	1	0	-0.715416	0.137952	-3.193998
7	1	0	0.820771	1.886351	-1.889692
8	1	0	2.847682	0.541288	-0.719463
9	1	0	2.501291	-2.102629	-1.276015
10	1	0	0.300374	-2.330255	-2.849324
11	42	0	0.114059	-0.694789	-0.238858
12	7	0	-1.972099	-0.395683	-0.278758
13	7	0	-0.716403	0.933805	0.897397
14	6	0	-3.101143	-1.056637	-0.931954
15	6	0	-3.950721	-0.115910	-1.805275
16	6	0	-0.317379	1.959792	1.854909
17	6	0	0.917932	2.709417	1.344437
18	6	0	-1.975204	0.635281	0.583872
19	6	0	-3.182687	1.353030	1.143622
20	1	0	-4.661433	-0.696778	-2.402903
21	1	0	-3.314725	0.452083	-2.491514
22	1	0	-4.528687	0.599234	-1.212548
23	1	0	1.220488	3.482441	2.058177
24	1	0	0.715497	3.190157	0.382509
25	1	0	1.754016	2.015905	1.212385
26	1	0	-3.241973	2.371267	0.742628

27	1	0	-3.110763	1.431118	2.232073
28	1	0	-4.108927	0.837543	0.900557
29	6	0	-3.950978	-1.886080	0.047860
30	1	0	-3.309077	-2.550029	0.633449
31	1	0	-4.514583	-1.257939	0.744906
32	1	0	-4.673304	-2.499153	-0.502163
33	1	0	-2.626365	-1.773527	-1.611602
34	1	0	-1.131110	2.692999	1.955112
35	6	0	-0.056131	1.337264	3.236314
36	1	0	-0.950456	0.835990	3.619809
37	1	0	0.740030	0.589777	3.167637
38	1	0	0.243881	2.104179	3.958996
39	7	0	0.326049	-1.995603	1.281395
40	6	0	0.474484	-2.784248	2.183395
41	8	0	0.622874	-3.564965	3.067634

Optimized Cartesian coordinates for **Int13**.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.777669	-1.646487	-2.106274
2	6	0	0.445178	-1.167448	-2.648536
3	6	0	1.498470	-1.850338	-1.996592
4	6	0	0.940063	-2.751433	-1.044259
5	6	0	-0.480587	-2.632113	-1.119150
6	1	0	-1.765766	-1.302279	-2.374599
7	1	0	0.551193	-0.396218	-3.398588
8	1	0	2.553507	-1.660760	-2.130125
9	1	0	1.493133	-3.422879	-0.402441
10	1	0	-1.198915	-3.212008	-0.556051
11	42	0	0.323585	-0.625352	-0.165693
12	7	0	-1.698069	0.216098	-0.030904
13	7	0	-0.005094	1.548920	-0.313114
14	6	0	-2.929326	-0.334664	0.543819
15	6	0	-4.166755	-0.084010	-0.339737
16	6	0	0.734959	2.788566	-0.554918
17	6	0	1.725593	2.614576	-1.713144
18	6	0	-1.312854	1.493001	-0.100022
19	6	0	-2.207426	2.705712	0.015035
20	1	0	-5.013235	-0.673994	0.027475
21	1	0	-3.970217	-0.378679	-1.375141
22	1	0	-4.475874	0.965141	-0.344346
23	1	0	2.246020	3.557393	-1.912444

24	1	0	1.201960	2.315120	-2.627144
25	1	0	2.466918	1.849737	-1.470167
26	1	0	-1.767531	3.448104	0.686041
27	1	0	-3.195435	2.446585	0.388094
28	1	0	-2.330156	3.177582	-0.966285
29	6	0	-3.161241	0.060518	2.013232
30	1	0	-2.289743	-0.196776	2.619970
31	1	0	-3.355633	1.131386	2.127557
32	1	0	-4.026985	-0.476895	2.415439
33	1	0	-2.768372	-1.418947	0.537347
34	1	0	0.011226	3.557631	-0.861143
35	6	0	1.430551	3.289183	0.721816
36	1	0	0.709654	3.418278	1.535790
37	1	0	2.194752	2.585266	1.058148
38	1	0	1.912953	4.255515	0.537794
39	7	0	0.130063	-1.164182	1.523679
40	8	0	-0.018551	-1.673303	2.588178
41	7	0	2.329091	-0.128926	0.138685
42	6	0	3.178485	0.123328	0.955945
43	8	0	4.067976	0.408552	1.695642

Optimized Cartesian coordinates for CO.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.276319	2.000000	0.000000
2	8	0	0.861625	2.000000	0.000000

Optimized Cartesian coordinates for N_2O.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.362128	0.037138	1.153911
2	7	0	-0.403257	-0.240889	0.615522
3	8	0	0.604706	-0.533150	0.049569

Optimized Cartesian coordinates for N_2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.357645	2.309533	0.119949

2	7	0	-0.747856	2.309533	0.119949

Optimized Cartesian coordinates for CO_2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.183674	1.397959	0.000000
2	8	0	-3.352830	1.397959	0.000000
3	8	0	-1.014518	1.397959	0.000000