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Structure, isomerization and dimerization processes of narigenin flavonoids

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Content

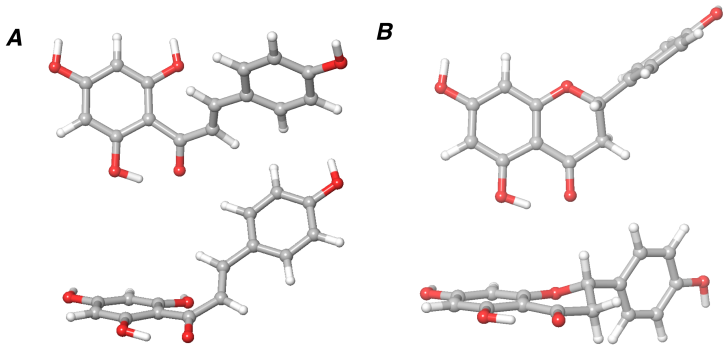


Figure S1. Top and lateral views of (A) naringenin chalcone (**1**) and (B) naringenin (**2**) structures computed at B3LYP(PCM=octanol)/6-31+G(d,p) level.

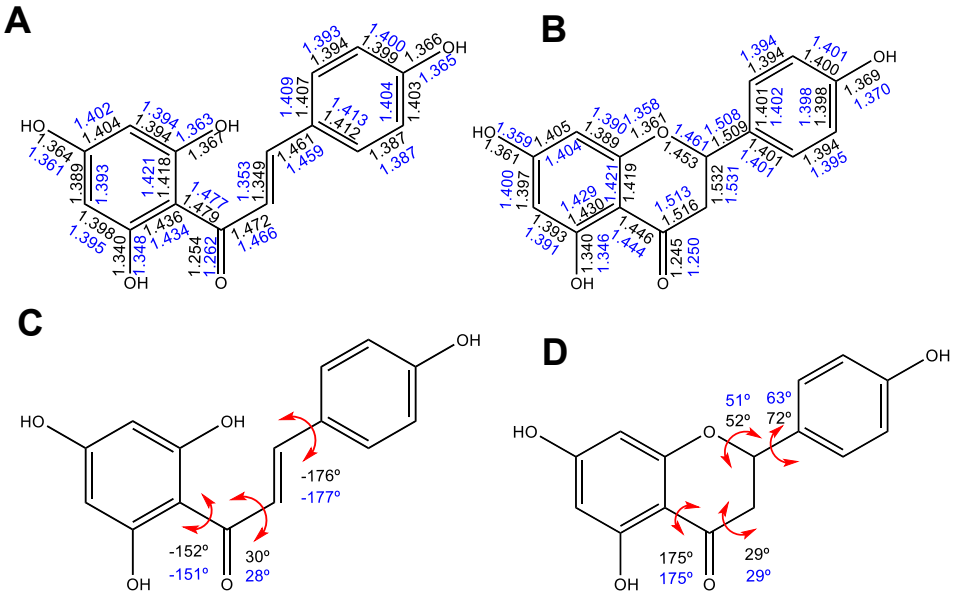


Figure S2. Main relevant (A,B) bond distances (Å) and (C,D) dihedral angles (deg) of naringenin chalcone (**1**) and naringenin (**2**). Values in black and blue were computed at B3LYP/6-31+G(d,p) and B3LYP(PCM,*n*-octanol)/6-31+G(d,p) levels, respectively.

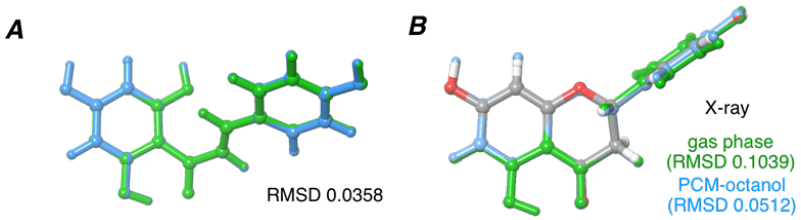


Figure S3. Superposition of (A) naringenin chalcone (**1**) and (B) naringenin (**2**) structures computed at B3LYP/6-31+G(d,p) (in green) and B3LYP(PCM=octanol)/6-31+G(d,p) (in blue) level. Naringenin X-ray structure (taken from ref.[30]) is represented with grey carbon, red oxygen and white hydrogen atoms and was used as reference for computing the RMDS.

More details about electronic and molecular structure of naringenin chalcone (1) and naringenin (2)

The higher conjugation of naringenin chalcone (**1**) in comparation to naringenin (**2**) skeleton leads to a longer carbonyl bond and a shorter C1'-C2 bond distance (see Fig.S2).

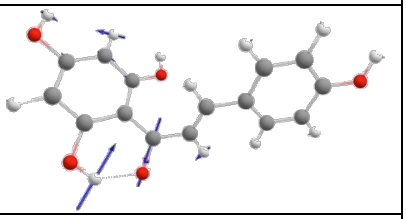
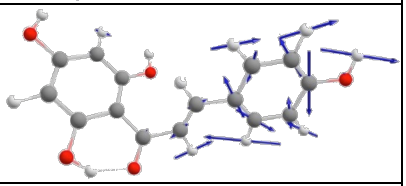
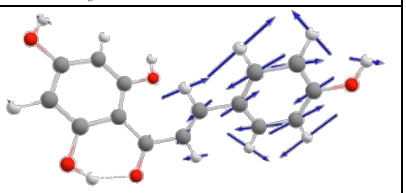
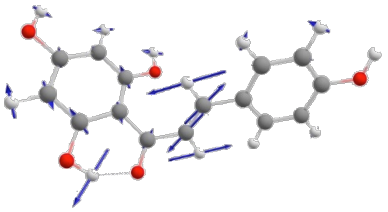
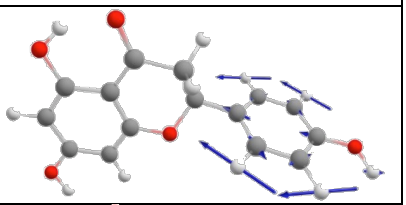
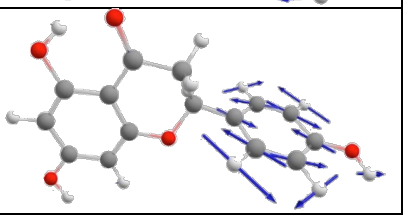
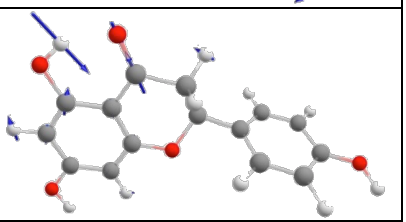
In naringenin (**2**) spectra (Fig. 3B) a weak lowest-energy absorption band at 336 nm was shown, being associated to a HOMO→LUMO one-electron excitation (S0→S1 transition); although both HOMO and LUMO electron density is mainly localized on the A and C rings, a slight delocalization over the B ring is also found for HOMO which also implies a small intramolecular charge-transfer character for this transition.

The smaller value of HOMO–LUMO gap of naringenin chalcone (**1**) rather than the computed to naringenin (**2**) is caused by an increase in electron donor and electron acceptor nature, which is reflected by the destabilization of HOMO and stabilization of LUMO orbitals in 1 when compared with **2**. In fact, the HOMO–LUMO transition of naringenin chalcone implies an intramolecular charge transfer character as mentioned in the main manuscript.

Table S1. Theoretical absorption bands (in nm) calculated at B3LYP(PCM,*n*-octanol)/6-31+G(d,p), ωb97xd(PCM,*n*-octanol)/6-31+G(d,p) and M06HF(PCM,*n*-octanol)/6-31+G(d,p) levels. Experimental values are included for comparison.

Naringenin chalcone			
B3LYP	**ωb97xd**	**M06HF**	**Experimental**
373.7	320.3	289.7	371
246.7	213.5	206.5	247
212.1	197.3	200.0	214
205.4	189.1	183.3	204
Naringenin			
326.4	288.2	261.7	336
276.6	259.6	249.2	292
221.7	207.7	197.6	229
210.1	183.0	182.6	214

Table S2. Raman band assignment of the naringenin chalcone and naringenin spectra computed at B3LYP/6-31+G(d,p) level.

Naringenin chalcone			
Theoretical ṽ (cm^{-1})	**Experimental ṽ (cm^{-1})**	**Assignment**	**Eigenvectors**
1555	1567	C=O stretching + in-plane O-H bending (H bonding)	
1563	1588	C-C stretching of ring B (vibrational **mode 8b**) + in-plane C-H bending	
1592	1607	C-C stretching of ring B (vibrational **mode 8a**) coupled with vinyl C-C stretching + in-plane C-H bending	
1624	1625	C-C stretching of vinyl group coupled with in-plane O-H bending (H bonding), C=O stretching and C–C stretching of ring A	
Naringenin			
Theoretical ṽ (cm^{-1})	**Experimental ṽ (cm^{-1})**	**Assignment**	**Eigenvectors**
1577	1592	C-C stretching of ring B (vibration **mode 8b**) + in-plane bending C-H	
1601	1619	C-C stretching of ring B (vibration **mode 8a**) + in-plane C-H bending	
1623	1636	C=O stretching + in plane O-H bending (H bonding) + and C–C stretching of ring A	

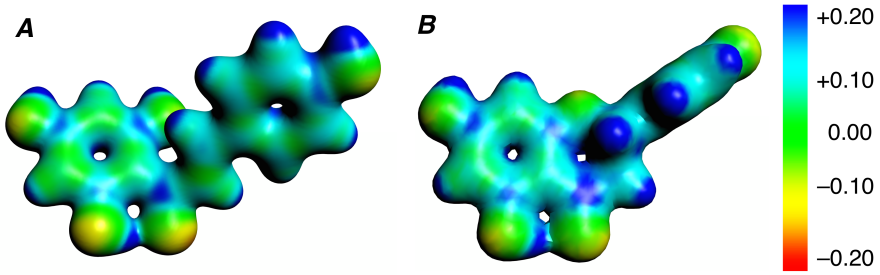


Figure S4. Electrostatic potential (ESP) surface of 0.03 a.u. electron density of naringenin chalcone (**1**) and naringenin (**2**) computed at B3LYP/6-31+G(d,p) level.

Evaluation of H–bond network on the cyclization step.

The main geometrical features and relative activation (Gibbs) energies of all H–bonding networks obtained after (MM/MC) conformational search– Molecular Dynamic simulations are collected in Figure S5.

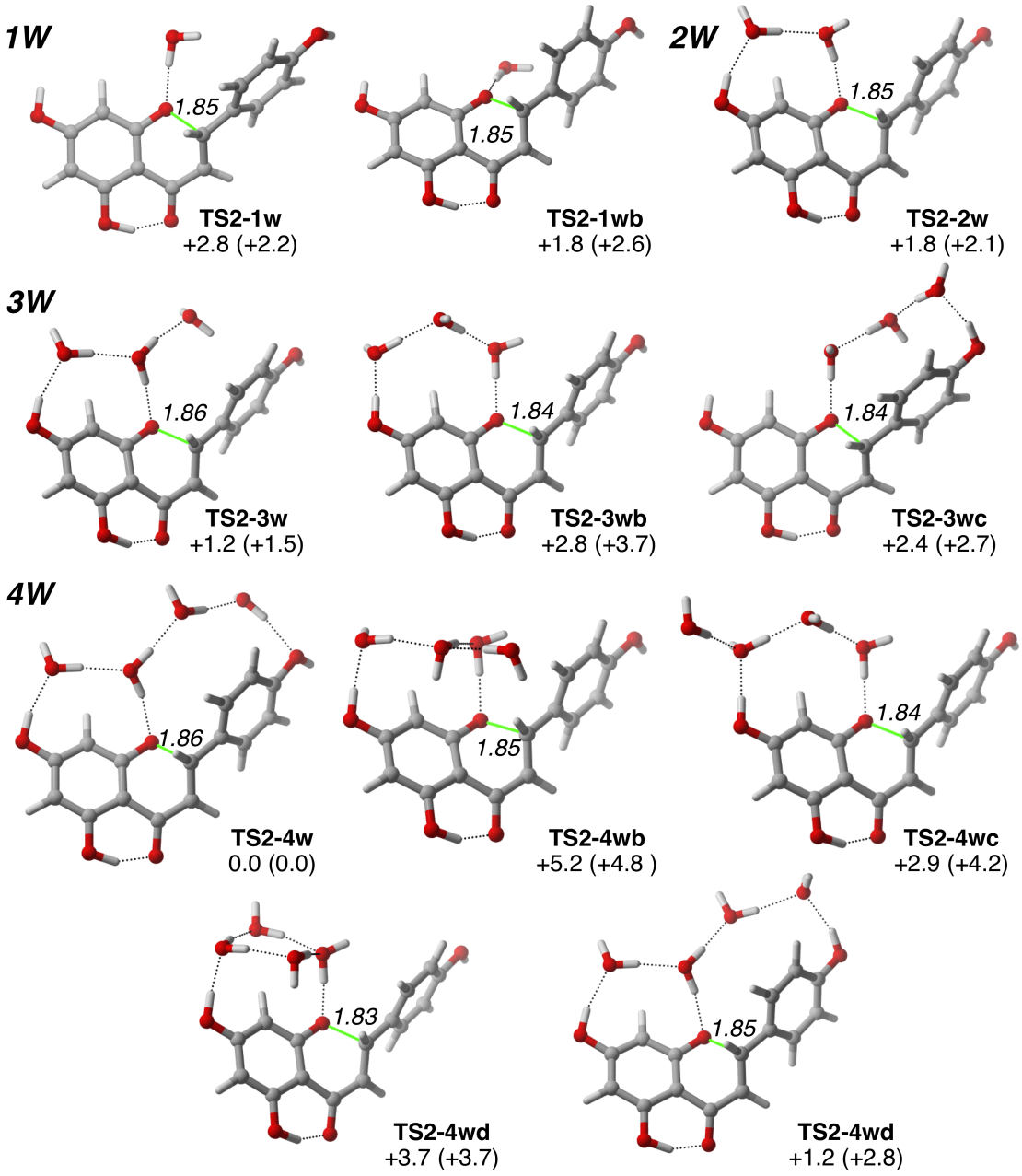
As far as one explicit molecule of water is considered in the calculations, the most stable compounds imply an H–bonding interaction with negatively charged O1, being *inplane* in **TS2-1w** and *out– of–plane* in **TS2-1wb**. Inclusion of a second water molecule creates a H–bonding network between OH–C7 and O1 that remains constant in the most stable systems including additional explicit water molecules. Remarkably, only **TS2-2w** can be found when considering two water molecules. In the case of 3 explicit water molecules, generation of a 3 water H–bonding network between OH–C7 and O1 implies an increase higher than 2 kcal mol^{-1} in the activation Gibbs energy barrier (Energy difference between **TS2-3w** and **TS2-3wb**). This increase in the activation Gibbs energy is lower when a H–bonding interaction between rings A and B is considered (O1 – OH–C4' network, **TS2-3wc**).

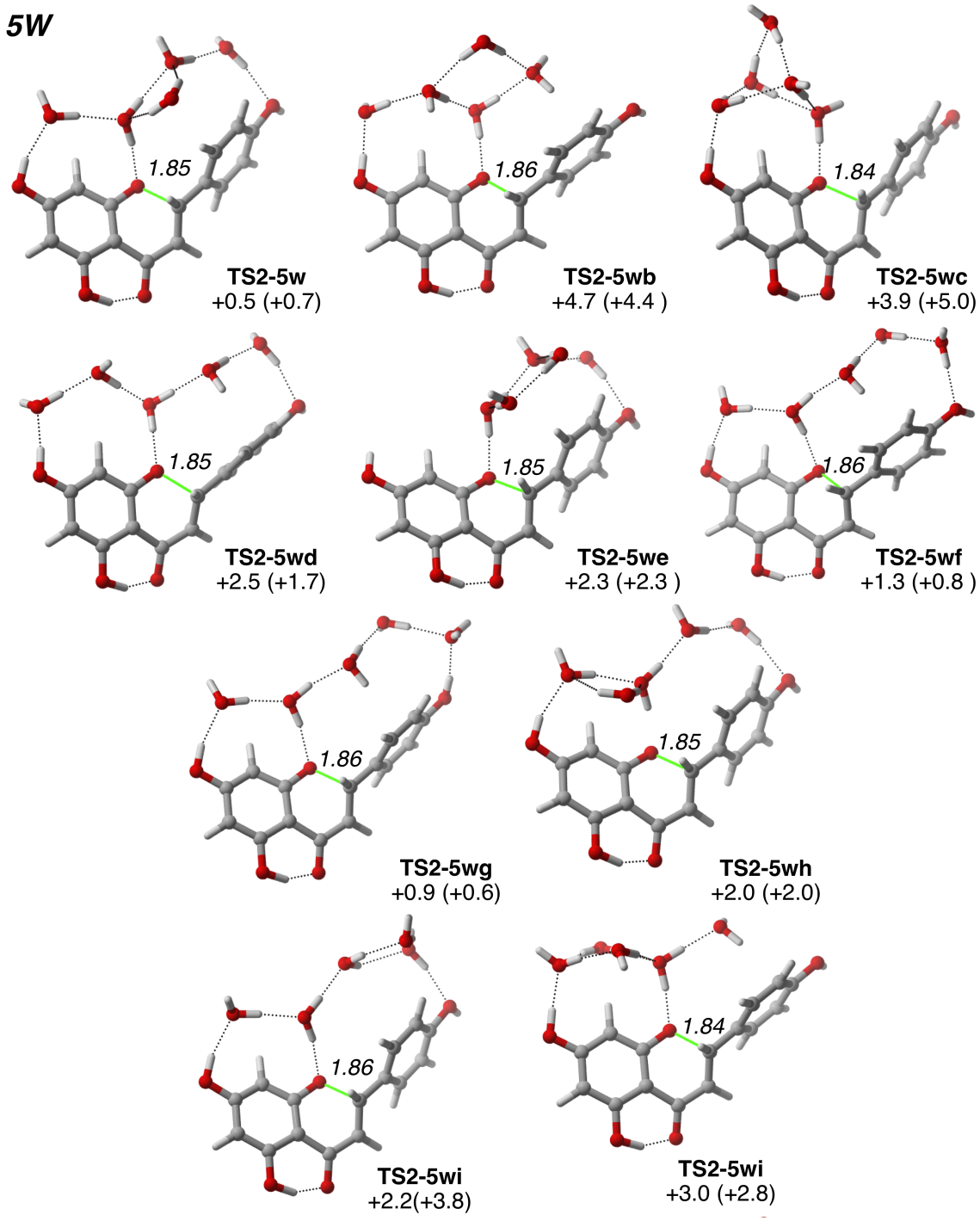
Our calculations shown that fusion of the two water network observed in **TS2-2w** and the three water network of **TS2-3wc** onto a four water network forms the most stable transition structure (**TS2-4w**) where a four water H-bonding network that connects OH–C7 – O1 – OH–C4' is observed. Noteworthy, this network can be found in all transition structures with higher amount of water molecules. Changing the OH–C4' H–bonding acceptor character implies also an increase in the activation energy (**TS2-4wd**).

Increasing the amount of explicit water molecules in the model system implies an increase in the computed activation Gibbs energy in all cases. For instance, for n = 5 ten different H–bonded networks were tested. And in all cases the OH–C7 – O1 – OH–C4' network remains in the less energetic structure (**TS2-5w**). We assume that slightly increase in the energy due to the formation of a 3 membered water cycle within the OH–C7 – O1 – OH–C4' network that increases its rigidity, thus affecting the barrier (associated not only

with a O1–C2 bond formation but also with a reduction in the C4a–C4–C3–C2 dihedral angle due to the cyclization process).

Consideration of *n* = 6, 7 explicit water implies a higher increase in the activation barrier.




5W
1.85
TS2-5w
+0.5 (+0.7)
1.86
TS2-5wb
+4.7 (+4.4)
1.84
TS2-5wc
+3.9 (+5.0)
1.85
TS2-5wd
+2.5 (+1.7)
1.85
TS2-5we
+2.3 (+2.3)
1.86
TS2-5wf
+1.3 (+0.8)
1.86
TS2-5wg
+0.9 (+0.6)
1.85
TS2-5wh
+2.0 (+2.0)
1.86
TS2-5wi
+2.2(+3.8)
1.84
TS2-5wi
+3.0 (+2.8)

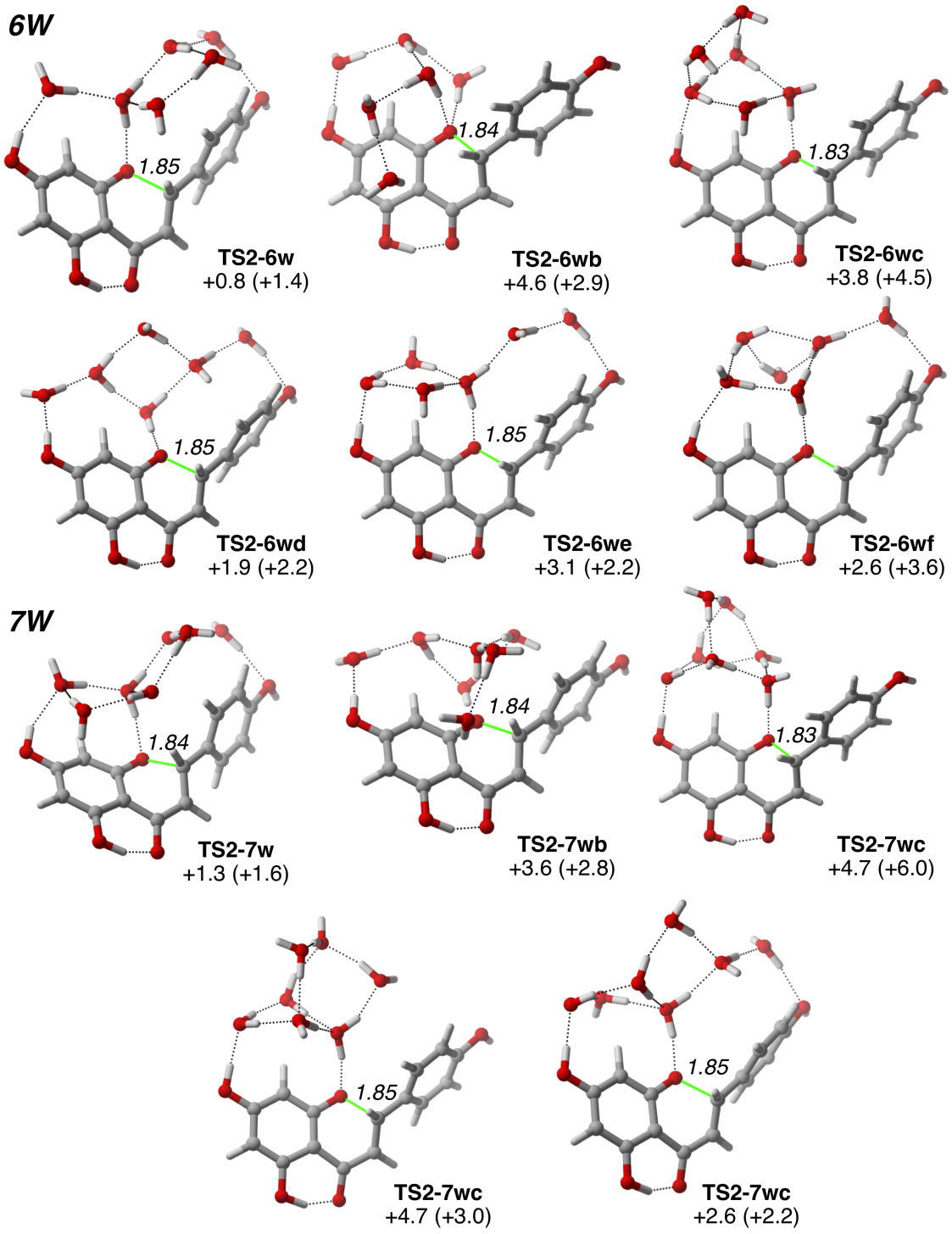


Figure S5. Main geometrical features and relative activation (Gibbs) energies of all transition structures associated with the cyclization of INT1 considering n=1–7 explicit water molecules. See Fig. 6 caption for further details.

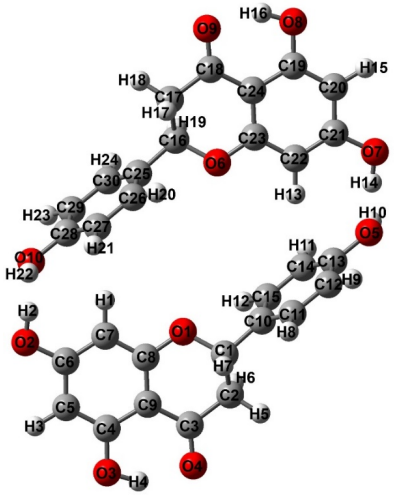


Figure S6. Numeration for naringenin dimers included in **Table S3.**

Table S3. Comparison between intermolecular interactions computed whithin different DFT levels of theory and these obtained by X-ray from naringenin cluster (taken from ref.[30] in the main text). Atom numbers are described in Figure S5.

Dimer	Interaction	Interaction length (Å) from XRD data	Interaction length (Å) calculated at M062X/6-31+G(d,p)	Interaction length (Å) calculated at ωb97xd/6-31+G(d,p)	Interaction length (Å) calculated at B3LYP-D3/6-31+G(d,p)
(2,2)-a	H22-O10•••O2	2.805	2.844	2.827	2.827
	H22-O10•••H2	2.041	1.961	1.909	1.894
(2,2)-b	C16-H19•••H1	2.316	2.276	2.302	2.340
	C16-H19•••C7	2.786	2.755	2.782	2.847
(2,2)-e	C30-H24•••O2	2.595	3.274	2.709	4.949
(2,2)-f	C15-H11•••O9	2.712	2.985	2.968	2.857
	O5-H10•••O9	1.950	1.972	1.914	1.881
	O5-H10•••C18	2.848	2.903	2.817	2.780

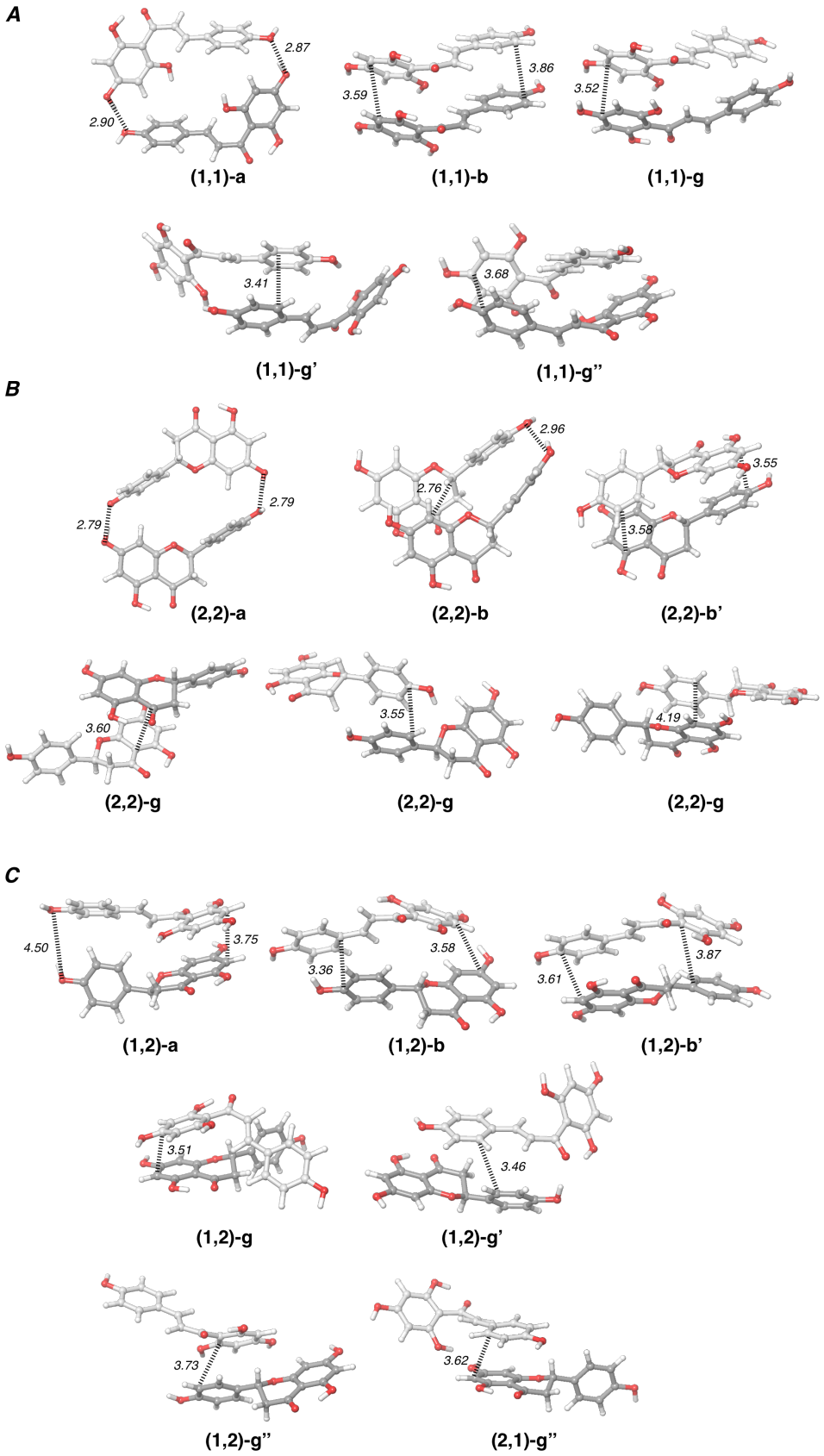


Figure S7. Main geometrical features of all (X,Y) dimers computed at ωB97XD(PCM, *n*-octanol)/6-31+G(d,p) level.

Table S4. Total electronic energies[a] (E, in a.u.), zero point correction of the energy[b] (ZPCE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of **1** and **2** discussed in the main text.

Structure	E	ZPCE	TCGFE	NIMAG(ν)
1	-955.009371	0.241495	0.195446	0
2	-955.029375	0.243867	0.199595	0

[a]Computed at B3LYP(PCM,octanol)/6-31+G** level. [b]Computed at 298.15 K. [c] If NIMAG=1, the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Table S5. Total electronic energies[a] (E, in a.u.), zero point correction of the energy[b] (ZPCE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of the cyclization reaction of **INT1** in gas phase discussed in the main text.

Structure	E	ZPCE	TCGFE	NIMAG(ν)
INT1-gp	-954.4842539	0.227381	0.179305	0
TS2-gp	-954.4337768	0.227079	0.182942	1 (-373.1110)
INT2-gp	-954.4748578	0.227436	0.182469	0

[a]Computed at B3LYP-D3/6-31G+(d,p) level. [b]Computed at 298.15 K. [c] If NIMAG=1 the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Table S6. Total electronic energies[a] (E, in a.u.), zero point correction of the energy[b] (ZPCE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of the cyclization reaction of **INT1** in octanol.

Structure	E	ZPCE	TCGFE	NIMAG(ν)
INT1-o	-954.5622558	0.227691	0.180839	0
TS2-o	-954.5111232	0.227217	0.18351	1 (-384.5567)
INT2-o	-954.5526025	0.228211	0.183656	0

[a]Computed at B3LYP-D3(PCM,octanol)/6-31G+(d,p) level. [b]Computed at 298.15 K. [c] If NIMAG=1 the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Table S7. Total electronic energies[a] (E, in a.u.), zero point correction of the energies[b] (ZPCE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of the cyclization reaction of **INT1** in water discussed in the main text.

Structure	E	ZPCE	TCGFE	NIMAG(ν)
INT1-w	-954.572209	0.227683	0.181098	0
TS2-w	-954.520987	0.227225	0.18351	1 (-384.0088)
INT2-w	-954.562403	0.228325	0.183943	0
INT1-1w	-1031.031639	0.252326	0.202229	0
TS2-1w	-1031.006529	0.251808	0.203603	1 (-420.1960)
INT2-1w	-1031.016365	0.252677	0.203951	0
INT1-1wb	-1031.030242	0.251923	0.200025	0
TS2-1wb	-1031.006025	0.251473	0.202896	1 (-413.1906)
INT2-1wb	-1031.016292	0.252503	0.203432	0
INT1-2wb	-1183.938511	0.302234	0.244474	0
TS2-2w	-1183.915522	0.302009	0.246752	1 (-406.4194)
INT2-2w	-1183.925831	0.302937	0.246732	0
INT1-2w	-1107.486131	0.277640	0.224238	0
TS2-2wb	-1107.462000	0.277302	0.226342	1 (-412.0947)
INT2-2wb	-1107.471538	0.278230	0.226579	0
INT1-2wc	-1183.946007	0.302613	0.246735	0
TS2-2wc	-1183.921277	0.302568	0.249265	1 (-428.8266)
INT2-2wc	-1183.929911	0.303598	0.249437	0
INT1-3w	-1183.949657	0.302241	0.244052	0
TS2-3w	-1183.924540	0.302491	0.247737	1 (-428.8866)
INT2-3w	-1183.933732	0.303457	0.247722	0
INT1-4w	-1260.391466	0.32713	0.265782	0
TS2-4w	-1260.370626	0.327229	0.267921	1 (-409.953)
INT2-4w	-1260.380926	0.328294	0.268686	0
INT1-4wb	-1260.432322	0.327362	0.268405	0
TS2-4wb	-1260.403093	0.327118	0.269867	1 (-436.1513)
INT2-4wb	-1260.412494	0.328232	0.27013	0
INT1-4wc	-1260.400862	0.32634	0.260873	0
TS2-4wc	-1260.375523	0.326577	0.265248	1 (-430.5348)
INT2-4wc	-1260.38469	0.327684	0.265179	0
INT1-4wd	-1260.409077	0.328633	0.269139	0
TS2-4wd	-1260.382548	0.328924	0.272599	1 (-432.4934)
INT2-4wd	-1260.390806	0.329657	0.271024	0
INT1-4we	-1260.392858	0.326334	0.263073	0
TS2-4we	-1260.37078	0.327108	0.268414	1 (-411.8318)
INT2-4we	-1260.380166	0.328033	0.268593	0
INT1-5w	-1336.847011	0.352579	0.288832	0
TS2-5w	-1336.825562	0.352835	0.291408	1 (-415.7500)
INT2-5w	-1336.834916	0.353731	0.291316	0
INT1-5wb	-1336.891280	0.351850	0.289071	0
TS2-5wb	-1336.862574	0.351518	0.290298	1 (-430.3716)
INT2-5wb	-1336.873648	0.353480	0.291655	0

INT1-5wc	-1336.86423	0.353844	0.2903	0
TS2-5wc	-1336.837542	0.354284	0.294473	1 (-433.0527)
INT2-5wc	-1336.846261	0.355639	0.29505	0
INT1-5wd	-1336.858688	0.352757	0.289608	0
TS2-5wd	-1336.833645	0.352655	0.290223	1 (-423.4180)
INT2-5wd	-1336.844696	0.353798	0.290877	0
INT1-5we	-1336.852958	0.353075	0.289402	0
TS2-5we	-1336.828472	0.353072	0.291483	1 (-419.3362)
INT2-5we	-1336.838012	0.354147	0.291887	0
INT1-5wf	-1336.849433	0.352976	0.288418	0
TS2-5wf	-1336.825915	0.352392	0.289103	1 (-406.6509)
INT2-5wf	-1336.836846	0.353359	0.288968	0
INT1-5wg	-1336.848237	0.352024	0.287521	0
TS2-5wg	-1336.826337	0.352507	0.289473	1 (-410.3543)
INT2-5wg	-1336.836674	0.353284	0.288869	0
INT1-5wh	-1336.849753	0.352428	0.288261	0
TS2-5wh	-1336.825662	0.352368	0.290298	1 (-417.3751)
INT2-5wh	-1336.83489	0.353277	0.289752	0
INT1-5wi	-1336.849159	0.352557	0.286757	0
TS2-5wi	-1336.825038	0.352825	0.291579	1 (-406.2921)
INT2-5wi	-1336.835142	0.353638	0.291382	0
INT1-5wj	-1336.861731	0.353721	0.291407	0
TS2-5wj	-1336.835663	0.353319	0.292467	1 (-428.6549)
INT2-5wj	-1336.845671	0.354359	0.292447	0
INT1-6w	-1413.307668	0.377968	0.311222	0
TS2-6w	-1413.2863	0.378759	0.314975	1 (-419.9690)
INT2-6w	-1413.295467	0.379919	0.315942	0
INT1-6wb	-1413.355155	0.377730	0.313327	0
TS2-6wb	-1413.32565	0.376460	0.311451	1 (-427.8643)
INT2-6wb	-1413.334801	0.376868	0.311452	0
INT1-6wc	-1413.321199	0.37879	0.311135	0
TS2-6wc	-1413.294508	0.379083	0.314679	1 (-433.3977)
INT2-6wc	-1413.303103	0.380479	0.315404	0
INT1-6wd	-1413.316703	0.378669	0.312343	0
TS2-6wd	-1413.292778	0.378658	0.314292	1 (-420.1094)
INT2-6wd	-1413.303591	0.379984	0.315387	0
INT1-6we	-1413.318892	0.379303	0.314918	0
TS2-6we	-1413.292759	0.379027	0.315272	1 (-423.4868)
INT2-6we	-1413.302727	0.379927	0.313745	0
INT1-6wf	-1413.318892	0.379303	0.314918	0
TS2-6wf	-1413.292759	0.379027	0.315272	1 (-405.5166)
INT2-6wf	-1413.302727	0.379927	0.313745	0
INT1-7w	-1489.770012	0.404903	0.337823	0
TS2-7w	-1489.747169	0.405052	0.340476	1 (-422.5613)
INT2-7w	-1489.754988	0.405962	0.340519	0
INT1-7wb	-1489.813758	0.403093	0.335076	0
TS2-7wb	-1489.787939	0.402225	0.336728	1 (-434.2627)
INT2-7wb	-1489.796569	0.403346	0.336720	0
INT1-7wc	-1489.778515	0.403371	0.332287	0

TS2-7wc	-1489.751463	0.404665	0.337803	1 (-437.2486)
INT2-7wc	-1489.759592	0.405772	0.337048	0
INT1-7wd	-1489.777881	0.404802	0.335268	0
TS2-7wd	-1489.752778	0.404846	0.337887	1 (-424.2405)
INT2-7wd	-1489.762392	0.406211	0.338402	0
INT1-7we	-1489.774249	0.404661	0.336604	0
TS2-7we	-1489.749372	0.404874	0.338123	1 (-429.3527)
INT2-7we	-1489.759598	0.405948	0.338273	0
1·4H_2O[d]	-1260.422650	0.323595	0.263562	0
TS1·4H_2O[d]	-1260.419001	0.321399	0.260924	1 (-717.2124)
INT1'·4H_2O[d]	-1260.437207	0.327649	0.269318	0
INT1·4H_2O[d]	-1260.429428	0.326518	0.265436	0
INT2·4H_2O[d]	-1260.414194	0.327160	0.267345	0
TS3·4H_2O[d]	-1260.403014	0.322723	0.264942	1 (-1492.8676)
2·4H_2O[d]	-1260.431800	0.326691	0.267797	0

[a]Computed at B3LYP-D3(PCM, water)/6-31G+(d,p) level. [b]Computed at 298.15 K [c] If NIMAG=1 the imaginary frequency ν (in parentheses) is given in cm^{-1}. [d] Computed with the radii=pauling option for the generation of the cavity.

Table S8. Total electronic energies[a] (E, in a.u.), zero point correction of the energy[b] (ZPCE), thermal corrections to Gibbs free energies[b] (TCGFE, in a.u.), and number of imaginary frequencies[c] (NIMAG) of **1** and **2** the aggregation analysis discussed in the main text.

Structure	E	ZPCE	TCGFE	NIMAG(ν)
1	-954.691516	0.245099	0.198595	0
2	-954.719940	0.247551	0.203310	0
(1,1)-a	-1909.400840	0.492761	0.423244	0
(1,1)-b	-1909.407960	0.491782	0.423406	0
(1,1)-g	-1909.413640	0.491992	0.422055	0
(1,1)-g'	-1909.401252	0.492333	0.423151	0
(1,1)-g''	-1909.408266	0.493014	0.424681	0
(2,2)-a	-1909.461817	0.497515	0.430233	0
(2,2)-b	-1909.461030	0.496711	0.430612	0
(2,2)-b'	-1909.466295	0.496812	0.431356	0
(2,2)-g	-1909.460870	0.496532	0.427799	0
(2,2)-g'	-1909.456948	0.496865	0.427694	0
(2,2)-g''	-1909.458716	0.496562	0.428168	0
(1,2)-a	-1909.432842	0.495203	0.426761	0
(1,2)-b	-1909.435768	0.494169	0.424899	0
(1,2)-b'	-1909.434954	0.494483	0.42758	0
(1,2)-g	-1909.434136	0.494441	0.424836	0
(1,2)-g'	-1909.432251	0.494826	0.426807	0
(1,2)-g''	-1909.427663	0.493702	0.422575	0
(2,1)-g''	-1909.434691	0.495400	0.427694	0

[a]Computed at wB97XD(PCM,octanol)/6-31G+(d,p) level. [b]Computed at 298.15 K. [c] If NIMAG=1 the imaginary frequency ν (in parentheses) is given in cm^{-1}.

Cartesian coordinates of all the stationary points collected in the main text

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.094761	-1.388026	-0.194664
2	6	0	-4.262238	-0.118670	-0.742959
3	6	0	-3.292796	0.855869	-0.505982
4	6	0	-2.087432	0.566102	0.214483
5	6	0	-2.002106	-0.722311	0.808897
6	6	0	-2.981496	-1.691956	0.601260
7	8	0	-5.072131	-2.303594	-0.439009
8	8	0	-3.524775	2.087419	-1.002134
9	8	0	-0.954105	-0.983125	1.640192
10	6	0	-1.065432	1.627308	0.314057
11	6	0	0.376311	1.387889	0.430002
12	6	0	1.021118	0.299792	-0.049985
13	6	0	2.943007	-1.107411	-0.695099
14	6	0	2.461736	0.076180	-0.100700
15	6	0	3.413161	0.981549	0.420708
16	6	0	4.773407	0.717162	0.350668
17	6	0	5.225960	-0.469538	-0.248611
18	6	0	4.305534	-1.385232	-0.772458
19	8	0	6.574710	-0.672780	-0.288644
20	8	0	-1.427346	2.831763	0.210635
21	1	0	-5.148447	0.126428	-1.316065
22	1	0	-2.891899	-2.666306	1.074583
23	1	0	-4.869521	-3.144565	-0.004467
24	1	0	-2.821210	2.678330	-0.614869
25	1	0	-1.043176	-1.871706	2.013534
26	1	0	0.923484	2.253442	0.793706
27	1	0	0.423504	-0.505929	-0.468669
28	1	0	2.234983	-1.822675	-1.104668
29	1	0	3.087312	1.904606	0.888763
30	1	0	5.499156	1.416231	0.753314
31	1	0	4.651810	-2.304994	-1.236045
32	1	0	6.779336	-1.512556	-0.725118

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.050053	-0.749054	-0.026255
2	6	0	-0.698845	0.412793	0.446249
3	6	0	-0.203345	1.674848	-0.264345
4	6	0	1.295862	1.828571	-0.131498
5	6	0	3.487793	0.627396	0.009364
6	6	0	4.218237	-0.556097	0.024642
7	6	0	3.529155	-1.774893	0.014930
8	6	0	2.126838	-1.839263	0.004782
9	6	0	1.404844	-0.651580	-0.003889
10	6	0	2.059133	0.609320	-0.010587
11	8	0	1.830988	2.958253	-0.165983
12	8	0	4.145884	1.801892	-0.002455
13	8	0	4.289446	-2.900995	0.029394
14	6	0	-2.165732	0.124038	0.249833
15	6	0	-3.041261	0.143753	1.343835
16	6	0	-4.405339	-0.100299	1.183383
17	6	0	-4.910393	-0.382112	-0.089875
18	6	0	-4.049567	-0.412872	-1.195101
19	6	0	-2.690104	-0.156937	-1.020158
20	8	0	-6.254213	-0.623223	-0.197358

21	1	0	-0.490810	0.504768	1.520036
22	1	0	-0.444558	1.630981	-1.335027
23	1	0	-0.696239	2.559943	0.146609
24	1	0	5.301512	-0.535635	0.035782
25	1	0	1.602482	-2.788804	0.019350
26	1	0	3.456009	2.517537	-0.053504
27	1	0	3.730375	-3.691783	0.013360
28	1	0	-2.655595	0.352334	2.338218
29	1	0	-5.079831	-0.082817	2.033305
30	1	0	-4.440913	-0.634789	-2.184622
31	1	0	-2.034577	-0.190508	-1.885404
32	1	0	-6.488778	-0.816196	-1.116226

INT1-gp

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.523013	-1.140929	-0.109808
2	6	0	4.636577	0.257147	-0.083695
3	6	0	3.479721	1.021899	0.005399
4	6	0	2.146603	0.432042	0.062682
5	6	0	2.065969	-1.046622	0.090004
6	6	0	3.303080	-1.775521	-0.036478
7	8	0	5.707273	-1.851300	-0.205301
8	8	0	3.648898	2.358643	0.022523
9	8	0	0.992368	-1.703875	0.229450
10	6	0	1.024369	1.349746	0.055011
11	6	0	-0.438860	1.082969	-0.046507
12	6	0	-1.194869	-0.013839	0.161261
13	6	0	-2.661752	-0.057366	0.076939
14	6	0	-3.494659	1.076225	-0.040689
15	6	0	-4.879577	0.963603	-0.121415
16	6	0	-5.479170	-0.299756	-0.082756
17	6	0	-4.684063	-1.441423	0.041999
18	6	0	-3.296192	-1.313328	0.123400
19	8	0	-6.856384	-0.356540	-0.164801
20	8	0	1.234754	2.618344	0.084699
21	1	0	5.602433	0.744473	-0.133993
22	1	0	3.223260	-2.860495	-0.030279
23	1	0	5.487522	-2.791983	-0.211270
24	1	0	2.700206	2.732704	0.069929
25	1	0	-0.928674	2.027215	-0.281739
26	1	0	-0.674308	-0.941718	0.380385
27	1	0	-3.050983	2.066562	-0.059486
28	1	0	-5.510593	1.842926	-0.208075
29	1	0	-5.144977	-2.427526	0.076368
30	1	0	-2.681637	-2.204270	0.219137
31	1	0	-7.138652	-1.279142	-0.125619

TS2-gp

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.286422	-1.866740	1.456544
2	6	0	3.182709	-3.070106	2.152044
3	6	0	3.985778	-4.140646	1.739112
4	6	0	4.952546	-4.010063	0.697905
5	6	0	5.038928	-2.746677	-0.000609
6	6	0	4.166524	-1.699341	0.390739
7	8	0	2.472152	-0.824840	1.871296
8	8	0	3.808868	-5.335649	2.340145
9	8	0	5.877133	-2.504503	-0.987721
10	6	0	5.613852	-5.234749	0.184305
11	6	0	6.624622	-5.063319	-0.794083
12	6	0	7.238514	-3.803157	-0.905507
13	6	0	8.130991	-3.478105	-2.042542
14	6	0	7.915422	-3.997497	-3.331452

15	6	0	8.758640	-3.683612	-4.394607
16	6	0	9.841562	-2.823556	-4.187667
17	6	0	10.068337	-2.278441	-2.921793
18	6	0	9.211684	-2.602557	-1.866938
19	8	0	10.650578	-2.537655	-5.270256
20	8	0	5.181792	-6.386217	0.550297
21	1	0	2.462505	-3.201394	2.950988
22	1	0	4.243949	-0.748860	-0.132644
23	1	0	2.621436	-0.078035	1.277293
24	1	0	4.311103	-5.992535	1.735849
25	1	0	6.818257	-5.865910	-1.498039
26	1	0	7.542398	-3.310526	0.018439
27	1	0	7.062039	-4.647193	-3.497184
28	1	0	8.585509	-4.086046	-5.388102
29	1	0	10.905256	-1.600189	-2.760468
30	1	0	9.383657	-2.166490	-0.886434
31	1	0	11.343027	-1.925074	-4.991332

INT2-gp

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.086365	1.426082	2.016765
2	6	0	-3.277431	0.194738	2.637301
3	6	0	-2.394037	-0.860679	2.343016
4	6	0	-1.299876	-0.658892	1.461673
5	6	0	-1.153925	0.594267	0.852533
6	6	0	-2.036668	1.648971	1.117124
7	8	0	-3.979702	2.440485	2.329862
8	8	0	-2.590931	-2.076759	2.867936
9	8	0	-0.169270	0.819208	-0.070853
10	6	0	-0.424754	-1.797801	1.068938
11	6	0	0.649449	-1.484418	0.268117
12	6	0	1.012101	-0.042645	0.063057
13	6	0	1.848408	0.183087	-1.177457
14	6	0	1.298054	-0.027091	-2.450654
15	6	0	2.058630	0.147554	-3.604904
16	6	0	3.402091	0.522858	-3.496653
17	6	0	3.971774	0.730286	-2.239614
18	6	0	3.187049	0.566513	-1.090370
19	8	0	4.118451	0.676608	-4.669955
20	8	0	-0.776298	-2.984468	1.486234
21	1	0	-4.109592	0.036516	3.313678
22	1	0	-1.884362	2.611041	0.635084
23	1	0	-3.749551	3.218558	1.806933
24	1	0	-1.857848	-2.671414	2.365688
25	1	0	1.326519	-2.251607	-0.092038
26	1	0	1.563710	0.384997	0.926642
27	1	0	0.258397	-0.330888	-2.518196
28	1	0	1.633077	-0.007956	-4.591616
29	1	0	5.017539	1.022355	-2.153918
30	1	0	3.630223	0.737980	-0.112287
31	1	0	5.026076	0.925596	-4.454714

INT1-o

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.152155	-1.374325	0.151715
2	6	0	4.363112	-0.058914	0.607062
3	6	0	3.362904	0.879343	0.395781
4	6	0	2.100931	0.541753	-0.219198
5	6	0	1.944361	-0.810714	-0.791114
6	6	0	3.003067	-1.747881	-0.519881
7	8	0	5.175394	-2.261429	0.394390
8	8	0	3.601678	2.144567	0.823913
9	8	0	0.957684	-1.153823	-1.514193
10	6	0	1.082406	1.565417	-0.268931
11	6	0	-0.367980	1.321686	-0.425859
12	6	0	-1.033085	0.261189	0.071429

13	6	0	-2.482333	0.058695	0.101994
14	6	0	-3.415546	0.990563	-0.402995
15	6	0	-4.782334	0.746168	-0.354255
16	6	0	-5.260572	-0.447046	0.207440
17	6	0	-4.359873	-1.388769	0.715996
18	6	0	-2.990385	-1.130039	0.660225
19	8	0	-6.618267	-0.629265	0.228671
20	8	0	1.377036	2.798151	-0.087148
21	1	0	5.289346	0.222235	1.094032
22	1	0	2.888389	-2.756134	-0.910331
23	1	0	4.941398	-3.129371	0.035909
24	1	0	2.804109	2.678479	0.516677
25	1	0	-0.899604	2.179099	-0.832510
26	1	0	-0.447545	-0.548777	0.497330
27	1	0	-3.070428	1.921745	-0.840527
28	1	0	-5.493002	1.467637	-0.744723
29	1	0	-4.725170	-2.315329	1.151287
30	1	0	-2.298334	-1.868499	1.055982
31	1	0	-6.838318	-1.479446	0.635363

TS2-o

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.303909	-1.851598	1.486873
2	6	0	3.205832	-3.063287	2.176709
3	6	0	3.990799	-4.134234	1.742154
4	6	0	4.934639	-4.008432	0.681802
5	6	0	5.015199	-2.742414	-0.010206
6	6	0	4.164274	-1.687792	0.402753
7	8	0	2.509098	-0.819878	1.931871
8	8	0	3.823127	-5.337443	2.344025
9	8	0	5.833593	-2.517000	-1.020970
10	6	0	5.580425	-5.229006	0.145528
11	6	0	6.592867	-5.067518	-0.819012
12	6	0	7.225380	-3.809113	-0.935522
13	6	0	8.124535	-3.486912	-2.061657
14	6	0	7.961440	-4.054141	-3.339662
15	6	0	8.818199	-3.734267	-4.388150
16	6	0	9.863505	-2.824523	-4.178114
17	6	0	10.039532	-2.236549	-2.920383
18	6	0	9.169874	-2.566545	-1.880588
19	8	0	10.678024	-2.544545	-5.244085
20	8	0	5.120416	-6.386397	0.499554
21	1	0	2.502923	-3.189601	2.992419
22	1	0	4.231969	-0.734569	-0.114609
23	1	0	2.636366	-0.046259	1.364730
24	1	0	4.298476	-5.991378	1.714854
25	1	0	6.799790	-5.876254	-1.512673
26	1	0	7.515867	-3.312639	-0.010775
27	1	0	7.145857	-4.748106	-3.516197
28	1	0	8.686941	-4.173560	-5.372072
29	1	0	10.846368	-1.526387	-2.757070
30	1	0	9.308521	-2.103010	-0.907474
31	1	0	11.358443	-1.906322	-4.986473

INT2-o

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.553738	-1.733734	-0.152251
2	6	0	4.200339	-0.498254	-0.084470
3	6	0	3.426926	0.667777	0.010111
4	6	0	2.013907	0.600210	0.076553
5	6	0	1.405122	-0.663359	-0.002405
6	6	0	2.156986	-1.837355	-0.119654
7	8	0	4.354512	-2.850336	-0.245484
8	8	0	4.024164	1.879319	0.012866
9	8	0	0.042787	-0.781255	-0.027359
10	6	0	1.184442	1.833996	0.076335

11	6	0	-0.163949	1.661511	0.246112
12	6	0	-0.689665	0.311378	0.648082
13	6	0	-2.153718	0.094505	0.342490
14	6	0	-2.675548	0.388007	-0.927007
15	6	0	-4.019583	0.171888	-1.222959
16	6	0	-4.872220	-0.341413	-0.236765
17	6	0	-4.373358	-0.639537	1.034946
18	6	0	-3.019234	-0.423335	1.310975
19	8	0	-6.189532	-0.528683	-0.579205
20	8	0	1.815083	2.975446	-0.121430
21	1	0	5.282077	-0.437604	-0.129287
22	1	0	1.655347	-2.798883	-0.170302
23	1	0	3.805441	-3.644253	-0.306245
24	1	0	3.207116	2.541680	-0.048035
25	1	0	-0.847873	2.504218	0.230308
26	1	0	-0.532320	0.112137	1.724465
27	1	0	-2.014759	0.793948	-1.687207
28	1	0	-4.422259	0.398332	-2.205377
29	1	0	-5.033820	-1.037412	1.801398
30	1	0	-2.636102	-0.661862	2.300057
31	1	0	-6.684059	-0.879930	0.174574

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.125604	-1.392715	0.151976
2	6	0	4.344603	-0.082653	0.619112
3	6	0	3.356569	0.867409	0.403509
4	6	0	2.097579	0.547530	-0.225310
5	6	0	1.934838	-0.797645	-0.809642
6	6	0	2.979584	-1.747801	-0.536485
7	8	0	5.135813	-2.290624	0.399315
8	8	0	3.604912	2.127797	0.842854
9	8	0	0.952216	-1.124876	-1.549663
10	6	0	1.086952	1.581925	-0.271257
11	6	0	-0.364128	1.347487	-0.416293
12	6	0	-1.025131	0.281280	0.077238
13	6	0	-2.472170	0.070751	0.110014
14	6	0	-3.411120	0.998080	-0.393751
15	6	0	-4.775734	0.742901	-0.347849
16	6	0	-5.246026	-0.456578	0.208989
17	6	0	-4.339060	-1.393419	0.717059
18	6	0	-2.971938	-1.123777	0.664694
19	8	0	-6.600550	-0.648559	0.225283
20	8	0	1.397594	2.811520	-0.094797
21	1	0	5.268069	0.185492	1.118730
22	1	0	2.860135	-2.751848	-0.936030
23	1	0	4.899775	-3.156168	0.035517
24	1	0	2.819525	2.673507	0.527525
25	1	0	-0.898819	2.208013	-0.811998
26	1	0	-0.434688	-0.528555	0.496904
27	1	0	-3.072926	1.933236	-0.828219
28	1	0	-5.490964	1.460410	-0.737189
29	1	0	-4.698226	-2.323478	1.149216
30	1	0	-2.275651	-1.857960	1.061057
31	1	0	-6.818641	-1.501356	0.628550

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.308016	-1.848771	1.490834
2	6	0	3.211733	-3.061437	2.180784
3	6	0	3.992195	-4.133210	1.741971
4	6	0	4.930182	-4.009278	0.676660
5	6	0	5.008558	-2.743510	-0.015696
6	6	0	4.162606	-1.687014	0.401221
7	8	0	2.518408	-0.818101	1.941835
8	8	0	3.826762	-5.337294	2.345342

9	8	0	5.821599	-2.523284	-1.033011
10	6	0	5.574541	-5.229309	0.138228
11	6	0	6.588753	-5.069345	-0.822549
12	6	0	7.222534	-3.810156	-0.940118
13	6	0	8.123254	-3.488171	-2.063328
14	6	0	7.967766	-4.061688	-3.339922
15	6	0	8.826122	-3.740096	-4.386267
16	6	0	9.866239	-2.823574	-4.175636
17	6	0	10.034995	-2.230057	-2.918847
18	6	0	9.163607	-2.561298	-1.881381
19	8	0	10.681248	-2.544033	-5.238953
20	8	0	5.109875	-6.387658	0.489951
21	1	0	2.514468	-3.185536	3.001779
22	1	0	4.227711	-0.733706	-0.116003
23	1	0	2.643646	-0.039920	1.379902
24	1	0	4.296502	-5.991370	1.713066
25	1	0	6.801446	-5.879848	-1.512543
26	1	0	7.507333	-3.310753	-0.015353
27	1	0	7.158362	-4.762642	-3.518064
28	1	0	8.700909	-4.184308	-5.368735
29	1	0	10.837627	-1.515689	-2.755079
30	1	0	9.297651	-2.094309	-0.909255
31	1	0	11.361542	-1.904316	-4.983253

INT2-w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.548921	-1.739022	-0.160435
2	6	0	4.198925	-0.505019	-0.082140
3	6	0	3.428820	0.661822	0.016899
4	6	0	2.015707	0.599674	0.075796
5	6	0	1.403325	-0.662271	-0.013596
6	6	0	2.151396	-1.837744	-0.135365
7	8	0	4.347348	-2.854714	-0.256518
8	8	0	4.031628	1.872836	0.031822
9	8	0	0.040440	-0.773614	-0.045961
10	6	0	1.189005	1.834798	0.080978
11	6	0	-0.159281	1.665934	0.249952
12	6	0	-0.689598	0.314297	0.642549
13	6	0	-2.154553	0.101398	0.340967
14	6	0	-2.690096	0.434273	-0.913080
15	6	0	-4.034456	0.214843	-1.205471
16	6	0	-4.873801	-0.342231	-0.231232
17	6	0	-4.361312	-0.678539	1.026022
18	6	0	-3.007444	-0.458170	1.298289
19	8	0	-6.190161	-0.531540	-0.570682
20	8	0	1.822807	2.977767	-0.111486
21	1	0	5.281196	-0.447974	-0.120544
22	1	0	1.647782	-2.797606	-0.194051
23	1	0	3.800525	-3.650591	-0.317893
24	1	0	3.220781	2.537336	-0.029676
25	1	0	-0.841077	2.510513	0.239220
26	1	0	-0.527429	0.106210	1.715924
27	1	0	-2.041769	0.873550	-1.665473
28	1	0	-4.447074	0.471871	-2.176163
29	1	0	-5.011325	-1.108253	1.783733
30	1	0	-2.614510	-0.726611	2.275744
31	1	0	-6.676947	-0.918581	0.170966

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.854803	0.641972	1.085377
2	6	0	2.349859	-0.351251	0.219366
3	6	0	3.278569	-1.064585	-0.566750
4	6	0	4.642456	-0.803928	-0.489353
5	6	0	5.117278	0.189877	0.381384
6	6	0	4.217601	0.914497	1.171191

7	6	0	0.905641	-0.573426	0.162364
8	6	0	0.250214	-1.555918	-0.487102
9	6	0	-1.207454	-1.770166	-0.388436
10	8	0	-1.572556	-2.990096	-0.330676
11	8	0	6.444631	0.495899	0.497517
12	6	0	-2.170510	-0.694680	-0.252275
13	6	0	-1.946066	0.666429	-0.743049
14	6	0	-2.897016	1.662156	-0.361451
15	6	0	-4.041337	1.330823	0.350187
16	6	0	-4.332950	0.007426	0.724510
17	6	0	-3.420438	-0.986699	0.396872
18	8	0	-0.968864	0.966111	-1.522257
19	8	0	-3.733741	-2.260318	0.746740
20	8	0	-4.975511	2.271661	0.702265
21	8	0	0.943116	2.744969	-1.020218
22	1	0	-5.254578	-0.236697	1.239479
23	1	0	-2.727447	2.681114	-0.699603
24	1	0	-4.695559	3.145521	0.393710
25	1	0	-3.005047	-2.829700	0.361802
26	1	0	0.782731	-2.354094	-0.998756
27	1	0	0.308668	0.149642	0.713758
28	1	0	2.163828	1.207607	1.705108
29	1	0	4.594164	1.681381	1.840130
30	1	0	5.340465	-1.363407	-1.106350
31	1	0	2.934437	-1.828420	-1.256428
32	1	0	6.975929	-0.056939	-0.093625
33	1	0	0.201135	2.100650	-1.191154
34	1	0	1.680784	2.202345	-0.712058

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.485114	0.548946	-0.206314
2	6	0	-2.117112	-0.709364	0.068664
3	6	0	-3.532655	-0.725738	0.202107
4	6	0	-4.297804	0.442952	0.152212
5	6	0	-3.648464	1.652238	-0.105951
6	6	0	-2.266189	1.716447	-0.303286
7	6	0	-1.375746	-1.993454	-0.038913
8	8	0	-2.050451	-3.078360	-0.259875
9	8	0	-4.174856	-1.909698	0.359962
10	8	0	-4.433976	2.777100	-0.153093
11	8	0	-0.167527	0.653904	-0.398997
12	6	0	0.023594	-1.939937	-0.002391
13	6	0	0.644524	-0.755320	0.485483
14	6	0	2.090016	-0.510160	0.311821
15	6	0	2.781105	-0.937031	-0.834453
16	6	0	4.135377	-0.658890	-1.005777
17	6	0	4.825269	0.065695	-0.023032
18	6	0	4.154726	0.507673	1.124918
19	6	0	2.800129	0.222107	1.280297
20	8	0	6.152505	0.376204	-0.131085
21	8	0	1.401360	2.893058	-0.234645
22	1	0	-5.374962	0.401217	0.266521
23	1	0	-1.774349	2.664529	-0.499287
24	1	0	-3.893056	3.551330	-0.364706
25	1	0	-3.461988	-2.605584	0.132852
26	1	0	0.607571	-2.751024	-0.424556
27	1	0	0.260323	-0.351340	1.423295
28	1	0	2.282136	0.574995	2.168092
29	1	0	4.700386	1.068839	1.876473
30	1	0	4.655060	-0.992281	-1.900160
31	1	0	2.249412	-1.480477	-1.609019
32	1	0	6.517506	0.027392	-0.957158
33	1	0	0.794273	2.117747	-0.294883
34	1	0	2.231320	2.519995	0.092090

INT2-1w

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.873323	0.160917	1.336682
2	6	0	2.035681	-0.448206	0.392294
3	6	0	2.587011	-0.829882	-0.838072
4	6	0	3.934458	-0.610616	-1.124720
5	6	0	4.754873	0.004354	-0.169136
6	6	0	4.223828	0.389668	1.067281
7	6	0	0.560275	-0.608931	0.668411
8	6	0	-0.040610	-1.912708	0.230563
9	6	0	-1.395211	-1.997516	0.042478
10	8	0	-2.090101	-3.094871	-0.189286
11	8	0	6.084974	0.252500	-0.386345
12	6	0	-2.151755	-0.717162	0.064182
13	6	0	-1.474558	0.511084	0.012896
14	6	0	-2.148438	1.731030	-0.075239
15	6	0	-3.549912	1.712398	-0.107092
16	6	0	-4.267348	0.514633	-0.068577
17	6	0	-3.566062	-0.697035	-0.001309
18	8	0	-0.102546	0.535551	-0.015395
19	8	0	-4.236484	-1.870728	-0.024012
20	8	0	-4.283336	2.872605	-0.171595
21	8	0	1.567212	2.821206	-0.326294
22	1	0	-5.350876	0.519771	-0.112558
23	1	0	-1.591599	2.662136	-0.103169
24	1	0	-3.693724	3.639123	-0.206320
25	1	0	-3.466517	-2.578419	-0.101455
26	1	0	0.591092	-2.794698	0.201328
27	1	0	0.383930	-0.407266	1.739676
28	1	0	2.463804	0.471275	2.294581
29	1	0	4.870217	0.861403	1.800385
30	1	0	4.347370	-0.910903	-2.084282
31	1	0	1.950581	-1.300601	-1.581223
32	1	0	6.344429	-0.043813	-1.270526
33	1	0	0.960398	2.060979	-0.232631
34	1	0	2.419802	2.478736	-0.024236

INT1-1wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.899859	0.669461	-0.432784
2	6	0	-2.033755	-0.775450	-0.227191
3	6	0	-3.284597	-1.270783	0.290311
4	6	0	-4.293507	-0.426093	0.734412
5	6	0	-4.103408	0.960721	0.616426
6	6	0	-2.959630	1.500633	0.048596
7	6	0	-1.002985	-1.746214	-0.547506
8	8	0	-1.298672	-2.978551	-0.708344
9	8	0	-3.509395	-2.604546	0.389577
10	8	0	-5.129856	1.748448	1.072099
11	8	0	-0.899060	1.192329	-1.046009
12	6	0	0.440797	-1.456059	-0.626393
13	6	0	1.085371	-0.542647	0.127643
14	6	0	2.527818	-0.313317	0.199619
15	6	0	3.475697	-1.073862	-0.516381
16	6	0	4.837261	-0.803413	-0.427254
17	6	0	5.289951	0.244457	0.389793
18	6	0	4.371376	1.012508	1.114167
19	6	0	3.011686	0.730135	1.016014
20	8	0	6.614814	0.559173	0.518955
21	8	0	-0.667096	3.789403	-1.485909
22	1	0	-5.212104	-0.832128	1.141151
23	1	0	-2.858675	2.575282	-0.073429
24	1	0	-4.914109	2.682603	0.937189
25	1	0	-2.721530	-3.038183	-0.060601
26	1	0	0.988039	-2.168219	-1.239470
27	1	0	0.485041	0.112295	0.752905
28	1	0	2.305406	1.333084	1.580446
29	1	0	4.732068	1.819728	1.743390
30	1	0	5.550558	-1.402904	-0.986580
31	1	0	3.150859	-1.891109	-1.152132
32	1	0	7.159333	-0.029535	-0.023458
33	1	0	-0.800307	2.809221	-1.314467

34	1	0	-1.523764	4.119352	-1.784720

TS2-1wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.794643	-0.795895	-0.743854
2	6	0	2.092076	-0.497008	0.436595
3	6	0	2.785980	0.151204	1.473385
4	6	0	4.135397	0.473432	1.353984
5	6	0	4.817374	0.161897	0.171275
6	6	0	4.143483	-0.473811	-0.882503
7	6	0	0.648948	-0.778687	0.576782
8	6	0	0.036366	-1.873904	-0.093622
9	6	0	-1.361797	-1.929578	-0.163353
10	8	0	-2.017585	-2.980169	-0.549575
11	8	0	6.138451	0.507018	0.099446
12	6	0	-2.119755	-0.678643	0.095422
13	6	0	-3.541645	-0.721552	0.150364
14	6	0	-4.319756	0.437402	0.207243
15	6	0	-3.675935	1.675248	0.134853
16	6	0	-2.287253	1.774872	0.023414
17	6	0	-1.492666	0.610918	0.024152
18	8	0	-4.174725	-1.920307	0.121318
19	8	0	-0.170275	0.760766	-0.053602
20	8	0	-4.475680	2.790158	0.184266
21	1	0	-5.400680	0.372618	0.256994
22	1	0	-1.797772	2.743288	-0.020285
23	1	0	-3.936658	3.589343	0.097471
24	1	0	-3.440801	-2.574992	-0.162075
25	1	0	0.627511	-2.612330	-0.624963
26	1	0	0.263789	-0.526741	1.565395
27	1	0	2.258145	0.407754	2.387927
28	1	0	4.667893	0.969216	2.159075
29	1	0	4.671036	-0.708640	-1.803070
30	1	0	2.277144	-1.269034	-1.572190
31	1	0	6.511263	0.253018	-0.757240
32	1	0	0.834925	1.715919	-1.141836
33	8	0	1.480960	2.189335	-1.715390
34	1	0	2.282258	1.650820	-1.661734

INT2-1wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.477276	0.525752	0.147849
2	6	0	-2.143137	-0.706451	0.062058
3	6	0	-3.555321	-0.690416	-0.042572
4	6	0	-4.266316	0.517228	-0.018262
5	6	0	-3.560043	1.718533	0.076012
6	6	0	-2.160548	1.743834	0.153580
7	6	0	-1.373813	-1.973086	-0.059209
8	8	0	-2.053443	-3.050795	-0.402593
9	8	0	-4.213268	-1.861536	-0.193826
10	8	0	-4.302962	2.874401	0.096198
11	8	0	-0.105828	0.568332	0.168254
12	6	0	-0.024045	-1.895748	0.161301
13	6	0	0.562982	-0.636468	0.729969
14	6	0	2.038231	-0.438703	0.473756
15	6	0	2.597432	-0.717144	-0.780868
16	6	0	3.943041	-0.456863	-1.045705
17	6	0	4.755000	0.083719	-0.038454
18	6	0	4.216217	0.360048	1.222976
19	6	0	2.866744	0.102388	1.465849
20	8	0	6.083365	0.360450	-0.229821
21	8	0	1.511565	2.436409	-1.249731
22	1	0	-5.348075	0.518520	-0.094416
23	1	0	-1.610654	2.676216	0.231772
24	1	0	-3.720149	3.645272	0.145663
25	1	0	-3.433487	-2.554150	-0.310924

26	1	0	0.613936	-2.768413	0.064305
27	1	0	0.384536	-0.546223	1.815792
28	1	0	2.450720	0.331423	2.443607
29	1	0	4.855958	0.776351	1.994515
30	1	0	4.361513	-0.674389	-2.024925
31	1	0	1.968564	-1.133414	-1.561997
32	1	0	6.349800	0.133448	-1.132265
33	1	0	0.927402	1.823634	-0.762094
34	1	0	2.329620	1.933904	-1.366550

INT1-2w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.067760	0.942595	-0.707629
2	6	0	-2.722718	-0.306602	-0.150390
3	6	0	-3.770725	-1.113860	0.339388
4	6	0	-5.095473	-0.694209	0.280142
5	6	0	-5.408917	0.556205	-0.275931
6	6	0	-4.389052	1.375859	-0.772431
7	6	0	-1.312278	-0.686449	-0.098156
8	6	0	-0.784065	-1.816532	0.415323
9	6	0	0.633580	-2.205437	0.301134
10	8	0	0.827859	-3.459925	0.160446
11	8	0	-6.690946	1.024670	-0.360466
12	6	0	1.748547	-1.275808	0.256809
13	6	0	1.726333	0.077111	0.813870
14	6	0	2.887909	0.872731	0.620901
15	6	0	3.952200	0.457652	-0.160825
16	6	0	4.031703	-0.861164	-0.641693
17	6	0	2.966813	-1.717525	-0.382458
18	8	0	0.730144	0.581373	1.464208
19	8	0	3.087274	-2.998493	-0.817140
20	8	0	4.961111	1.328729	-0.473097
21	8	0	0.776089	3.162703	0.726899
22	8	0	3.314315	3.719685	-0.491667
23	1	0	4.890612	-1.207782	-1.204683
24	1	0	2.901810	1.858095	1.063514
25	1	0	4.611631	2.237763	-0.357726
26	1	0	2.264078	-3.468381	-0.485988
27	1	0	-1.416947	-2.607794	0.810335
28	1	0	-0.628043	0.044750	-0.517863
29	1	0	-2.281612	1.585959	-1.093993
30	1	0	-4.642549	2.340094	-1.200928
31	1	0	-5.887977	-1.331849	0.662715
32	1	0	-3.554538	-2.084680	0.773405
33	1	0	-7.312969	0.383874	0.013280
34	1	0	0.701301	2.209533	1.039677
35	1	0	2.422524	3.561417	-0.106012
36	1	0	3.528505	4.642802	-0.305677
37	1	0	-0.019173	3.338847	0.208157

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.311259	0.030686	-0.415216
2	6	0	-1.793617	-1.238637	0.041936
3	6	0	-3.198135	-1.388802	0.212412
4	6	0	-4.085892	-0.316742	0.069663
5	6	0	-3.574748	0.913088	-0.358071
6	6	0	-2.225218	1.059760	-0.683677
7	6	0	-0.905318	-2.425737	0.105960
8	8	0	-1.442143	-3.603913	0.040195
9	8	0	-3.700672	-2.608389	0.537734
10	8	0	-4.418670	1.989493	-0.440683
11	8	0	-0.009565	0.297855	-0.597642
12	6	0	0.476829	-2.192279	0.126074
13	6	0	0.942495	-0.887224	0.457489
14	6	0	2.354536	-0.498925	0.267625

15	6	0	3.130255	-1.007445	-0.788019
16	6	0	4.454084	-0.611482	-0.966328
17	6	0	5.026306	0.315854	-0.083201
18	6	0	4.269796	0.841170	0.971478
19	6	0	2.946945	0.437199	1.133529
20	8	0	6.318381	0.749938	-0.204778
21	8	0	0.129876	2.961510	0.215146
22	8	0	-2.533862	4.012110	0.264004
23	1	0	-5.141669	-0.443956	0.281472
24	1	0	-1.860458	2.003490	-1.062983
25	1	0	-3.872862	2.802912	-0.373354
26	1	0	-2.917732	-3.243022	0.391748
27	1	0	1.162336	-2.973543	-0.185195
28	1	0	0.494693	-0.419130	1.335493
29	1	0	2.362857	0.850681	1.951537
30	1	0	4.724654	1.559506	1.645805
31	1	0	5.040627	-1.012684	-1.788709
32	1	0	2.690106	-1.712859	-1.485684
33	1	0	6.745845	0.335108	-0.967824
34	1	0	0.187896	2.008849	-0.043147
35	1	0	-1.608082	3.682296	0.287032
36	1	0	-2.486666	4.926404	-0.043654
37	1	0	0.689333	3.064197	0.995732

INT2-2w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.058714	0.445622	1.151689
2	6	0	2.313896	-0.370063	0.289723
3	6	0	2.940357	-0.868653	-0.860689
4	6	0	4.271631	-0.565721	-1.146680
5	6	0	5.000999	0.247523	-0.268242
6	6	0	4.393758	0.754404	0.885319
7	6	0	0.863945	-0.671431	0.578267
8	6	0	0.459106	-2.106465	0.397981
9	6	0	-0.870679	-2.416417	0.266222
10	8	0	-1.405680	-3.621010	0.270163
11	8	0	6.314221	0.578887	-0.486655
12	6	0	-1.794200	-1.271545	0.054235
13	6	0	-1.286970	-0.003862	-0.269471
14	6	0	-2.120185	1.060697	-0.597413
15	6	0	-3.506504	0.891717	-0.493906
16	6	0	-4.060337	-0.356807	-0.194011
17	6	0	-3.200394	-1.440143	0.043299
18	8	0	0.069577	0.226486	-0.307634
19	8	0	-3.710341	-2.673724	0.275398
20	8	0	-4.341324	1.964269	-0.672840
21	8	0	0.078042	3.040878	0.553618
22	8	0	-2.620968	4.021744	0.281265
23	1	0	-5.135508	-0.487289	-0.135201
24	1	0	-1.702871	2.013709	-0.886549
25	1	0	-3.823224	2.781560	-0.505501
26	1	0	-2.861662	-3.277216	0.306401
27	1	0	1.211228	-2.879266	0.520488
28	1	0	0.629366	-0.301710	1.592648
29	1	0	2.591082	0.845389	2.048074
30	1	0	4.969758	1.381564	1.558307
31	1	0	4.744207	-0.959834	-2.042764
32	1	0	2.377441	-1.503437	-1.538404
33	1	0	6.632785	0.174469	-1.306263
34	1	0	0.213186	2.102239	0.315691
35	1	0	-1.695994	3.728795	0.426041
36	1	0	-2.567006	4.927291	-0.050766
37	1	0	0.570181	3.180352	1.373327

INT1-3w

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

1	6	0	-3.263056	-1.616882	0.396865
2	6	0	-2.041355	-1.340098	-0.316468
3	6	0	-1.867540	-0.007254	-0.893324
4	6	0	-2.877640	0.951106	-0.605251
5	6	0	-3.930274	0.681875	0.252368
6	6	0	-4.174591	-0.620467	0.728398
7	6	0	-1.040023	-2.385687	-0.379419
8	8	0	-1.357202	-3.612769	-0.249037
9	8	0	-0.871085	0.332266	-1.637533
10	8	0	-4.770947	1.688304	0.647667
11	8	0	-3.526852	-2.875805	0.837372
12	6	0	0.408645	-2.109082	-0.472677
13	6	0	0.994503	-1.062857	0.142964
14	6	0	2.422187	-0.756571	0.216771
15	6	0	2.865719	0.219694	1.134021
16	6	0	4.211107	0.567876	1.239257
17	6	0	5.153079	-0.058161	0.412937
18	6	0	4.737892	-1.031343	-0.508425
19	6	0	3.391225	-1.370441	-0.601656
20	8	0	6.458314	0.323143	0.548075
21	8	0	-0.464639	2.915083	-0.848953
22	8	0	-2.748645	3.790546	0.586713
23	8	0	2.357391	3.134122	-0.399313
24	1	0	-5.034485	-0.843758	1.349334
25	1	0	-2.779766	1.935679	-1.040043
26	1	0	-4.292994	2.534891	0.520659
27	1	0	-2.795724	-3.448905	0.468295
28	1	0	0.993061	-2.900801	-0.935648
29	1	0	0.347405	-0.353195	0.653172
30	1	0	2.142066	0.705278	1.784033
31	1	0	4.541838	1.316472	1.951871
32	1	0	5.467179	-1.511979	-1.154925
33	1	0	3.091020	-2.113107	-1.333941
34	1	0	7.023496	-0.168380	-0.065464
35	1	0	-0.560718	1.982673	-1.188434
36	1	0	-1.917421	3.520289	0.130067
37	1	0	-2.824126	4.745557	0.465511
38	1	0	0.483928	3.031253	-0.651552
39	1	0	2.733827	2.292887	-0.095682
40	1	0	2.831485	3.345780	-1.215345

TS2-3w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.773116	-0.105751	1.190251
2	6	0	2.096644	-0.932413	0.277008
3	6	0	2.821287	-1.448992	-0.810471
4	6	0	4.175075	-1.166018	-0.977639
5	6	0	4.834917	-0.352029	-0.045325
6	6	0	4.130416	0.181514	1.043146
7	6	0	0.653727	-1.194811	0.448861
8	6	0	0.065675	-2.437936	0.087800
9	6	0	-1.335912	-2.528600	0.062583
10	8	0	-1.988885	-3.643209	-0.027283
11	8	0	6.161131	-0.039218	-0.145700
12	6	0	-2.097141	-1.255651	0.024346
13	6	0	-1.487754	-0.034866	-0.416190
14	6	0	-2.291534	1.088921	-0.657559
15	6	0	-3.645459	1.079112	-0.320292
16	6	0	-4.280659	-0.099008	0.088428
17	6	0	-3.508713	-1.260564	0.203255
18	8	0	-0.169233	0.100958	-0.602728
19	8	0	-4.134369	-2.427404	0.509945
20	8	0	-4.369316	2.241160	-0.371921
21	8	0	0.200518	2.697319	0.418551
22	8	0	-2.260373	4.085082	0.240967
23	1	0	-5.342506	-0.119203	0.307109
24	1	0	-1.828862	1.997311	-1.015354
25	1	0	-3.736667	2.990760	-0.324987
26	1	0	-3.425508	-3.137287	0.345518
27	1	0	0.669623	-3.272557	-0.253168
28	1	0	0.240338	-0.697196	1.327014
29	1	0	2.230374	0.319541	2.029983

30	1	0	4.655018	0.800938	1.764001
31	1	0	4.718828	-1.568929	-1.827873
32	1	0	2.315219	-2.068786	-1.543913
33	1	0	6.553160	-0.461061	-0.923999
34	1	0	0.149284	1.781471	0.060934
35	1	0	-1.367902	3.670733	0.290542
36	1	0	-2.126960	4.973149	-0.114136
37	1	0	1.120992	2.978809	0.251066
38	8	0	2.964033	3.116903	-0.098162
39	1	0	3.340029	2.236390	0.064885
40	1	0	3.185375	3.325750	-1.016196

INT2-3w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.556325	-1.246933	-0.047407
2	6	0	2.140288	-1.261857	-0.040375
3	6	0	1.480839	-0.060409	0.257515
4	6	0	2.171894	1.111528	0.543121
5	6	0	3.566172	1.120270	0.422035
6	6	0	4.272987	-0.055260	0.146668
7	6	0	1.364639	-2.519825	-0.204038
8	8	0	2.045704	-3.646904	-0.172517
9	8	0	0.107742	-0.004312	0.308432
10	8	0	4.254119	2.297809	0.559491
11	8	0	4.217528	-2.412101	-0.252056
12	6	0	0.004415	-2.379479	-0.333152
13	6	0	-0.563242	-1.007414	-0.560956
14	6	0	-2.040289	-0.854550	-0.295195
15	6	0	-2.869497	-0.212415	-1.223108
16	6	0	-4.229165	-0.011662	-0.965214
17	6	0	-4.774251	-0.456526	0.245761
18	6	0	-3.959546	-1.103539	1.185557
19	6	0	-2.606900	-1.299057	0.907302
20	8	0	-6.109029	-0.232507	0.453288
21	8	0	-0.297537	2.767331	-0.612374
22	8	0	2.182354	4.146825	-0.227124
23	8	0	-3.058345	3.032774	-0.074800
24	1	0	5.355375	-0.049292	0.076293
25	1	0	1.635740	2.009647	0.809166
26	1	0	3.619603	3.036363	0.437379
27	1	0	3.455781	-3.119173	-0.248857
28	1	0	-0.650769	-3.240034	-0.423609
29	1	0	-0.358077	-0.642234	-1.583161
30	1	0	-2.450642	0.145695	-2.159944
31	1	0	-4.872270	0.475046	-1.691837
32	1	0	-4.382686	-1.450437	2.124650
33	1	0	-1.976818	-1.799531	1.636396
34	1	0	-6.378177	-0.567285	1.320756
35	1	0	-0.238019	1.833229	-0.337329
36	1	0	1.287650	3.761684	-0.357581
37	1	0	2.045024	5.037532	0.120185
38	1	0	-1.227983	3.010993	-0.431317
39	1	0	-3.397507	2.133373	-0.217137
40	1	0	-3.294518	3.255885	0.836148

INT1-3wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.459220	-0.198547	0.412673
2	6	0	-1.255176	-1.639053	0.265051
3	6	0	-2.353609	-2.420684	-0.247577
4	6	0	-3.515656	-1.840181	-0.735635
5	6	0	-3.654083	-0.440480	-0.671269
6	6	0	-2.661611	0.357895	-0.110375
7	6	0	-0.035944	-2.337293	0.627319
8	8	0	-0.047629	-3.597467	0.838350
9	8	0	-2.269530	-3.774746	-0.297578

10	8	0	-4.812221	0.081168	-1.155177
11	8	0	-0.608423	0.557702	1.024407
12	6	0	1.305382	-1.725829	0.691293
13	6	0	1.731748	-0.717849	-0.096655
14	6	0	3.087160	-0.177762	-0.191708
15	6	0	4.180048	-0.670870	0.551518
16	6	0	5.448108	-0.112029	0.431796
17	6	0	5.658224	0.964702	-0.444221
18	6	0	4.592076	1.472562	-1.194995
19	6	0	3.328340	0.903121	-1.065383
20	8	0	6.880947	1.555904	-0.606479
21	8	0	-1.018180	3.084033	1.085931
22	8	0	-3.581789	3.838818	1.145842
23	8	0	-5.031428	2.767445	-0.882239
24	1	0	-4.311321	-2.458788	-1.134594
25	1	0	-2.813181	1.426372	-0.018689
26	1	0	-4.835318	1.066379	-1.049137
27	1	0	-1.413698	-4.002763	0.176724
28	1	0	1.996872	-2.278128	1.323348
29	1	0	1.000534	-0.233407	-0.737633
30	1	0	2.506064	1.304889	-1.651417
31	1	0	4.765122	2.305070	-1.869252
32	1	0	6.276148	-0.508191	1.013566
33	1	0	4.044623	-1.503966	1.233541
34	1	0	7.543509	1.129678	-0.043782
35	1	0	-0.863391	2.067769	1.067771
36	1	0	-3.948114	3.620793	2.012942
37	1	0	-4.499284	3.176825	-0.152674
38	1	0	-4.839725	3.280178	-1.678444
39	1	0	-2.625197	3.557560	1.169715
40	1	0	-0.452342	3.440652	1.782557

TS2-3wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.211322	-1.075787	-0.819373
2	6	0	2.432583	-0.699579	0.287542
3	6	0	2.983494	0.211363	1.207091
4	6	0	4.269819	0.719777	1.043729
5	6	0	5.031142	0.324948	-0.063921
6	6	0	4.499543	-0.575977	-0.997997
7	6	0	1.047197	-1.177707	0.468133
8	6	0	0.630839	-2.470208	0.036559
9	6	0	-0.742560	-2.748820	0.006123
10	8	0	-1.236342	-3.935169	-0.167963
11	8	0	6.285735	0.856237	-0.182570
12	6	0	-1.678012	-1.596405	0.072700
13	6	0	-3.072377	-1.823393	0.234246
14	6	0	-4.006272	-0.785753	0.175379
15	6	0	-3.560422	0.509045	-0.116251
16	6	0	-2.202410	0.767029	-0.353245
17	6	0	-1.257738	-0.265845	-0.250391
18	8	0	-3.521911	-3.088596	0.436229
19	8	0	0.031158	0.028818	-0.484217
20	8	0	-4.490636	1.501981	-0.158418
21	8	0	-0.945573	4.232195	0.647040
22	8	0	-3.397290	3.960301	-0.514853
23	1	0	-5.061465	-0.989049	0.320847
24	1	0	-1.867011	1.770390	-0.584462
25	1	0	-4.064575	2.379854	-0.327661
26	1	0	-2.713119	-3.672175	0.223436
27	1	0	1.340064	-3.193502	-0.351928
28	1	0	0.593883	-0.802549	1.387307
29	1	0	2.394292	0.524727	2.065129
30	1	0	4.692909	1.418295	1.758294
31	1	0	5.088576	-0.874623	-1.861037
32	1	0	2.800383	-1.757046	-1.557620
33	1	0	6.722815	0.522722	-0.979476
34	1	0	0.594164	1.588725	-0.371134
35	1	0	-0.997573	4.127457	1.606278
36	1	0	-2.498206	4.075274	-0.116342
37	1	0	-3.336307	4.283586	-1.423345

38	8	0	0.931532	2.525717	-0.307696
39	1	0	-0.240994	3.605114	0.340891
40	1	0	1.781904	2.464788	0.148468

INT2-3wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276753	-0.278564	-0.033246
2	6	0	-1.763833	-1.589723	0.079091
3	6	0	-3.167837	-1.771119	0.046668
4	6	0	-4.035933	-0.675452	-0.045356
5	6	0	-3.506099	0.617330	-0.140885
6	6	0	-2.116098	0.828531	-0.144097
7	6	0	-0.828906	-2.746151	0.091171
8	8	0	-1.357638	-3.941122	-0.085830
9	8	0	-3.664469	-3.030429	0.081678
10	8	0	-4.383770	1.656523	-0.222390
11	8	0	0.081001	-0.062641	-0.099363
12	6	0	0.502392	-2.457119	0.253401
13	6	0	0.903831	-1.063364	0.636441
14	6	0	2.338418	-0.686536	0.358055
15	6	0	2.965929	-1.050288	-0.840628
16	6	0	4.265380	-0.633187	-1.130409
17	6	0	4.958300	0.165549	-0.210689
18	6	0	4.349095	0.538807	0.992874
19	6	0	3.048888	0.111600	1.265857
20	8	0	6.235598	0.610265	-0.432439
21	8	0	1.144493	2.472252	-0.357562
22	8	0	-0.656961	4.287105	0.596334
23	8	0	-3.174704	4.078005	-0.435108
24	1	0	-5.109531	-0.829479	-0.062592
25	1	0	-1.701412	1.826203	-0.213611
26	1	0	-3.906421	2.519411	-0.308295
27	1	0	-2.807377	-3.622592	0.013317
28	1	0	1.256437	-3.237647	0.247212
29	1	0	0.687378	-0.843488	1.696906
30	1	0	2.577989	0.409103	2.199477
31	1	0	4.897576	1.154258	1.698729
32	1	0	4.739297	-0.923121	-2.064608
33	1	0	2.428135	-1.664937	-1.556059
34	1	0	6.559898	0.295187	-1.288274
35	1	0	0.785094	1.560338	-0.274522
36	1	0	-0.651393	4.243985	1.561720
37	1	0	-2.254547	4.166936	-0.083401
38	1	0	-3.161589	4.449607	-1.326947
39	1	0	0.025528	3.640830	0.289468
40	1	0	2.025901	2.433873	0.039432

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.225224	-0.233162	1.353944
2	6	0	1.633390	-1.168096	0.481379
3	6	0	2.490912	-1.958482	-0.313157
4	6	0	3.870810	-1.777584	-0.281196
5	6	0	4.431524	-0.792433	0.547192
6	6	0	3.603059	-0.047229	1.397541
7	6	0	0.177987	-1.187087	0.369981
8	6	0	-0.586344	-1.956247	-0.429917
9	6	0	-2.058024	-1.864011	-0.464301
10	8	0	-2.682122	-2.967999	-0.585350
11	8	0	5.777907	-0.561737	0.480401
12	6	0	-2.775112	-0.613312	-0.284838
13	6	0	-2.208301	0.703734	-0.579940
14	6	0	-2.957497	1.845851	-0.167063
15	6	0	-4.221494	1.715445	0.392272
16	6	0	-4.832698	0.463187	0.572604
17	6	0	-4.124296	-0.675163	0.209264

18	8	0	-1.100267	0.851503	-1.220582
19	8	0	-4.743685	-1.871803	0.370604
20	8	0	-4.963391	2.804943	0.770523
21	8	0	0.803999	2.485537	-0.531525
22	8	0	5.460659	2.131772	0.089119
23	8	0	3.220201	1.639857	-1.464485
24	1	0	-5.838769	0.384765	0.967346
25	1	0	-2.533223	2.827525	-0.359643
26	1	0	-4.468597	3.618674	0.596108
27	1	0	-4.115844	-2.551990	-0.012524
28	1	0	-0.167459	-2.765006	-1.023860
29	1	0	-0.329616	-0.439686	0.975131
30	1	0	1.587919	0.379746	1.985764
31	1	0	4.039884	0.705499	2.045354
32	1	0	4.523535	-2.356278	-0.927013
33	1	0	2.076379	-2.694967	-0.994168
34	1	0	5.904142	0.417251	0.493131
35	1	0	0.030795	1.882653	-0.785447
36	1	0	3.172748	0.672996	-1.452375
37	1	0	0.814418	2.502719	0.434175
38	1	0	2.342502	1.941836	-1.112417
39	1	0	4.650582	2.042185	-0.471875
40	1	0	6.109352	2.603037	-0.449930

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.933235	0.512556	-0.149609
2	6	0	-2.788673	-0.618351	0.050485
3	6	0	-4.186896	-0.382334	0.152203
4	6	0	-4.724534	0.908063	0.141870
5	6	0	-3.859038	1.987771	-0.043211
6	6	0	-2.482354	1.806670	-0.208023
7	6	0	-2.287727	-2.011346	-0.094941
8	8	0	-3.143499	-2.945569	-0.376857
9	8	0	-5.036760	-1.434876	0.239322
10	8	0	-4.424410	3.238566	-0.052850
11	8	0	-0.608519	0.378854	-0.308833
12	6	0	-0.906293	-2.213729	-0.023317
13	6	0	-0.091939	-1.176014	0.521483
14	6	0	1.377354	-1.183654	0.379429
15	6	0	2.019483	-1.764419	-0.728375
16	6	0	3.400526	-1.673426	-0.888193
17	6	0	4.170463	-0.981235	0.059005
18	6	0	3.549472	-0.421231	1.186166
19	6	0	2.168822	-0.517372	1.330341
20	8	0	5.512952	-0.857164	-0.157134
21	8	0	1.068268	2.451781	0.081058
22	8	0	3.465738	2.031496	-1.172707
23	1	0	-5.794203	1.059352	0.231267
24	1	0	-1.821215	2.656585	-0.347766
25	1	0	-3.744545	3.908348	-0.213409
26	1	0	-4.451955	-2.239613	-0.001438
27	1	0	-0.468602	-3.109093	-0.451540
28	1	0	-0.417253	-0.750978	1.472747
29	1	0	1.691463	-0.055961	2.190916
30	1	0	4.147382	0.113353	1.916745
31	1	0	3.892337	-2.099954	-1.756787
32	1	0	1.429589	-2.265405	-1.489345
33	1	0	5.798909	0.026296	0.180035
34	1	0	0.445309	1.687630	-0.050489
35	1	0	3.397135	1.137142	-1.536457
36	1	0	1.178890	2.533083	1.037592
37	1	0	2.609229	2.175987	-0.697327
38	8	0	5.695243	1.797636	0.431957
39	1	0	4.900373	1.995709	-0.122987
40	1	0	6.422457	2.310025	0.054723

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.244618	-0.560030	1.383104
2	6	0	1.346251	-1.084634	0.444771
3	6	0	1.859530	-1.601443	-0.752878
4	6	0	3.229388	-1.574095	-1.019971
5	6	0	4.111917	-1.018216	-0.083280
6	6	0	3.616168	-0.529298	1.133739
7	6	0	-0.140012	-1.002748	0.692856
8	6	0	-0.947380	-2.168518	0.205107
9	6	0	-2.291612	-2.014520	-0.008341
10	8	0	-3.157809	-2.970729	-0.283801
11	8	0	5.445057	-0.958141	-0.392080
12	6	0	-2.819120	-0.624816	0.038177
13	6	0	-1.943598	0.471849	0.039577
14	6	0	-2.399806	1.790557	-0.020543
15	6	0	-3.783326	2.009578	-0.080875
16	6	0	-4.693258	0.950513	-0.093567
17	6	0	-4.208203	-0.363647	-0.052525
18	8	0	-0.583979	0.263157	0.035255
19	8	0	-5.066292	-1.405172	-0.125396
20	8	0	-4.308318	3.278566	-0.124468
21	8	0	1.119968	2.468836	0.290803
22	8	0	5.773670	1.676458	0.260996
23	8	0	3.428577	2.029417	-1.159269
24	1	0	-5.758937	1.140124	-0.158925
25	1	0	-1.694569	2.615406	-0.008388
26	1	0	-3.596189	3.933436	-0.138054
27	1	0	-4.424565	-2.231644	-0.209217
28	1	0	-0.478015	-3.145965	0.161639
29	1	0	-0.303595	-0.801342	1.766151
30	1	0	1.865733	-0.156189	2.318869
31	1	0	4.302083	-0.103873	1.859073
32	1	0	3.624655	-1.954483	-1.956906
33	1	0	1.175994	-2.011615	-1.490072
34	1	0	5.795641	-0.099611	-0.054803
35	1	0	0.540867	1.678470	0.217705
36	1	0	3.300251	1.136994	-1.512972
37	1	0	1.302303	2.565916	1.235256
38	1	0	2.621325	2.197985	-0.616573
39	1	0	4.945253	1.917357	-0.221742
40	1	0	6.485434	2.176704	-0.159462

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.677725	-2.299979	-0.244863
2	6	0	1.778881	-1.431964	0.407704
3	6	0	2.316901	-0.344182	1.124670
4	6	0	3.685599	-0.105982	1.168208
5	6	0	4.548939	-0.957874	0.476452
6	6	0	4.050466	-2.068869	-0.216501
7	6	0	0.326334	-1.534335	0.308603
8	6	0	-0.415522	-2.454340	-0.338674
9	6	0	-1.890645	-2.391116	-0.357228
10	8	0	-2.507173	-3.502239	-0.269428
11	8	0	5.883458	-0.617001	0.475027
12	6	0	-2.605519	-1.128446	-0.368838
13	6	0	-3.905510	-1.085790	0.250802
14	6	0	-4.555710	0.109538	0.537748
15	6	0	-3.950122	1.308412	0.114569
16	6	0	-2.804569	1.303477	-0.662940
17	6	0	-2.059678	0.117973	-0.912273
18	8	0	-4.510503	-2.237408	0.647869
19	8	0	-0.965414	0.194485	-1.588830
20	8	0	-4.529528	2.494251	0.481365
21	8	0	0.060458	2.533679	-0.537515
22	8	0	2.857702	2.975272	-0.109022
23	8	0	5.467528	2.037325	-0.657805
24	8	0	-2.053697	3.994746	0.658784
25	1	0	-5.486882	0.111855	1.092587

26	1	0	-2.419099	2.232271	-1.060300
27	1	0	-3.837929	3.187243	0.422099
28	1	0	-3.919338	-2.977146	0.328801
29	1	0	0.020983	-3.339193	-0.795886
30	1	0	-0.208856	-0.716397	0.784346
31	1	0	1.645428	0.342528	1.631804
32	1	0	4.088391	0.747979	1.701980
33	1	0	4.729804	-2.730324	-0.747111
34	1	0	2.303730	-3.150528	-0.805790
35	1	0	6.406439	-1.265947	-0.018673
36	1	0	-0.198388	1.673588	-0.960538
37	1	0	-1.282387	3.514165	0.278105
38	1	0	-1.872686	4.935023	0.534273
39	1	0	1.028775	2.540565	-0.417297
40	1	0	3.718278	2.547639	-0.306902
41	1	0	3.000995	3.916897	-0.271782
42	1	0	5.702412	2.051305	-1.595294
43	1	0	5.772251	1.174459	-0.322620

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.006760	-0.776747	0.154216
2	6	0	-2.619238	-1.051135	0.001611
3	6	0	-1.773620	0.023669	-0.431372
4	6	0	-2.334280	1.284035	-0.684510
5	6	0	-3.669664	1.542307	-0.373213
6	6	0	-4.532206	0.513778	0.023451
7	6	0	-2.123161	-2.449075	0.066016
8	8	0	-2.979987	-3.414593	-0.038848
9	8	0	-0.453720	-0.109513	-0.599762
10	8	0	-4.149870	2.823913	-0.438291
11	8	0	-4.855664	-1.795773	0.451811
12	6	0	-0.732073	-2.634267	0.134200
13	6	0	0.068734	-1.517820	0.497613
14	6	0	1.538100	-1.493618	0.362183
15	6	0	2.283236	-0.624501	1.177638
16	6	0	3.656217	-0.474805	1.011931
17	6	0	4.303210	-1.192357	0.002689
18	6	0	3.591426	-2.081046	-0.811118
19	6	0	2.216369	-2.222592	-0.628438
20	8	0	5.647775	-0.941730	-0.169099
21	8	0	0.434216	2.422562	0.327427
22	8	0	-1.733854	4.228454	0.200087
23	8	0	3.188914	2.939742	0.603003
24	1	0	-5.581063	0.704190	0.221888
25	1	0	-1.693995	2.081292	-1.033022
26	1	0	-3.382905	3.434880	-0.382559
27	1	0	-4.297919	-2.632170	0.302606
28	1	0	-0.293356	-3.573739	-0.185785
29	1	0	-0.277580	-0.934841	1.351905
30	1	0	1.774829	-0.039936	1.938929
31	1	0	4.224895	0.209083	1.632713
32	1	0	4.102366	-2.634488	-1.594089
33	1	0	1.661784	-2.885382	-1.284868
34	1	0	6.014408	-1.490760	-0.878112
35	1	0	0.265452	1.512232	-0.000714
36	1	0	-0.936070	3.652246	0.245503
37	1	0	-1.436299	5.072912	-0.161774
38	1	0	1.404574	2.545005	0.374533
39	1	0	3.952438	2.517217	0.150940
40	1	0	3.373428	3.888043	0.588298
41	8	0	5.488952	1.903995	-0.614337
42	1	0	5.554941	2.091270	-1.560328
43	1	0	5.678236	0.951537	-0.519373

INT2-4w

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

1	6	0	2.050359	-1.995202	-0.746861
2	6	0	1.486660	-1.429256	0.403748
3	6	0	2.334336	-0.799402	1.324448
4	6	0	3.706949	-0.709265	1.099324
5	6	0	4.241672	-1.248329	-0.072500
6	6	0	3.422291	-1.910421	-0.992434
7	6	0	-0.006929	-1.358639	0.597524
8	6	0	-0.807998	-2.575372	0.236003
9	6	0	-2.164348	-2.436992	0.062815
10	8	0	-3.049202	-3.402757	-0.077437
11	8	0	5.594233	-1.060440	-0.280675
12	6	0	-2.676814	-1.042337	-0.013062
13	6	0	-4.062231	-0.749908	-0.039729
14	6	0	-4.526783	0.570274	-0.157431
15	6	0	-3.595204	1.601505	-0.322347
16	6	0	-2.225734	1.328633	-0.403499
17	6	0	-1.787237	0.026489	-0.197047
18	8	0	-4.944229	-1.774992	0.053848
19	8	0	-0.431133	-0.186165	-0.215106
20	8	0	-4.035257	2.898159	-0.390147
21	8	0	0.627215	2.459955	0.657574
22	8	0	3.078568	2.840552	-0.625191
23	8	0	5.599926	1.801917	-0.062664
24	8	0	-1.599366	4.265101	0.455692
25	1	0	-5.589906	0.781944	-0.117917
26	1	0	-1.513216	2.118050	-0.582360
27	1	0	-3.267608	3.488712	-0.237428
28	1	0	-4.334458	-2.614987	0.010004
29	1	0	-0.335308	-3.551725	0.273522
30	1	0	-0.202617	-1.035003	1.635592
31	1	0	1.913700	-0.351632	2.220816
32	1	0	4.360296	-0.205272	1.803876
33	1	0	3.847583	-2.335988	-1.897459
34	1	0	1.405538	-2.487508	-1.468486
35	1	0	5.873677	-1.467782	-1.113819
36	1	0	0.384161	1.546217	0.419647
37	1	0	-0.783948	3.719832	0.525825
38	1	0	-1.311127	5.150929	0.200770
39	1	0	1.510324	2.602801	0.252439
40	1	0	3.944690	2.426028	-0.411166
41	1	0	2.971497	2.741001	-1.580255
42	1	0	6.307227	2.263937	-0.532003
43	1	0	5.759531	0.849137	-0.202455

INT1-4wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.673555	1.280534	-0.497924
2	6	0	-2.619453	0.509423	0.037018
3	6	0	-2.942790	-0.747509	0.591712
4	6	0	-4.252768	-1.217821	0.620864
5	6	0	-5.279185	-0.431853	0.084804
6	6	0	-4.986175	0.821638	-0.476624
7	6	0	-1.223391	0.937877	0.029165
8	6	0	-0.736998	2.151823	-0.313678
9	6	0	0.679658	2.525453	-0.178558
10	8	0	0.910451	3.727347	0.178451
11	8	0	-6.550530	-0.935620	0.131144
12	6	0	1.770480	1.571571	-0.315481
13	6	0	2.950823	1.774446	0.473432
14	6	0	3.936062	0.801367	0.602000
15	6	0	3.791485	-0.395739	-0.117248
16	6	0	2.736545	-0.580025	-1.011641
17	6	0	1.716189	0.396819	-1.170493
18	8	0	3.118079	2.921618	1.186841
19	8	0	0.796976	0.225835	-2.073379
20	8	0	4.733786	-1.363299	0.076093
21	8	0	1.027072	-2.504465	0.605323
22	8	0	-0.258505	-1.619519	2.936985
23	8	0	3.443563	-3.779850	-0.289975
24	1	0	4.781416	0.957712	1.262281
25	1	0	2.700047	-1.464543	-1.638398

26	1	0	4.366822	-2.240691	-0.194137
27	1	0	2.364928	3.519497	0.927752
28	1	0	-1.397696	2.977587	-0.565268
29	1	0	-0.511563	0.178207	0.343957
30	1	0	-2.153906	-1.361498	1.015379
31	1	0	-4.489087	-2.185491	1.051356
32	1	0	-5.784090	1.425864	-0.898756
33	1	0	-3.468314	2.247487	-0.945145
34	1	0	-7.176323	-0.315338	-0.272531
35	1	0	-0.038154	-1.174737	-1.838723
36	1	0	1.582898	-1.715708	0.451192
37	1	0	2.545684	-3.500164	-0.008318
38	1	0	3.347803	-4.060583	-1.211553
39	1	0	0.157439	-1.937938	2.104843
40	1	0	-0.541727	-0.714744	2.745076
41	8	0	-0.529534	-2.025001	-1.624570
42	1	0	0.390812	-2.457907	-0.152037
43	1	0	-1.409402	-1.741407	-1.336363

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.217700	1.295353	-0.848448
2	6	0	-2.400227	0.653224	0.098322
3	6	0	-2.937357	-0.429639	0.818761
4	6	0	-4.250459	-0.848591	0.622427
5	6	0	-5.049870	-0.188489	-0.319820
6	6	0	-4.531040	0.882904	-1.061793
7	6	0	-1.002430	1.058693	0.328524
8	6	0	-0.586619	2.425049	0.236164
9	6	0	0.780521	2.703194	0.228540
10	8	0	1.280101	3.903068	0.335088
11	8	0	-6.333293	-0.636814	-0.478566
12	6	0	1.711243	1.571360	-0.008285
13	6	0	3.101383	1.725764	0.225063
14	6	0	4.020882	0.710913	-0.052906
15	6	0	3.558468	-0.465761	-0.649537
16	6	0	2.207612	-0.620772	-0.995316
17	6	0	1.274904	0.372210	-0.654940
18	8	0	3.567423	2.895780	0.742753
19	8	0	-0.019516	0.169166	-0.962977
20	8	0	4.464881	-1.460696	-0.884800
21	8	0	1.167008	-2.816441	0.983925
22	8	0	-0.326442	-2.069311	3.279536
23	8	0	3.141448	-3.870850	-0.812463
24	1	0	5.071437	0.840563	0.182487
25	1	0	1.870882	-1.517293	-1.501960
26	1	0	3.997784	-2.325913	-0.994127
27	1	0	2.777923	3.529288	0.677446
28	1	0	-1.308235	3.223430	0.096312
29	1	0	-0.515156	0.453590	1.094179
30	1	0	-2.318323	-0.946495	1.546360
31	1	0	-4.663838	-1.678023	1.186899
32	1	0	-5.152273	1.381301	-1.800515
33	1	0	-2.820077	2.119266	-1.432376
34	1	0	-6.798833	-0.100934	-1.138468
35	1	0	-0.565578	-1.434339	-0.951820
36	1	0	1.636893	-1.972656	0.862957
37	1	0	2.430049	-3.648467	-0.172933
38	1	0	2.684099	-4.098652	-1.634971
39	1	0	0.204465	-2.354182	2.504841
40	1	0	-0.430264	-1.113461	3.172215
41	8	0	-0.804102	-2.397752	-0.870569
42	1	0	0.417424	-2.755145	0.337117
43	1	0	-1.694296	-2.403551	-0.489600

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.046635	-1.226428	-0.911097
2	6	0	2.378548	-0.559872	0.125501
3	6	0	3.068773	0.432090	0.835341
4	6	0	4.391229	0.754598	0.526879
5	6	0	5.039870	0.080720	-0.513941
6	6	0	4.366836	-0.913738	-1.236906
7	6	0	0.936816	-0.859281	0.446004
8	6	0	0.576775	-2.315038	0.536973
9	6	0	-0.739272	-2.679991	0.444638
10	8	0	-1.231874	-3.893557	0.649205
11	8	0	6.338696	0.436912	-0.782773
12	6	0	-1.698177	-1.618234	0.046476
13	6	0	-3.096534	-1.818406	0.087807
14	6	0	-3.987751	-0.822438	-0.327638
15	6	0	-3.478866	0.377197	-0.835095
16	6	0	-2.094455	0.583950	-0.954622
17	6	0	-1.230333	-0.406149	-0.488943
18	8	0	-3.579665	-3.007461	0.538368
19	8	0	0.125208	-0.195955	-0.617132
20	8	0	-4.371519	1.342123	-1.212577
21	8	0	-1.339069	2.920931	1.052400
22	8	0	0.205510	2.361350	3.385926
23	8	0	-3.189682	3.807456	-0.951403
24	1	0	-5.058428	-0.979617	-0.253561
25	1	0	-1.707256	1.494791	-1.393056
26	1	0	-3.926761	2.225472	-1.239900
27	1	0	-2.731849	-3.581166	0.659197
28	1	0	1.348782	-3.031514	0.799867
29	1	0	0.662592	-0.310572	1.361789
30	1	0	2.566743	0.963107	1.639772
31	1	0	4.923495	1.521239	1.080892
32	1	0	4.871137	-1.435528	-2.045303
33	1	0	2.528117	-1.997772	-1.472737
34	1	0	6.686743	-0.085633	-1.521030
35	1	0	0.645977	1.546870	-0.709709
36	1	0	-1.759191	2.046676	0.985038
37	1	0	-2.536625	3.629433	-0.239917
38	1	0	-2.665663	4.082154	-1.717775
39	1	0	-0.357240	2.599968	2.619536
40	1	0	0.555041	1.485264	3.169921
41	8	0	0.789240	2.517067	-0.643793
42	1	0	-0.552097	2.851471	0.455237
43	1	0	1.651157	2.610533	-0.212288

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.330517	-1.309334	0.856960
2	6	0	-3.328505	-0.022108	0.279886
3	6	0	-4.559261	0.484539	-0.187560
4	6	0	-5.731994	-0.256536	-0.086815
5	6	0	-5.703676	-1.535729	0.491071
6	6	0	-4.496438	-2.062275	0.964033
7	6	0	-2.063635	0.704550	0.186700
8	6	0	-1.854269	1.923675	-0.350889
9	6	0	-0.580388	2.664277	-0.282183
10	8	0	-0.711245	3.929368	-0.167084
11	8	0	-6.822372	-2.311821	0.619398
12	6	0	0.735683	2.051967	-0.242434
13	6	0	1.049383	0.728057	-0.776997
14	6	0	2.349797	0.204506	-0.527219
15	6	0	3.323206	0.948105	0.132530
16	6	0	3.071656	2.264052	0.562872
17	6	0	1.812648	2.807639	0.347211
18	8	0	0.205408	0.052217	-1.485558
19	8	0	1.614325	4.088868	0.749671
20	8	0	4.569718	0.455213	0.368104
21	8	0	0.674967	-2.420311	-1.944903
22	8	0	2.603288	-3.545008	-0.486135
23	8	0	4.886302	-2.161417	-0.407558
24	8	0	6.412298	-2.904674	1.836007

25	1	0	3.849370	2.852520	1.035822
26	1	0	2.584539	-0.782450	-0.906531
27	1	0	4.647784	-0.473970	0.045355
28	1	0	0.690144	4.324003	0.435392
29	1	0	-2.677318	2.519643	-0.738216
30	1	0	-1.205282	0.179732	0.596505
31	1	0	-2.397170	-1.726733	1.225315
32	1	0	-4.485604	-3.052211	1.408464
33	1	0	-6.669688	0.152556	-0.453859
34	1	0	-4.607790	1.471365	-0.636275
35	1	0	-7.598018	-1.852850	0.265994
36	1	0	0.496480	-1.425165	-1.757735
37	1	0	2.259437	-3.706110	0.402556
38	1	0	4.036400	-2.682169	-0.462626
39	1	0	5.341138	-2.283287	-1.252194
40	1	0	5.890344	-2.688155	1.035444
41	1	0	6.545634	-3.860645	1.804949
42	1	0	1.856027	-3.130293	-1.003423
43	1	0	-0.180092	-2.867566	-1.903477

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.772052	0.820255	-0.303739
2	6	0	0.829017	2.200241	0.074109
3	6	0	2.114991	2.788627	0.220593
4	6	0	3.291456	2.044424	0.096921
5	6	0	3.200168	0.691251	-0.248271
6	6	0	1.955982	0.085932	-0.473565
7	6	0	-0.384069	3.058855	0.079612
8	8	0	-0.232646	4.340402	-0.047724
9	8	0	2.213775	4.118816	0.472906
10	8	0	4.362463	-0.012620	-0.354477
11	8	0	-0.396666	0.198091	-0.526310
12	6	0	-1.629714	2.418109	0.123315
13	6	0	-1.667910	1.044602	0.501707
14	6	0	-2.877749	0.215974	0.328010
15	6	0	-3.766366	0.409875	-0.742529
16	6	0	-4.875808	-0.414826	-0.917016
17	6	0	-5.110492	-1.463595	-0.015959
18	6	0	-4.233733	-1.679834	1.054990
19	6	0	-3.129164	-0.846814	1.214693
20	8	0	-6.176351	-2.312372	-0.132623
21	8	0	-0.579467	-2.452600	-0.439004
22	8	0	1.708538	-3.594189	0.429388
23	8	0	3.935692	-2.701051	-0.772240
24	8	0	6.221274	-3.553555	0.634807
25	1	0	4.257074	2.518423	0.233660
26	1	0	1.895163	-0.960054	-0.747264
27	1	0	4.178907	-0.961205	-0.550911
28	1	0	1.271597	4.470519	0.302912
29	1	0	-2.520089	2.937369	-0.215255
30	1	0	-1.101252	0.770501	1.393310
31	1	0	-2.448140	-1.021557	2.043708
32	1	0	-4.426949	-2.495505	1.744094
33	1	0	-5.552448	-0.254140	-1.752264
34	1	0	-3.580988	1.206546	-1.455916
35	1	0	-6.713612	-2.080232	-0.903730
36	1	0	-0.512724	-1.457198	-0.470569
37	1	0	1.761138	-3.488731	1.388667
38	1	0	3.098334	-3.039727	-0.351197
39	1	0	3.916064	-2.987191	-1.695843
40	1	0	5.419398	-3.303166	0.130750
41	1	0	6.226358	-4.519210	0.646392
42	1	0	0.849874	-3.178900	0.152764
43	1	0	-1.402556	-2.642381	0.031696

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Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.195710	-0.811223	1.286701
2	6	0	-2.767681	0.194589	0.408634
3	6	0	-3.510893	0.420384	-0.757377
4	6	0	-4.649914	-0.332284	-1.044261
5	6	0	-5.060530	-1.334581	-0.155002
6	6	0	-4.332338	-1.574580	1.015978
7	6	0	-1.487743	0.947655	0.677282
8	6	0	-1.509972	2.415368	0.367070
9	6	0	-0.322151	3.077253	0.185687
10	8	0	-0.158999	4.380031	0.062600
11	8	0	-6.168157	-2.110739	-0.376479
12	6	0	0.899660	2.235603	0.082780
13	6	0	0.797290	0.847340	-0.091840
14	6	0	1.909606	0.030744	-0.288004
15	6	0	3.181501	0.627863	-0.309861
16	6	0	3.330438	2.010834	-0.153038
17	6	0	2.192929	2.809463	0.024522
18	8	0	-0.445688	0.258457	-0.134889
19	8	0	2.315205	4.154380	0.119407
20	8	0	4.313138	-0.115763	-0.476288
21	8	0	-0.751772	-2.460303	-0.491152
22	8	0	1.524605	-3.721113	0.299485
23	8	0	3.812367	-2.808623	-0.774450
24	8	0	5.997961	-3.617148	0.811992
25	1	0	4.315556	2.463397	-0.189281
26	1	0	1.790558	-1.038989	-0.404299
27	1	0	4.091676	-1.068747	-0.594584
28	1	0	1.323501	4.481558	0.106908
29	1	0	-2.453150	2.949131	0.424983
30	1	0	-1.177806	0.745349	1.717732
31	1	0	-2.630190	-1.005842	2.194600
32	1	0	-4.662812	-2.350785	1.698728
33	1	0	-5.215814	-0.145996	-1.953266
34	1	0	-3.190322	1.192907	-1.449711
35	1	0	-6.593398	-1.863648	-1.210237
36	1	0	-0.665324	-1.487654	-0.371078
37	1	0	1.554619	-3.724535	1.265516
38	1	0	2.954417	-3.150171	-0.403586
39	1	0	3.856547	-3.113227	-1.691323
40	1	0	5.234577	-3.382985	0.244787
41	1	0	6.029388	-4.582374	0.814744
42	1	0	0.672196	-3.283211	0.051284
43	1	0	-1.590431	-2.694180	-0.069360

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.138340	0.895043	0.724580
2	6	0	2.969220	-0.380047	0.144913
3	6	0	4.121296	-1.039006	-0.332330
4	6	0	5.379002	-0.452351	-0.241566
5	6	0	5.517333	0.820462	0.334625
6	6	0	4.390729	1.494963	0.819376
7	6	0	1.621401	-0.936384	0.058309
8	6	0	1.240082	-2.085273	-0.537823
9	6	0	-0.122219	-2.644984	-0.472273
10	8	0	-0.183374	-3.917797	-0.452340
11	8	0	6.726201	1.448676	0.451791
12	6	0	-1.328378	-1.845465	-0.326380
13	6	0	-1.455994	-0.463511	-0.767227
14	6	0	-2.623525	0.246157	-0.382723
15	6	0	-3.641145	-0.353685	0.356599
16	6	0	-3.590374	-1.720327	0.681833
17	6	0	-2.467517	-2.452288	0.311338
18	8	0	-0.562539	0.118853	-1.507929
19	8	0	-2.457589	-3.773312	0.623687
20	8	0	-4.732265	0.351520	0.760949
21	8	0	-0.454413	2.583411	-0.974567
22	8	0	-4.007368	2.987786	0.806337
23	8	0	-2.838601	3.755488	-1.617176
24	8	0	-1.348619	2.405721	1.644736

25	1	0	-4.404990	-2.198082	1.213803
26	1	0	-2.734694	1.267525	-0.719931
27	1	0	-4.550326	1.324755	0.686785
28	1	0	-1.611940	-4.134886	0.226964
29	1	0	1.965523	-2.758243	-0.988762
30	1	0	0.850360	-0.329097	0.523714
31	1	0	2.267649	1.425870	1.100660
32	1	0	4.509376	2.477879	1.263659
33	1	0	6.254712	-0.978209	-0.612405
34	1	0	4.040420	-2.025582	-0.777074
35	1	0	7.433995	0.897507	0.087489
36	1	0	-0.470555	1.577467	-1.254140
37	1	0	-1.476238	1.446256	1.692677
38	1	0	-3.139466	2.880856	1.253597
39	1	0	-3.756543	3.344050	-0.074602
40	1	0	-1.916308	3.430010	-1.472094
41	1	0	-2.765241	4.695481	-1.827483
42	1	0	-0.933924	2.536536	0.758923
43	1	0	0.417221	2.937309	-1.193190

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.169090	0.448216	-0.359219
2	6	0	1.556425	1.781171	-0.018737
3	6	0	2.946093	2.045049	0.121623
4	6	0	3.907123	1.032240	0.040979
5	6	0	3.492500	-0.269327	-0.261089
6	6	0	2.139631	-0.553726	-0.501468
7	6	0	0.583580	2.905245	-0.039419
8	8	0	1.038336	4.108781	-0.200613
9	8	0	3.362550	3.318693	0.335934
10	8	0	4.438897	-1.247672	-0.318349
11	8	0	-0.119752	0.115841	-0.571352
12	6	0	-0.776786	2.579614	0.018706
13	6	0	-1.140098	1.261803	0.429418
14	6	0	-2.516367	0.748730	0.273781
15	6	0	-3.333121	1.127029	-0.804758
16	6	0	-4.613999	0.600940	-0.957823
17	6	0	-5.099682	-0.327821	-0.025802
18	6	0	-4.299304	-0.725629	1.052737
19	6	0	-3.020448	-0.191781	1.190285
20	8	0	-6.345543	-0.884155	-0.119395
21	8	0	-0.615528	-2.377395	0.097220
22	8	0	1.412829	-2.576580	2.014534
23	8	0	3.200419	-3.638056	0.086682
24	8	0	0.955437	-3.938478	-1.558997
25	1	0	4.956664	1.259699	0.191249
26	1	0	1.834141	-1.552992	-0.780125
27	1	0	4.009374	-2.142181	-0.285582
28	1	0	2.532355	3.882115	0.152176
29	1	0	-1.521618	3.289554	-0.324854
30	1	0	-0.656070	0.884870	1.332606
31	1	0	-2.401438	-0.506301	2.026557
32	1	0	-4.687021	-1.446155	1.765505
33	1	0	-5.232758	0.901373	-1.799063
34	1	0	-2.958149	1.831682	-1.540177
35	1	0	-6.813961	-0.542872	-0.894967
36	1	0	-0.500373	-1.419678	-0.186595
37	1	0	1.727944	-1.660668	2.012995
38	1	0	2.667811	-3.383142	0.871605
39	1	0	2.517359	-3.861781	-0.582796
40	1	0	0.272421	-3.474756	-1.022728
41	1	0	0.606213	-4.821197	-1.738641
42	1	0	0.614485	-2.553971	1.440864
43	1	0	-1.556363	-2.501960	0.281368

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Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.093368	0.097722	1.251129
2	6	0	2.439998	-0.754468	0.349480
3	6	0	3.110089	-1.119374	-0.825752
4	6	0	4.396192	-0.651892	-1.097772
5	6	0	5.031497	0.200175	-0.184118
6	6	0	4.379151	0.575415	0.995715
7	6	0	1.020726	-1.193805	0.612306
8	6	0	0.684160	-2.606308	0.236232
9	6	0	-0.631699	-2.956625	0.064855
10	8	0	-1.105309	-4.174679	-0.107528
11	8	0	6.292634	0.696527	-0.389479
12	6	0	-1.616557	-1.842989	0.034838
13	6	0	-1.186495	-0.513691	-0.085310
14	6	0	-2.072719	0.552020	-0.212101
15	6	0	-3.452658	0.287163	-0.203652
16	6	0	-3.927279	-1.026532	-0.103334
17	6	0	-3.011830	-2.083530	-0.005254
18	8	0	0.162755	-0.234102	-0.143206
19	8	0	-3.453686	-3.363086	0.035295
20	8	0	-4.364868	1.296038	-0.290318
21	8	0	0.727169	2.421734	0.130392
22	8	0	-3.097903	3.699536	-0.117760
23	8	0	-0.852109	3.699712	-1.803808
24	8	0	-1.189706	3.402956	1.929213
25	1	0	-4.993234	-1.227313	-0.116270
26	1	0	-1.705306	1.562999	-0.304378
27	1	0	-3.910136	2.178696	-0.266540
28	1	0	-2.572642	-3.918065	-0.022303
29	1	0	1.472224	-3.352417	0.243602
30	1	0	0.779099	-0.974236	1.667368
31	1	0	2.589641	0.395236	2.167510
32	1	0	4.883493	1.232430	1.697025
33	1	0	4.904411	-0.945139	-2.012796
34	1	0	2.617443	-1.776518	-1.535889
35	1	0	6.648510	0.378508	-1.231493
36	1	0	0.620436	1.444097	0.029201
37	1	0	-1.405393	2.717496	2.575762
38	1	0	-2.554630	3.659094	0.699864
39	1	0	-2.425834	3.800063	-0.826258
40	1	0	-0.169131	3.322426	-1.208453
41	1	0	-0.496832	4.539853	-2.122401
42	1	0	-0.442168	3.044750	1.402960
43	1	0	1.672589	2.581263	0.257506

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.325404	0.037157	-0.860808
2	6	0	-2.592896	-1.232199	-0.186329
3	6	0	-3.775715	-1.330564	0.630336
4	6	0	-4.547166	-0.221646	0.962195
5	6	0	-4.203896	1.016212	0.386224
6	6	0	-3.199845	1.117466	-0.561151
7	6	0	-1.714934	-2.384826	-0.253639
8	8	0	-2.153428	-3.560482	-0.031184
9	8	0	-4.136365	-2.525894	1.169650
10	8	0	-4.898602	2.131349	0.774663
11	8	0	-1.362814	0.219919	-1.699137
12	6	0	-0.257252	-2.272587	-0.457857
13	6	0	0.474876	-1.257214	0.044909
14	6	0	1.925790	-1.095394	0.010229
15	6	0	2.779614	-1.873631	-0.801033
16	6	0	4.152879	-1.664247	-0.813835
17	6	0	4.725601	-0.662209	-0.010995
18	6	0	3.897622	0.124875	0.806871
19	6	0	2.519992	-0.096368	0.808353
20	8	0	6.071346	-0.498099	-0.067902
21	8	0	6.839676	1.557289	1.561626
22	8	0	-0.625798	2.786634	-1.135050
23	8	0	-2.674686	3.996469	0.414418
24	8	0	2.236321	2.659788	-1.014729

25	1	0	-5.374405	-0.312614	1.656658
26	1	0	-3.032859	2.058390	-1.065690
27	1	0	-4.346230	2.910829	0.554904
28	1	0	-3.504924	-3.196892	0.782634
29	1	0	0.209045	-3.150233	-0.899438
30	1	0	-0.061359	-0.452760	0.543076
31	1	0	1.889082	0.514278	1.449848
32	1	0	4.335560	0.896979	1.431590
33	1	0	4.800594	-2.261091	-1.448336
34	1	0	2.362215	-2.642610	-1.443591
35	1	0	6.364369	0.237080	0.521090
36	1	0	-0.847048	1.849785	-1.395904
37	1	0	-1.918797	3.607860	-0.085424
38	1	0	-2.667230	4.942341	0.220073
39	1	0	0.344112	2.812656	-1.031776
40	1	0	2.521085	1.820378	-0.618596
41	1	0	2.717408	3.343764	-0.528879
42	1	0	7.210222	2.326318	1.105492
43	1	0	7.478368	1.330818	2.252624

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.131984	-2.318812	-0.635668
2	6	0	1.457991	-1.544193	0.325296
3	6	0	2.209912	-0.635856	1.088882
4	6	0	3.578765	-0.481069	0.895182
5	6	0	4.226525	-1.231523	-0.097175
6	6	0	3.501547	-2.173743	-0.843173
7	6	0	-0.008663	-1.542162	0.471770
8	6	0	-0.846063	-2.635505	0.109769
9	6	0	-2.230189	-2.408635	0.057999
10	8	0	-3.120401	-3.344989	-0.048875
11	8	0	5.554139	-1.074920	-0.371055
12	6	0	-2.685555	-0.994897	0.017422
13	6	0	-4.059903	-0.678189	0.198729
14	6	0	-4.544807	0.631246	0.096326
15	6	0	-3.655598	1.636873	-0.300322
16	6	0	-2.335337	1.339694	-0.639141
17	6	0	-1.814375	0.057395	-0.415496
18	8	0	-4.935577	-1.674426	0.496287
19	8	0	-0.502889	-0.119455	-0.609660
20	8	0	-4.093049	2.935398	-0.338236
21	8	0	0.542807	2.346792	0.320284
22	8	0	3.285655	2.758238	-0.345445
23	8	0	5.937860	1.640627	0.235187
24	8	0	-1.578604	4.234025	0.250276
25	1	0	-5.583408	0.852512	0.315871
26	1	0	-1.674617	2.119896	-0.987752
27	1	0	-3.304518	3.518055	-0.300389
28	1	0	-4.405805	-2.525539	0.325313
29	1	0	-0.438066	-3.586635	-0.216533
30	1	0	-0.334129	-0.958579	1.334228
31	1	0	1.707762	-0.020999	1.830442
32	1	0	4.140238	0.230355	1.491030
33	1	0	4.016257	-2.753530	-1.602958
34	1	0	1.574412	-3.017913	-1.251226
35	1	0	5.849085	-0.199822	-0.042886
36	1	0	0.291598	1.458396	-0.018370
37	1	0	-0.795424	3.636922	0.263059
38	1	0	-1.259883	5.091510	-0.059024
39	1	0	1.494930	2.457174	0.129930
40	1	0	4.115595	2.314338	-0.087985
41	1	0	3.523468	3.682671	-0.495725
42	1	0	6.524212	2.051137	-0.417833
43	1	0	6.281378	1.915978	1.098300

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Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.829709	0.043972	-0.224878
2	6	0	-2.744788	-0.989267	0.026245
3	6	0	-4.120907	-0.654839	0.031221
4	6	0	-4.548758	0.674582	-0.118113
5	6	0	-3.592121	1.669898	-0.348400
6	6	0	-2.234870	1.351791	-0.462617
7	6	0	-2.272284	-2.395818	0.138450
8	8	0	-3.190296	-3.337649	0.056880
9	8	0	-5.029804	-1.648244	0.187807
10	8	0	-3.995122	2.976711	-0.448047
11	8	0	-0.483431	-0.214140	-0.278318
12	6	0	-0.916374	-2.570700	0.280837
13	6	0	-0.072827	-1.365990	0.576536
14	6	0	1.414582	-1.471171	0.362375
15	6	0	1.972413	-2.210324	-0.690052
16	6	0	3.335743	-2.133632	-0.978553
17	6	0	4.164140	-1.297955	-0.216875
18	6	0	3.629824	-0.592134	0.870020
19	6	0	2.266322	-0.679948	1.143912
20	8	0	5.484549	-1.201377	-0.562845
21	8	0	5.997977	1.477483	0.139728
22	8	0	0.677371	2.420510	0.479717
23	8	0	-1.490202	4.307774	0.259414
24	8	0	3.372964	2.696141	-0.343103
25	1	0	-5.603250	0.920624	-0.053700
26	1	0	-1.505284	2.112243	-0.691863
27	1	0	-3.205246	3.547937	-0.343566
28	1	0	-4.446603	-2.507954	0.154768
29	1	0	-0.474346	-3.560003	0.343896
30	1	0	-0.245328	-0.991063	1.601653
31	1	0	1.853824	-0.102590	1.967375
32	1	0	4.273063	0.032632	1.480541
33	1	0	3.763663	-2.686957	-1.808928
34	1	0	1.327158	-2.828961	-1.306787
35	1	0	5.841536	-0.358009	-0.216164
36	1	0	0.427377	1.508831	0.240481
37	1	0	-0.691273	3.740789	0.332089
38	1	0	-1.185995	5.159214	-0.080323
39	1	0	1.621981	2.509622	0.237755
40	1	0	4.183665	2.207358	-0.105395
41	1	0	3.659673	3.602911	-0.514493
42	1	0	6.578205	1.899436	-0.511382
43	1	0	6.372821	1.705482	1.003524

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.122408	-0.039020	-0.950296
2	6	0	-2.683465	-1.239902	-0.328888
3	6	0	-3.985858	-1.138851	0.279881
4	6	0	-4.629075	0.079480	0.471792
5	6	0	-4.016359	1.237992	-0.041351
6	6	0	-2.860573	1.165851	-0.800641
7	6	0	-1.993539	-2.515322	-0.251728
8	8	0	-2.633165	-3.604616	-0.088472
9	8	0	-4.604959	-2.251798	0.755270
10	8	0	-4.600623	2.449605	0.214209
11	8	0	-1.016793	-0.015116	-1.616358
12	6	0	-0.520938	-2.614182	-0.263397
13	6	0	0.259917	-1.683057	0.318875
14	6	0	1.716872	-1.611828	0.373291
15	6	0	2.575869	-2.502747	-0.301583
16	6	0	3.952725	-2.294612	-0.326725
17	6	0	4.494435	-1.183771	0.333419
18	6	0	3.671209	-0.312062	1.048996
19	6	0	2.297885	-0.526800	1.059996
20	8	0	5.832676	-0.861585	0.275841
21	8	0	0.030047	2.306231	-0.727902
22	8	0	2.880784	2.842238	-0.362096
23	8	0	5.441091	1.804920	-0.830034
24	8	0	-2.128831	4.014366	0.156670

25	8	0	1.115870	2.562036	1.923942
26	1	0	-5.566195	0.128523	1.014240
27	1	0	-2.469140	2.056169	-1.272465
28	1	0	-3.923863	3.142177	0.065745
29	1	0	-4.024339	-3.019714	0.484786
30	1	0	-0.117801	-3.532218	-0.684529
31	1	0	-0.241892	-0.830518	0.769641
32	1	0	1.662208	0.183341	1.580330
33	1	0	4.107463	0.540333	1.559292
34	1	0	4.600190	-2.972314	-0.876530
35	1	0	2.167118	-3.350974	-0.841551
36	1	0	6.326567	-1.518426	-0.236975
37	1	0	-0.274451	1.436513	-1.120789
38	1	0	-1.349397	3.513340	-0.165132
39	1	0	-1.937951	4.946927	-0.005856
40	1	0	0.988719	2.385614	-0.878381
41	1	0	3.737107	2.385449	-0.522355
42	1	0	3.048554	3.772102	-0.567260
43	1	0	5.704705	1.835728	-1.759486
44	1	0	5.722357	0.930181	-0.504270
45	1	0	0.449892	2.385162	1.234021
46	1	0	1.921188	2.685334	1.389112

TS2-5w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.008032	-2.439753	-0.675298
2	6	0	1.393261	-1.626374	0.290842
3	6	0	2.199269	-0.750320	1.037773
4	6	0	3.572840	-0.678406	0.829074
5	6	0	4.157849	-1.480645	-0.153716
6	6	0	3.382640	-2.375155	-0.900632
7	6	0	-0.071449	-1.581735	0.469692
8	6	0	-0.917931	-2.699905	0.228289
9	6	0	-2.303574	-2.478018	0.189828
10	8	0	-3.193157	-3.419570	0.197322
11	8	0	5.509130	-1.310142	-0.367348
12	6	0	-2.760376	-1.074895	0.020124
13	6	0	-4.132974	-0.743033	0.189685
14	6	0	-4.623028	0.548280	-0.038227
15	6	0	-3.743468	1.509116	-0.549095
16	6	0	-2.426717	1.180801	-0.874935
17	6	0	-1.898653	-0.070262	-0.528312
18	8	0	-5.001577	-1.703969	0.600239
19	8	0	-0.586575	-0.262038	-0.722212
20	8	0	-4.186387	2.795147	-0.714526
21	8	0	0.433959	2.231803	-0.024849
22	8	0	3.233706	2.735933	0.085567
23	8	0	5.553270	1.520716	-0.839903
24	8	0	-1.681000	4.145695	-0.261399
25	1	0	-5.658747	0.789453	0.173692
26	1	0	-1.775120	1.922135	-1.313938
27	1	0	-3.400553	3.382169	-0.738925
28	1	0	-4.473588	-2.568091	0.508757
29	1	0	-0.515966	-3.677899	-0.015404
30	1	0	-0.367359	-0.921491	1.286169
31	1	0	1.747120	-0.094208	1.775464
32	1	0	4.190203	0.007951	1.399085
33	1	0	3.844709	-2.994825	-1.664119
34	1	0	1.404195	-3.109883	-1.278823
35	1	0	5.828720	-1.906370	-1.060740
36	1	0	0.183843	1.316827	-0.299550
37	1	0	-0.905520	3.545207	-0.197089
38	1	0	-1.355286	4.967087	-0.651125
39	1	0	1.383349	2.343790	-0.228149
40	1	0	4.015787	2.242173	-0.253884
41	1	0	3.435396	3.669982	-0.061276
42	1	0	5.752672	1.721788	-1.764101
43	1	0	5.669009	0.555958	-0.745650
44	8	0	1.730776	2.346075	2.552736
45	1	0	0.994428	2.271910	1.918613
46	1	0	2.491222	2.460957	1.955427

INT2-5w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.926143	-0.056891	-0.359039
2	6	0	-2.839612	-1.045556	0.035876
3	6	0	-4.213360	-0.701435	0.040341
4	6	0	-4.637571	0.605801	-0.247874
5	6	0	-3.682866	1.559410	-0.617475
6	6	0	-2.331152	1.217697	-0.736554
7	6	0	-2.373555	-2.433111	0.301928
8	8	0	-3.298138	-3.369667	0.357054
9	8	0	-5.122679	-1.661498	0.336621
10	8	0	-4.081793	2.850228	-0.850175
11	8	0	-0.580496	-0.331240	-0.416708
12	6	0	-1.015714	-2.601580	0.428024
13	6	0	-0.155140	-1.379452	0.555554
14	6	0	1.323420	-1.547133	0.314988
15	6	0	1.813329	-2.343284	-0.728327
16	6	0	3.175954	-2.371530	-1.032434
17	6	0	4.059871	-1.590831	-0.280709
18	6	0	3.597256	-0.815415	0.783977
19	6	0	2.233611	-0.795937	1.070466
20	8	0	5.409095	-1.509486	-0.566650
21	8	0	0.559803	2.296955	0.138933
22	8	0	3.369075	2.655309	0.067022
23	8	0	5.547393	1.322856	-1.010925
24	8	0	-1.586129	4.208303	-0.240590
25	8	0	2.096211	2.319558	2.650446
26	1	0	-5.687768	0.868353	-0.179303
27	1	0	-1.605870	1.941393	-1.074498
28	1	0	-3.290029	3.426422	-0.800559
29	1	0	-4.545594	-2.524592	0.389310
30	1	0	-0.575924	-3.579843	0.593955
31	1	0	-0.289105	-0.885057	1.534201
32	1	0	1.877182	-0.161164	1.876655
33	1	0	4.298657	-0.220351	1.359795
34	1	0	3.544940	-2.977872	-1.855330
35	1	0	1.119420	-2.930839	-1.321763
36	1	0	5.640861	-2.095922	-1.301856
37	1	0	0.309741	1.375907	-0.071694
38	1	0	-0.799326	3.635677	-0.116990
39	1	0	-1.261681	5.033276	-0.624121
40	1	0	1.503963	2.387814	-0.103008
41	1	0	4.094115	2.113292	-0.323607
42	1	0	3.623904	3.575480	-0.085381
43	1	0	5.695941	1.518984	-1.945691
44	1	0	5.627915	0.353417	-0.925703
45	1	0	1.276008	2.296512	2.128815
46	1	0	2.773940	2.394052	1.954095

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.386959	-1.843352	0.442352
2	6	0	-2.392547	-1.120970	-0.250770
3	6	0	-2.805352	-0.021238	-1.032187
4	6	0	-4.145585	0.348284	-1.122373
5	6	0	-5.111285	-0.382900	-0.419329
6	6	0	-4.728209	-1.484197	0.362668
7	6	0	-0.967819	-1.431825	-0.177526
8	6	0	-0.382392	-2.511331	0.386300
9	6	0	1.063650	-2.778379	0.299018
10	8	0	1.397158	-3.999664	0.141459
11	8	0	-6.412369	0.025517	-0.526580
12	6	0	2.063533	-1.725224	0.266443
13	6	0	3.265526	-1.953897	-0.483313
14	6	0	4.163611	-0.934466	-0.770742
15	6	0	3.914234	0.347898	-0.247504
16	6	0	2.836984	0.587269	0.602456

17	6	0	1.902355	-0.433842	0.919313
18	8	0	3.538313	-3.188332	-0.990780
19	8	0	0.971482	-0.212051	1.799840
20	8	0	4.795981	1.333043	-0.579938
21	8	0	1.039280	3.067959	-0.624805
22	8	0	-1.702528	3.683373	-1.245456
23	8	0	3.693111	3.796703	-0.135271
24	1	0	5.034644	-1.124518	-1.387520
25	1	0	2.721736	1.554924	1.075207
26	1	0	4.433708	2.221268	-0.329851
27	1	0	2.835844	-3.794803	-0.627177
28	1	0	-0.969176	-3.326719	0.801651
29	1	0	-0.318423	-0.694096	-0.644564
30	1	0	-2.061152	0.562495	-1.566273
31	1	0	-4.449452	1.201600	-1.719606
32	1	0	-5.479728	-2.044777	0.911250
33	1	0	-3.111301	-2.688568	1.064490
34	1	0	-6.991254	-0.537730	0.009488
35	1	0	0.413930	1.315701	1.810696
36	1	0	1.255894	2.237589	-1.076388
37	1	0	2.733087	3.624171	-0.285247
38	1	0	3.762915	4.088708	0.785006
39	1	0	-0.743298	3.519589	-1.145804
40	1	0	-2.098715	3.291092	-0.442857
41	8	0	-2.676686	2.381594	1.121555
42	1	0	-3.095420	1.575413	0.776743
43	1	0	-3.323465	2.786005	1.717761
44	8	0	0.090136	2.268512	1.756162
45	1	0	0.717028	2.778842	0.277206
46	1	0	-0.876901	2.229628	1.617469

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.623919	-1.912677	-0.895344
2	6	0	1.969338	-1.452040	0.261186
3	6	0	2.727959	-0.770755	1.228651
4	6	0	4.101534	-0.583998	1.071210
5	6	0	4.734501	-1.061025	-0.085488
6	6	0	3.990326	-1.716854	-1.077446
7	6	0	0.523005	-1.652586	0.467184
8	6	0	-0.125404	-2.864953	0.086932
9	6	0	-1.523539	-2.902269	0.088427
10	8	0	-2.214761	-3.999633	-0.039636
11	8	0	6.080764	-0.850767	-0.198278
12	6	0	-2.248390	-1.609798	0.128898
13	6	0	-3.651860	-1.582761	0.343974
14	6	0	-4.399777	-0.407172	0.258032
15	6	0	-3.749846	0.773117	-0.123175
16	6	0	-2.381105	0.780995	-0.419623
17	6	0	-1.616219	-0.387782	-0.275353
18	8	0	-4.305888	-2.742839	0.634232
19	8	0	-0.303288	-0.326362	-0.543504
20	8	0	-4.497160	1.912244	-0.192199
21	8	0	-0.504050	3.706953	0.504674
22	8	0	2.205231	4.361711	1.352973
23	8	0	-3.011790	4.166075	-0.652387
24	1	0	-5.466595	-0.418138	0.452607
25	1	0	-1.897461	1.696971	-0.729330
26	1	0	-3.930276	2.699153	-0.396894
27	1	0	-3.630520	-3.468397	0.421502
28	1	0	0.442732	-3.712578	-0.283174
29	1	0	0.154360	-1.164974	1.369592
30	1	0	2.241024	-0.388797	2.121282
31	1	0	4.688896	-0.080704	1.832667
32	1	0	4.481652	-2.069801	-1.979689
33	1	0	2.053964	-2.419928	-1.667428
34	1	0	6.411001	-1.218628	-1.032059
35	1	0	0.420482	1.172194	-0.983565
36	1	0	-0.782788	3.135475	1.236060
37	1	0	-2.107507	4.060359	-0.273007
38	1	0	-2.880969	4.309751	-1.600675

39	1	0	1.262170	4.251502	1.123213
40	1	0	2.664632	3.667634	0.841087
41	8	0	3.381394	2.308632	-0.255820
42	1	0	3.637540	1.450669	0.125792
43	1	0	4.077959	2.534558	-0.889140
44	8	0	0.754561	2.072821	-1.227713
45	1	0	-0.060725	3.094482	-0.147046
46	1	0	1.693692	2.101862	-0.948919

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.300498	-1.653983	-1.037548
2	6	0	1.842149	-1.368067	0.256961
3	6	0	2.781335	-1.025723	1.236030
4	6	0	4.148051	-0.974741	0.941332
5	6	0	4.585170	-1.258492	-0.358197
6	6	0	3.657214	-1.594448	-1.354066
7	6	0	0.371289	-1.417275	0.588139
8	6	0	-0.281738	-2.760060	0.395857
9	6	0	-1.645789	-2.826297	0.288631
10	8	0	-2.376067	-3.932554	0.264586
11	8	0	5.933266	-1.185100	-0.600385
12	6	0	-2.366733	-1.535431	0.151434
13	6	0	-3.777202	-1.452414	0.187094
14	6	0	-4.442869	-0.237165	-0.010786
15	6	0	-3.693243	0.913040	-0.285144
16	6	0	-2.293251	0.859186	-0.370191
17	6	0	-1.657257	-0.358234	-0.140220
18	8	0	-4.498376	-2.586444	0.404025
19	8	0	-0.288325	-0.402054	-0.265877
20	8	0	-4.367329	2.088150	-0.460266
21	8	0	-0.268071	3.689020	0.583260
22	8	0	2.448854	4.188230	1.558348
23	8	0	-2.708278	4.263699	-0.681097
24	1	0	-5.525563	-0.191524	0.037915
25	1	0	-1.718140	1.744931	-0.597992
26	1	0	-3.736315	2.843749	-0.570310
27	1	0	-3.787427	-3.330478	0.384971
28	1	0	0.327482	-3.655235	0.476065
29	1	0	0.233930	-1.039960	1.614726
30	1	0	2.448162	-0.790633	2.243110
31	1	0	4.875167	-0.719426	1.705684
32	1	0	3.996781	-1.810194	-2.363142
33	1	0	1.585588	-1.919086	-1.810685
34	1	0	6.119534	-1.380591	-1.530958
35	1	0	0.635920	1.081265	-0.800272
36	1	0	-0.593724	3.145962	1.317013
37	1	0	-1.830698	4.110567	-0.258945
38	1	0	-2.518831	4.468667	-1.607970
39	1	0	1.514493	4.135540	1.280122
40	1	0	2.894165	3.475290	1.060402
41	8	0	3.592052	2.100876	-0.032212
42	1	0	3.812923	1.215076	0.306322
43	1	0	4.294876	2.325372	-0.659172
44	8	0	0.995268	1.953957	-1.065665
45	1	0	0.173237	3.047318	-0.037643
46	1	0	1.928738	1.961760	-0.762940

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.319597	-3.326384	0.291683
2	6	0	-0.427329	-2.326996	-0.243638
3	6	0	-0.950553	-0.974615	-0.404632
4	6	0	-2.242441	-0.697846	0.115603
5	6	0	-3.029399	-1.685165	0.700746
6	6	0	-2.580223	-3.015619	0.784950

7	6	0	0.915285	-2.741367	-0.612067
8	8	0	1.180797	-3.973605	-0.813945
9	8	0	-0.296400	-0.043943	-1.029805
10	8	0	-4.269107	-1.412302	1.186554
11	8	0	-0.933549	-4.625870	0.358675
12	6	0	2.083038	-1.844664	-0.692580
13	6	0	2.270706	-0.757379	0.083412
14	6	0	3.463403	0.084387	0.158390
15	6	0	3.452042	1.204932	1.015196
16	6	0	4.547787	2.057036	1.120829
17	6	0	5.696019	1.801931	0.362502
18	6	0	5.737280	0.691125	-0.495053
19	6	0	4.634981	-0.151580	-0.590985
20	8	0	6.746106	2.667388	0.498842
21	8	0	-1.485416	2.165007	-1.141130
22	8	0	-4.871471	1.210664	0.795050
23	8	0	-2.696740	3.046475	1.096162
24	8	0	-4.337162	4.697937	-0.412289
25	8	0	-4.237739	2.199896	-1.750840
26	1	0	-3.211356	-3.792281	1.201308
27	1	0	-2.631486	0.304794	0.015629
28	1	0	-4.490352	-0.453479	1.050439
29	1	0	-0.054915	-4.666193	-0.125769
30	1	0	2.877666	-2.230008	-1.327100
31	1	0	1.452571	-0.449113	0.728149
32	1	0	2.563805	1.411762	1.606219
33	1	0	4.526826	2.917848	1.781272
34	1	0	6.630021	0.491026	-1.081452
35	1	0	4.692216	-1.004848	-1.258997
36	1	0	7.483160	2.401682	-0.069947
37	1	0	-0.971113	1.246383	-1.107150
38	1	0	-2.123210	3.274584	1.838932
39	1	0	-4.189187	1.786619	1.192559
40	1	0	-4.803024	1.436438	-0.161349
41	1	0	-3.260480	2.112304	-1.699456
42	1	0	-4.402013	3.127336	-1.481634
43	1	0	-2.112237	2.734540	0.354021
44	1	0	-0.929292	2.796062	-1.616692
45	1	0	-5.170913	4.921105	0.022165
46	1	0	-3.777227	4.273476	0.274526

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.031318	0.126537	1.166690
2	6	0	2.628167	-0.903562	0.297688
3	6	0	3.480135	-1.243422	-0.766441
4	6	0	4.699467	-0.594882	-0.949249
5	6	0	5.085073	0.422495	-0.064235
6	6	0	4.246943	0.784625	0.998092
7	6	0	1.310363	-1.544505	0.481981
8	6	0	1.065079	-2.894216	0.090622
9	6	0	-0.260227	-3.346036	0.044283
10	8	0	-0.598220	-4.589620	-0.100580
11	8	0	6.265808	1.101356	-0.189455
12	6	0	-1.334999	-2.319986	0.057122
13	6	0	-1.077417	-0.958280	-0.294162
14	6	0	-2.137289	-0.052522	-0.434953
15	6	0	-3.456959	-0.463853	-0.199369
16	6	0	-3.746825	-1.797458	0.111683
17	6	0	-2.693675	-2.712827	0.202878
18	8	0	0.171589	-0.507848	-0.519028
19	8	0	-2.987284	-4.018867	0.428191
20	8	0	-4.491893	0.418550	-0.267615
21	8	0	0.446677	2.069344	-0.112053
22	8	0	-3.507318	2.950398	-0.229745
23	8	0	-1.242707	3.709929	-1.726708
24	8	0	-1.336027	3.216324	1.604206
25	1	0	-4.770542	-2.124461	0.256648
26	1	0	-1.925272	0.975588	-0.694818
27	1	0	-4.145650	1.346187	-0.333485
28	1	0	-2.107165	-4.502152	0.249003
29	1	0	1.867933	-3.535924	-0.256372

30	1	0	0.802532	-1.199779	1.384669
31	1	0	2.381627	0.415155	1.988815
32	1	0	4.556321	1.575291	1.673879
33	1	0	5.346494	-0.868659	-1.778254
34	1	0	3.181738	-2.015919	-1.467877
35	1	0	6.766314	0.777970	-0.952557
36	1	0	0.386487	1.077071	-0.266460
37	1	0	-1.254510	2.998161	2.541651
38	1	0	-2.965317	3.005486	0.582340
39	1	0	-2.859606	3.190869	-0.929197
40	1	0	-0.577256	3.102036	-1.344553
41	1	0	-1.137548	4.529570	-1.199602
42	1	0	-0.637082	2.708902	1.122242
43	1	0	1.385816	2.273026	-0.005023
44	8	0	-1.021016	5.658964	0.311886
45	1	0	-1.767559	6.261707	0.426867
46	1	0	-1.159554	4.929010	0.953509

INT2-5wc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.864060	-2.624821	0.023236
2	6	0	-1.485194	-2.303944	0.065107
3	6	0	-1.132169	-0.953342	-0.064686
4	6	0	-2.076855	0.060129	-0.199277
5	6	0	-3.439049	-0.285149	-0.198786
6	6	0	-3.838037	-1.622964	-0.089284
7	6	0	-0.437631	-3.358232	0.108797
8	8	0	-0.840705	-4.603507	-0.049774
9	8	0	0.198221	-0.598089	-0.125191
10	8	0	-4.407362	0.668412	-0.301073
11	8	0	-3.231693	-3.927079	0.074660
12	6	0	0.855741	-2.931810	0.277776
13	6	0	1.113265	-1.497724	0.635500
14	6	0	2.502946	-0.979989	0.356312
15	6	0	3.107140	-0.070803	1.236405
16	6	0	4.359261	0.480673	0.962738
17	6	0	5.027044	0.122611	-0.213841
18	6	0	4.440675	-0.785205	-1.106022
19	6	0	3.187625	-1.325929	-0.816182
20	8	0	6.253969	0.691054	-0.438402
21	8	0	0.644245	2.086439	0.018851
22	8	0	-3.277860	3.140969	-0.230072
23	8	0	-1.120741	3.456224	1.627995
24	8	0	-0.644015	5.766203	0.147317
25	8	0	-0.970854	3.700836	-1.742730
26	1	0	-4.890621	-1.884605	-0.107576
27	1	0	-1.767405	1.091395	-0.292069
28	1	0	-4.000116	1.572910	-0.309457
29	1	0	-2.319302	-4.430848	0.026617
30	1	0	1.684655	-3.632049	0.295410
31	1	0	0.866836	-1.279731	1.689760
32	1	0	2.590735	0.213930	2.149757
33	1	0	4.825581	1.181897	1.647354
34	1	0	4.960977	-1.063739	-2.018850
35	1	0	2.732397	-2.025737	-1.510317
36	1	0	6.623114	0.377302	-1.276363
37	1	0	0.556723	1.103370	-0.029043
38	1	0	-1.065732	3.317648	2.582511
39	1	0	-2.760352	3.238990	0.592918
40	1	0	-2.604570	3.311548	-0.926559
41	1	0	-0.336636	3.080554	-1.333393
42	1	0	-0.815682	4.543291	-1.264900
43	1	0	-0.434580	2.884370	1.210581
44	1	0	1.590033	2.267603	0.110091
45	1	0	-1.342623	6.431919	0.197560
46	1	0	-0.843277	5.107283	0.846557

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.485070	-0.413117	1.433647
2	6	0	2.034219	-1.344342	0.475498
3	6	0	2.998484	-1.942533	-0.362050
4	6	0	4.347603	-1.607864	-0.264620
5	6	0	4.758459	-0.660475	0.682083
6	6	0	3.829805	-0.074339	1.545869
7	6	0	0.596496	-1.580817	0.348746
8	6	0	-0.031923	-2.497641	-0.410897
9	6	0	-1.505429	-2.641400	-0.421062
10	8	0	-1.950644	-3.835010	-0.402297
11	8	0	6.058318	-0.216044	0.770734
12	6	0	-2.389737	-1.500891	-0.338861
13	6	0	-2.015274	-0.154489	-0.771620
14	6	0	-2.867960	0.917390	-0.383546
15	6	0	-4.066432	0.689163	0.285424
16	6	0	-4.512191	-0.618305	0.573111
17	6	0	-3.693437	-1.687986	0.240107
18	8	0	-0.978114	0.068106	-1.503026
19	8	0	-4.139736	-2.939557	0.525659
20	8	0	-4.879724	1.712118	0.663828
21	8	0	-3.621620	4.114365	0.424849
22	8	0	-0.910831	3.912448	0.623804
23	8	0	0.201400	2.392444	-1.256570
24	8	0	2.906006	1.533889	-1.493980
25	8	0	5.281403	2.400299	-0.250165
26	1	0	-5.470863	-0.785236	1.050740
27	1	0	-2.583656	1.923565	-0.666922
28	1	0	-4.431784	2.582991	0.514679
29	1	0	-3.437354	-3.561871	0.180161
30	1	0	0.511105	-3.261667	-0.962345
31	1	0	-0.025542	-0.896714	0.922031
32	1	0	1.763050	0.068387	2.086985
33	1	0	4.164521	0.660284	2.270535
34	1	0	5.072277	-2.057238	-0.937607
35	1	0	2.693226	-2.655709	-1.120695
36	1	0	6.637016	-0.720397	0.179472
37	1	0	-0.270794	1.506355	-1.364203
38	1	0	-0.655228	3.566718	1.489029
39	1	0	-2.633288	4.050872	0.476645
40	1	0	-3.818443	4.652826	-0.352810
41	1	0	5.782211	1.637558	0.091348
42	1	0	5.888255	2.877880	-0.831496
43	1	0	2.864773	0.591551	-1.276601
44	1	0	3.716766	1.863494	-1.049441
45	1	0	-0.463113	3.325157	-0.050871
46	1	0	1.158680	2.192607	-1.262279

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.787320	-0.220606	-0.021520
2	6	0	-2.458995	-1.487027	0.080253
3	6	0	-3.878593	-1.471965	0.192881
4	6	0	-4.607094	-0.284561	0.272764
5	6	0	-3.925330	0.934710	0.167481
6	6	0	-2.533624	0.971973	0.005947
7	6	0	-1.762737	-2.764124	-0.209196
8	8	0	-2.467172	-3.789910	-0.571138
9	8	0	-4.559196	-2.647111	0.194695
10	8	0	-4.668231	2.072555	0.236473
11	8	0	-0.461332	-0.126050	-0.163966
12	6	0	-0.358890	-2.757220	-0.187607
13	6	0	0.304182	-1.687468	0.470099
14	6	0	1.759295	-1.484427	0.302606
15	6	0	2.372701	-1.633958	-0.951801
16	6	0	3.738872	-1.415655	-1.116994
17	6	0	4.514464	-1.050676	-0.011553
18	6	0	3.931225	-0.906255	1.251087
19	6	0	2.558044	-1.109378	1.395793
20	8	0	5.861250	-0.772737	-0.118513

21	8	0	0.781222	2.200473	-0.856449
22	8	0	-0.631920	4.319928	-0.032043
23	8	0	-3.319505	4.348354	-0.308238
24	8	0	3.091098	2.291240	0.693322
25	8	0	5.736966	2.114602	-0.173529
26	1	0	-5.687655	-0.308966	0.360021
27	1	0	-2.012799	1.919883	-0.057126
28	1	0	-4.120308	2.875421	0.042620
29	1	0	-3.868345	-3.329331	-0.118637
30	1	0	0.195291	-3.500369	-0.751703
31	1	0	-0.050691	-1.422317	1.466738
32	1	0	2.102682	-0.983653	2.374415
33	1	0	4.551933	-0.629597	2.097312
34	1	0	4.197102	-1.511393	-2.097447
35	1	0	1.767882	-1.901721	-1.812195
36	1	0	6.203639	-1.076667	-0.972823
37	1	0	0.346818	1.347616	-0.607401
38	1	0	-0.352935	4.494545	0.876356
39	1	0	-2.331179	4.337787	-0.228295
40	1	0	-3.516552	4.705278	-1.184259
41	1	0	5.955579	1.163665	-0.174738
42	1	0	5.952710	2.435841	-1.059406
43	1	0	3.034095	1.463739	1.193105
44	1	0	4.001204	2.288799	0.321137
45	1	0	-0.112756	3.521991	-0.331953
46	1	0	1.641652	2.218520	-0.382054

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.636469	-1.293154	1.297157
2	6	0	1.668197	-1.289896	0.286283
3	6	0	2.089986	-1.210717	-1.047484
4	6	0	3.442645	-1.109102	-1.370066
5	6	0	4.393854	-1.107799	-0.344724
6	6	0	3.999400	-1.213429	0.990553
7	6	0	0.197890	-1.389340	0.618002
8	6	0	-0.431355	-2.686275	0.191394
9	6	0	-1.791804	-2.752117	0.032313
10	8	0	-2.503846	-3.838872	-0.192540
11	8	0	5.744720	-0.950468	-0.594041
12	6	0	-2.527184	-1.461670	0.078319
13	6	0	-1.834103	-0.242126	0.019612
14	6	0	-2.487460	0.988354	-0.049183
15	6	0	-3.893887	1.000402	-0.058586
16	6	0	-4.623598	-0.193743	-0.009270
17	6	0	-3.941970	-1.415624	0.041362
18	8	0	-0.458675	-0.237674	-0.035534
19	8	0	-4.633962	-2.579733	0.027632
20	8	0	-4.598849	2.164950	-0.106143
21	8	0	-3.099112	4.389395	-0.416825
22	8	0	-0.536327	4.243880	0.438592
23	8	0	0.918113	2.197261	-0.516046
24	8	0	3.265967	2.062675	0.935877
25	8	0	5.863353	1.883295	-0.063539
26	1	0	-5.707850	-0.173609	-0.035604
27	1	0	-1.919158	1.909712	-0.077987
28	1	0	-4.000967	2.947455	-0.215598
29	1	0	-3.883027	-3.298038	-0.070169
30	1	0	0.191674	-3.573465	0.139266
31	1	0	0.070532	-1.197923	1.698498
32	1	0	2.329432	-1.358272	2.337691
33	1	0	4.752159	-1.215205	1.772226
34	1	0	3.755513	-1.019350	-2.406776
35	1	0	1.347638	-1.208739	-1.839116
36	1	0	5.933149	-1.084363	-1.535113
37	1	0	0.491837	1.331336	-0.357004
38	1	0	-0.461760	4.230554	1.401830
39	1	0	-2.153343	4.349473	-0.122974
40	1	0	-3.088787	4.730806	-1.320677
41	1	0	6.011793	0.942746	-0.277721
42	1	0	6.098005	2.376696	-0.860946
43	1	0	3.197800	1.182241	1.334794

44	1	0	4.158280	2.072826	0.522534
45	1	0	0.009308	3.480108	0.107503
46	1	0	1.794226	2.154763	-0.068196

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.441139	0.337742	-0.901869
2	6	0	-3.027805	-0.864494	-0.307947
3	6	0	-4.351337	-0.769032	0.247948
4	6	0	-5.008326	0.446333	0.392755
5	6	0	-4.372663	1.608243	-0.076211
6	6	0	-3.138472	1.568817	-0.709597
7	6	0	-2.355845	-2.150800	-0.242496
8	8	0	-3.019854	-3.228948	-0.094622
9	8	0	-4.995284	-1.879409	0.688683
10	8	0	-5.060758	2.781707	0.099656
11	8	0	-1.360168	0.310624	-1.601635
12	6	0	-0.889502	-2.305988	-0.241084
13	6	0	-0.044930	-1.408146	0.304088
14	6	0	1.410990	-1.486134	0.394337
15	6	0	2.172423	-2.561598	-0.107637
16	6	0	3.563468	-2.534149	-0.077972
17	6	0	4.220167	-1.420407	0.461737
18	6	0	3.492646	-0.355675	0.995935
19	6	0	2.102764	-0.395105	0.957813
20	8	0	5.593395	-1.293844	0.449539
21	8	0	0.329899	2.222740	-0.983248
22	8	0	0.186877	2.468039	1.678862
23	8	0	3.227655	2.271117	-1.149136
24	8	0	5.668596	0.963790	-1.336901
25	8	0	2.970323	3.040735	1.613055
26	1	0	-5.993469	0.490825	0.841861
27	1	0	-2.695867	2.471935	-1.121064
28	1	0	-4.549169	3.520736	-0.260121
29	1	0	-4.405169	-2.648542	0.433507
30	1	0	-0.543484	-3.269619	-0.607553
31	1	0	-0.471119	-0.488914	0.696822
32	1	0	1.540664	0.445002	1.352363
33	1	0	4.008628	0.504600	1.408598
34	1	0	4.136993	-3.360901	-0.487822
35	1	0	1.679285	-3.423841	-0.544567
36	1	0	6.012351	-2.103033	0.120082
37	1	0	-0.278098	1.478732	-1.280632
38	1	0	0.145216	2.400819	0.685152
39	1	0	-0.422358	3.174599	1.928526
40	1	0	1.253631	1.961382	-1.144705
41	1	0	4.047491	1.730891	-1.233512
42	1	0	3.374194	3.046124	-1.708649
43	1	0	5.920854	0.670959	-2.222930
44	1	0	5.805896	0.193679	-0.753585
45	1	0	2.014799	2.899048	1.769195
46	1	0	3.098658	2.795475	0.676221

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.581119	-2.381885	-0.627894
2	6	0	1.093920	-1.440370	0.294456
3	6	0	2.018370	-0.621243	0.964513
4	6	0	3.386573	-0.739218	0.735466
5	6	0	3.844768	-1.680953	-0.188794
6	6	0	2.946932	-2.508927	-0.872229
7	6	0	-0.353394	-1.255002	0.524648
8	6	0	-1.263769	-2.347304	0.441127
9	6	0	-2.636177	-2.074778	0.403235
10	8	0	-3.555915	-2.979208	0.537802
11	8	0	5.204988	-1.720905	-0.418547

12	6	0	-3.052453	-0.686374	0.073686
13	6	0	-4.422716	-0.321527	0.181597
14	6	0	-4.898882	0.917803	-0.255514
15	6	0	-4.004926	1.790327	-0.879255
16	6	0	-2.660619	1.455685	-1.065424
17	6	0	-2.165642	0.229785	-0.581978
18	8	0	-5.309802	-1.204592	0.703073
19	8	0	-0.868411	-0.043551	-0.775453
20	8	0	-4.508869	2.996189	-1.299315
21	8	0	0.663569	2.176399	-0.397548
22	8	0	3.485981	2.385874	-0.631269
23	8	0	5.627775	0.885172	-1.476374
24	8	0	0.611598	2.321313	2.300606
25	1	0	-5.947198	1.172986	-0.150735
26	1	0	-1.975451	2.148381	-1.544101
27	1	0	-3.816585	3.509641	-1.739681
28	1	0	-4.791030	-2.085225	0.727414
29	1	0	-0.911987	-3.366139	0.317924
30	1	0	-0.564638	-0.494849	1.277861
31	1	0	1.662580	0.125182	1.667356
32	1	0	4.091421	-0.095623	1.250664
33	1	0	3.311730	-3.230173	-1.598229
34	1	0	0.884497	-3.007815	-1.176162
35	1	0	5.431446	-2.446459	-1.019651
36	1	0	0.189922	1.337584	-0.618515
37	1	0	0.538314	2.322074	1.310122
38	1	0	0.136866	3.103954	2.608911
39	1	0	1.613347	2.050900	-0.589643
40	1	0	4.214598	1.810939	-0.968019
41	1	0	3.651621	3.262457	-1.004409
42	1	0	5.746309	0.832803	-2.434343
43	1	0	5.618196	-0.038297	-1.157146
44	8	0	3.451484	2.458084	2.242583
45	1	0	2.486196	2.436658	2.400500
46	1	0	3.532031	2.436698	1.269576

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.186517	0.269981	-0.382059
2	6	0	-3.133006	-0.657788	0.079719
3	6	0	-4.501526	-0.301679	0.005591
4	6	0	-4.893925	0.956685	-0.470614
5	6	0	-3.914815	1.851054	-0.908418
6	6	0	-2.552110	1.522886	-0.879308
7	6	0	-2.712179	-2.019207	0.505661
8	8	0	-3.667079	-2.917074	0.656240
9	8	0	-5.434035	-1.205664	0.380504
10	8	0	-4.349443	3.072645	-1.363643
11	8	0	-0.853801	-0.068188	-0.412032
12	6	0	-1.367190	-2.220644	0.670361
13	6	0	-0.441282	-1.040365	0.641086
14	6	0	1.008207	-1.351846	0.356754
15	6	0	1.372160	-2.306100	-0.602681
16	6	0	2.712057	-2.532237	-0.920664
17	6	0	3.702714	-1.791928	-0.267922
18	6	0	3.364934	-0.844120	0.699360
19	6	0	2.020776	-0.630467	1.002778
20	8	0	5.045882	-1.930565	-0.566984
21	8	0	0.822049	2.197894	-0.385369
22	8	0	0.877607	2.471463	2.326374
23	8	0	3.621274	2.284997	-0.690642
24	8	0	5.586868	0.632402	-1.653689
25	8	0	3.717990	2.362474	2.185681
26	1	0	-5.944213	1.222474	-0.517749
27	1	0	-1.792311	2.221635	-1.214006
28	1	0	-3.597145	3.605067	-1.658383
29	1	0	-4.865693	-2.070194	0.553563
30	1	0	-0.971356	-3.190036	0.955594
31	1	0	-0.492135	-0.447392	1.570688
32	1	0	1.759261	0.121722	1.740954
33	1	0	4.142164	-0.270411	1.192775
34	1	0	2.983771	-3.266780	-1.674189

35	1	0	0.597686	-2.871572	-1.111615
36	1	0	5.184388	-2.664970	-1.183347
37	1	0	0.357906	1.346796	-0.513897
38	1	0	0.764003	2.438816	1.343283
39	1	0	0.485027	3.304932	2.616700
40	1	0	1.768916	2.055576	-0.590761
41	1	0	4.284385	1.656669	-1.067073
42	1	0	3.833727	3.148372	-1.070956
43	1	0	5.641420	0.568954	-2.616751
44	1	0	5.527373	-0.287427	-1.327560
45	1	0	2.759669	2.422991	2.372196
46	1	0	3.764867	2.326351	1.211151

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.430890	0.158473	-0.877796
2	6	0	-2.900924	-1.122794	-0.347012
3	6	0	-4.169403	-1.152321	0.338859
4	6	0	-4.855706	0.005521	0.684847
5	6	0	-4.329799	1.238449	0.250519
6	6	0	-3.223786	1.300729	-0.578657
7	6	0	-2.146644	-2.352263	-0.436067
8	8	0	-2.709097	-3.490640	-0.335902
9	8	0	-4.701476	-2.338629	0.735588
10	8	0	-4.949803	2.389267	0.657741
11	8	0	-1.369334	0.296751	-1.593238
12	6	0	-0.669011	-2.374251	-0.529052
13	6	0	0.110249	-1.547233	0.192422
14	6	0	1.573155	-1.536580	0.255139
15	6	0	2.387539	-2.144335	-0.720526
16	6	0	3.776255	-2.069638	-0.652094
17	6	0	4.381443	-1.378006	0.403756
18	6	0	3.601897	-0.773458	1.393087
19	6	0	2.212464	-0.853611	1.310361
20	8	0	5.748499	-1.240413	0.507847
21	8	0	6.477221	1.498599	0.336846
22	8	0	4.471596	2.806498	-1.023333
23	8	0	2.092281	2.320995	0.264705
24	8	0	-0.465864	2.782170	-0.796863
25	8	0	-2.546756	4.042065	0.649452
26	1	0	-5.757633	-0.044878	1.283871
27	1	0	-2.912228	2.252432	-0.983650
28	1	0	-4.305887	3.121625	0.553340
29	1	0	-4.098036	-3.043595	0.364070
30	1	0	-0.253418	-3.206443	-1.092663
31	1	0	-0.383109	-0.789319	0.797632
32	1	0	1.609012	-0.387759	2.085685
33	1	0	4.084753	-0.243852	2.207729
34	1	0	4.386916	-2.529328	-1.424156
35	1	0	1.933758	-2.660381	-1.560383
36	1	0	6.199418	-1.740455	-0.189118
37	1	0	-0.738611	1.887588	-1.134514
38	1	0	-1.783898	3.621025	0.184385
39	1	0	-2.429205	4.995507	0.551588
40	1	0	0.439016	2.667596	-0.437958
41	1	0	2.152641	1.383180	0.498597
42	1	0	2.920208	2.510143	-0.236299
43	1	0	6.653543	1.865873	1.213519
44	1	0	6.283063	0.550772	0.474902
45	1	0	4.521120	2.533341	-1.948814
46	1	0	5.199419	2.331523	-0.557218

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.819645	-2.094006	-0.843651
2	6	0	1.212097	-1.567074	0.307518

3	6	0	2.039141	-1.046875	1.317623
4	6	0	3.429641	-1.067512	1.198201
5	6	0	4.008056	-1.596249	0.039498
6	6	0	3.206000	-2.107672	-0.986380
7	6	0	-0.258433	-1.527333	0.453251
8	6	0	-1.071471	-2.607866	0.020126
9	6	0	-2.463673	-2.419140	-0.027778
10	8	0	-3.317878	-3.379786	-0.177892
11	8	0	5.382914	-1.577000	-0.043810
12	6	0	-2.957538	-1.021257	-0.022619
13	6	0	-4.349272	-0.757321	0.118015
14	6	0	-4.878760	0.533984	0.024663
15	6	0	-4.015677	1.578452	-0.326170
16	6	0	-2.673780	1.336787	-0.622769
17	6	0	-2.107119	0.072737	-0.397699
18	8	0	-5.198926	-1.789273	0.363569
19	8	0	-0.782118	-0.040551	-0.540464
20	8	0	-4.503288	2.857680	-0.361516
21	8	0	0.014562	2.484365	0.488937
22	8	0	2.765050	2.305630	0.844213
23	8	0	6.600506	0.986021	-0.159605
24	8	0	-2.139827	4.286245	0.342059
25	1	0	-5.931728	0.712755	0.211655
26	1	0	-2.035354	2.149507	-0.937250
27	1	0	-3.742256	3.473610	-0.273770
28	1	0	-4.637724	-2.617880	0.185971
29	1	0	-0.634361	-3.525339	-0.360450
30	1	0	-0.579539	-0.998924	1.351545
31	1	0	1.589771	-0.629343	2.214743
32	1	0	4.068793	-0.689287	1.989874
33	1	0	3.661768	-2.505883	-1.888663
34	1	0	1.198689	-2.481066	-1.645226
35	1	0	5.684931	-2.057795	-0.829261
36	1	0	-0.164704	1.585010	0.136411
37	1	0	-1.339911	3.713602	0.401650
38	1	0	-1.845098	5.121509	-0.042855
39	1	0	0.988891	2.538989	0.590666
40	1	0	2.867137	1.348658	0.954847
41	1	0	3.422653	2.549158	0.150593
42	1	0	7.019193	1.208692	0.682783
43	1	0	6.201489	0.102005	-0.038050
44	8	0	4.751683	2.848160	-0.971374
45	1	0	4.550997	2.707565	-1.906028
46	1	0	5.441794	2.184606	-0.733100

INT2-5wf

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.141986	0.027335	-0.298212
2	6	0	-2.986560	-1.045453	0.024333
3	6	0	-4.380071	-0.795878	0.054513
4	6	0	-4.891912	0.497211	-0.136013
5	6	0	-4.005030	1.537252	-0.433669
6	6	0	-2.633916	1.296323	-0.581428
7	6	0	-2.428104	-2.413275	0.190189
8	8	0	-3.285246	-3.412851	0.180236
9	8	0	-5.222081	-1.833432	0.281085
10	8	0	-4.490514	2.812061	-0.565202
11	8	0	-0.779438	-0.147900	-0.374137
12	6	0	-1.061066	-2.496987	0.298282
13	6	0	-0.274139	-1.231531	0.499748
14	6	0	1.203867	-1.352018	0.218411
15	6	0	1.667578	-1.599812	-1.080136
16	6	0	3.032608	-1.696834	-1.351737
17	6	0	3.952062	-1.561512	-0.306362
18	6	0	3.513900	-1.326064	0.998572
19	6	0	2.142032	-1.216863	1.249358
20	8	0	5.315756	-1.640088	-0.510356
21	8	0	6.671804	0.784460	0.006713
22	8	0	4.850224	2.774639	-0.505367
23	8	0	2.737089	2.143121	1.123730
24	8	0	0.074393	2.543156	0.483783
25	8	0	-2.164829	4.288127	0.240875

26	1	0	-5.956450	0.684189	-0.045096
27	1	0	-1.963297	2.092783	-0.866425
28	1	0	-3.743195	3.435816	-0.436450
29	1	0	-4.590026	-2.657161	0.272538
30	1	0	-0.552096	-3.451341	0.388481
31	1	0	-0.398013	-0.829185	1.521355
32	1	0	1.802575	-1.025811	2.264250
33	1	0	4.240187	-1.228608	1.799055
34	1	0	3.379663	-1.873767	-2.366245
35	1	0	0.951271	-1.705156	-1.888637
36	1	0	5.510121	-1.894417	-1.424809
37	1	0	-0.112231	1.628492	0.203090
38	1	0	-1.342419	3.762844	0.356234
39	1	0	-1.890165	5.144323	-0.111786
40	1	0	1.031761	2.544984	0.706780
41	1	0	2.771127	1.175131	1.159270
42	1	0	3.462442	2.401320	0.506359
43	1	0	7.029376	0.807640	0.904521
44	1	0	6.251677	-0.092864	-0.096078
45	1	0	4.677639	2.786812	-1.456007
46	1	0	5.527221	2.072274	-0.356377

INT1-5wg

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.128372	-0.851591	1.268050
2	6	0	1.450330	-1.435509	0.179928
3	6	0	2.207617	-1.774565	-0.959707
4	6	0	3.571560	-1.510836	-1.023256
5	6	0	4.217530	-0.895816	0.057915
6	6	0	3.498827	-0.590575	1.222388
7	6	0	-0.006829	-1.565143	0.223678
8	6	0	-0.786704	-2.352381	-0.539778
9	6	0	-2.261804	-2.342778	-0.388946
10	8	0	-2.836436	-3.468390	-0.248320
11	8	0	5.531620	-0.549313	-0.105639
12	6	0	-2.982540	-1.094970	-0.289076
13	6	0	-2.496884	0.157975	-0.868600
14	6	0	-3.202098	1.339440	-0.510769
15	6	0	-4.251358	1.327501	0.391562
16	6	0	-4.808810	0.121019	0.862065
17	6	0	-4.200986	-1.068237	0.477597
18	8	0	-1.497607	0.234198	-1.677016
19	8	0	-4.751749	-2.231532	0.916805
20	8	0	-4.785613	2.506579	0.839169
21	8	0	6.543259	0.420245	2.209934
22	8	0	-0.372808	2.654396	-0.991454
23	8	0	2.344865	2.197355	-0.291019
24	8	0	4.836672	1.848779	-1.588336
25	8	0	-2.261104	4.032839	0.635090
26	1	0	-5.669224	0.115631	1.521231
27	1	0	-2.874386	2.275607	-0.939165
28	1	0	-4.120927	3.208321	0.680726
29	1	0	-4.198928	-2.962036	0.522384
30	1	0	-0.372544	-3.098961	-1.213780
31	1	0	-0.504328	-0.904057	0.932022
32	1	0	1.569178	-0.579045	2.159361
33	1	0	4.003218	-0.120185	2.060248
34	1	0	4.141738	-1.735862	-1.919032
35	1	0	1.714638	-2.207231	-1.824630
36	1	0	5.918929	-0.208945	0.739755
37	1	0	-0.718696	1.770009	-1.287539
38	1	0	-1.559760	3.576192	0.113533
39	1	0	-2.080399	4.978322	0.558336
40	1	0	0.577180	2.528617	-0.796978
41	1	0	2.332725	1.397141	0.255503
42	1	0	3.166862	2.119025	-0.821102
43	1	0	6.954791	1.293318	2.136480
44	1	0	7.192488	-0.138852	2.660219
45	1	0	4.819701	1.703504	-2.543876
46	1	0	5.241626	1.047049	-1.205722

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.177617	0.062284	-0.372955
2	6	0	-2.993808	-1.023721	0.090378
3	6	0	-4.374838	-0.763137	0.314432
4	6	0	-4.920099	0.521503	0.214507
5	6	0	-4.090541	1.557785	-0.229204
6	6	0	-2.768308	1.314592	-0.601623
7	6	0	-2.491288	-2.419395	0.087452
8	8	0	-3.349092	-3.387735	0.017284
9	8	0	-5.197924	-1.792599	0.646670
10	8	0	-4.590947	2.831824	-0.283141
11	8	0	-0.865211	-0.052667	-0.601387
12	6	0	-1.098957	-2.597700	0.049863
13	6	0	-0.269007	-1.497898	0.401883
14	6	0	1.189008	-1.524720	0.171221
15	6	0	1.738389	-2.049280	-1.012290
16	6	0	3.109246	-2.015699	-1.247667
17	6	0	3.972607	-1.455524	-0.293187
18	6	0	3.446547	-0.954344	0.908680
19	6	0	2.066367	-0.980118	1.122505
20	8	0	5.302109	-1.431483	-0.580767
21	8	0	6.693829	0.544687	0.806903
22	8	0	5.206627	2.561331	-0.554661
23	8	0	2.723333	2.317899	0.657119
24	8	0	0.062552	2.603211	-0.137205
25	8	0	-2.171421	4.321031	0.114062
26	1	0	-5.960645	0.699571	0.462001
27	1	0	-2.164015	2.118385	-0.993750
28	1	0	-3.832026	3.455403	-0.296156
29	1	0	-4.643067	-2.622643	0.452053
30	1	0	-0.676983	-3.523321	-0.328407
31	1	0	-0.541535	-0.950483	1.305239
32	1	0	1.665858	-0.576527	2.049392
33	1	0	4.111832	-0.551494	1.666528
34	1	0	3.527678	-2.400987	-2.172132
35	1	0	1.076738	-2.463466	-1.766893
36	1	0	5.786869	-0.836055	0.029548
37	1	0	-0.150282	1.654262	-0.278591
38	1	0	-1.350292	3.779912	0.066475
39	1	0	-1.957703	5.169282	-0.295346
40	1	0	1.011744	2.633864	0.104507
41	1	0	2.716703	1.355862	0.775886
42	1	0	3.560760	2.491179	0.171077
43	1	0	7.635803	0.531592	0.580712
44	1	0	6.658773	0.636010	1.770795
45	1	0	5.224599	2.338822	-1.495194
46	1	0	5.762139	1.889095	-0.110725

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.141185	-1.072996	-1.122344
2	6	0	-1.173621	-1.333140	-0.145852
3	6	0	-1.605241	-1.648956	1.151278
4	6	0	-2.959934	-1.670653	1.474430
5	6	0	-3.919847	-1.383729	0.492436
6	6	0	-3.507675	-1.104762	-0.818191
7	6	0	0.295991	-1.236950	-0.469336
8	6	0	1.086334	-2.501615	-0.281894
9	6	0	2.456468	-2.418992	-0.224857
10	8	0	3.313222	-3.419692	-0.239396
11	8	0	-5.233045	-1.401395	0.864143
12	6	0	3.022446	-1.050749	-0.087980
13	6	0	2.191082	0.024441	0.261506
14	6	0	2.696419	1.291727	0.528870
15	6	0	4.062946	1.528678	0.341463
16	6	0	4.936878	0.487058	0.012191

17	6	0	4.414944	-0.804334	-0.163531
18	8	0	0.833164	-0.148206	0.385149
19	8	0	5.246372	-1.844579	-0.416021
20	8	0	4.556561	2.801191	0.466382
21	8	0	-6.741920	0.341155	-0.713197
22	8	0	-0.114001	2.603202	-0.168614
23	8	0	-2.771840	2.230107	-0.899438
24	8	0	-5.174645	2.404339	0.479060
25	8	0	2.178045	4.318214	-0.144220
26	1	0	5.999022	0.670172	-0.109475
27	1	0	2.039024	2.088448	0.840079
28	1	0	3.804565	3.428092	0.397074
29	1	0	4.612336	-2.667167	-0.381614
30	1	0	0.573719	-3.456206	-0.346329
31	1	0	0.396638	-0.839674	-1.495356
32	1	0	-1.830326	-0.839321	-2.138066
33	1	0	-4.244768	-0.907756	-1.590765
34	1	0	-3.290853	-1.892179	2.484384
35	1	0	-0.865703	-1.859218	1.917990
36	1	0	-5.786781	-0.937201	0.202676
37	1	0	0.083859	1.662108	-0.007251
38	1	0	1.339164	3.809753	-0.191419
39	1	0	1.951944	5.173369	0.243853
40	1	0	-1.069453	2.628237	-0.392116
41	1	0	-2.733322	1.267430	-1.010584
42	1	0	-3.585900	2.374903	-0.366225
43	1	0	-7.678621	0.356098	-0.466930
44	1	0	-6.726310	0.340973	-1.681724
45	1	0	-5.103999	2.167666	1.413740
46	1	0	-5.755562	1.726603	0.078134

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.354938	-0.397255	1.094654
2	6	0	1.848723	-1.486574	0.355866
3	6	0	2.770634	-2.319600	-0.309083
4	6	0	4.136838	-2.052891	-0.272821
5	6	0	4.603649	-0.940728	0.439755
6	6	0	3.716954	-0.123022	1.143750
7	6	0	0.399258	-1.618137	0.249001
8	6	0	-0.322567	-2.549267	-0.405971
9	6	0	-1.796828	-2.498267	-0.425907
10	8	0	-2.411764	-3.607504	-0.326390
11	8	0	5.929369	-0.565740	0.446855
12	6	0	-2.519040	-1.236095	-0.456384
13	6	0	-1.988227	-0.002666	-1.036855
14	6	0	-2.751993	1.180141	-0.835792
15	6	0	-3.898537	1.201260	-0.057938
16	6	0	-4.476007	0.011627	0.424425
17	6	0	-3.813285	-1.186176	0.171385
18	8	0	-0.884665	0.074365	-1.700454
19	8	0	-4.404448	-2.328917	0.610021
20	8	0	-4.500710	2.390139	0.253287
21	8	0	0.087048	2.259598	-0.393554
22	8	0	2.812599	2.953860	-0.431212
23	8	0	5.468539	2.062176	-0.710795
24	8	0	-0.873950	1.183375	2.005095
25	8	0	-2.115706	4.047166	0.237732
26	1	0	-5.404670	0.020522	0.983069
27	1	0	-2.377979	2.096824	-1.270197
28	1	0	-3.835988	3.101123	0.129765
29	1	0	-3.818872	-3.074568	0.297245
30	1	0	0.126178	-3.427801	-0.863732
31	1	0	-0.150132	-0.814750	0.731653
32	1	0	1.659925	0.255857	1.613808
33	1	0	4.097638	0.730946	1.694185
34	1	0	4.835010	-2.686621	-0.812627
35	1	0	2.419639	-3.169120	-0.886376
36	1	0	6.470490	-1.197116	-0.050238
37	1	0	-0.143820	1.488334	-0.983092
38	1	0	-1.325198	3.520423	-0.007600

39	1	0	-1.998617	4.912041	-0.176039
40	1	0	1.053365	2.408379	-0.447180
41	1	0	3.694387	2.531099	-0.517671
42	1	0	2.927651	3.854741	-0.760744
43	1	0	5.783887	2.093856	-1.623943
44	1	0	5.779418	1.209982	-0.353981
45	1	0	-0.475677	1.590143	1.203519
46	1	0	-1.754187	0.913451	1.706998

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.710543	-0.186806	-0.601680
2	6	0	-2.530302	-1.242165	-0.085524
3	6	0	-3.925081	-0.994132	0.034673
4	6	0	-4.481858	0.266767	-0.208513
5	6	0	-3.643164	1.280324	-0.683978
6	6	0	-2.298037	1.033157	-0.963014
7	6	0	-1.995911	-2.614816	0.108344
8	8	0	-2.825081	-3.609462	0.079886
9	8	0	-4.749242	-2.006485	0.411696
10	8	0	-4.159395	2.537582	-0.860510
11	8	0	-0.383356	-0.304192	-0.749499
12	6	0	-0.602582	-2.749442	0.211024
13	6	0	0.157689	-1.577059	0.480094
14	6	0	1.628600	-1.525716	0.370520
15	6	0	2.341809	-2.310467	-0.550310
16	6	0	3.717979	-2.156520	-0.712056
17	6	0	4.395361	-1.200461	0.053296
18	6	0	3.712348	-0.423271	0.992238
19	6	0	2.338263	-0.585111	1.136692
20	8	0	5.739791	-0.939574	-0.104245
21	8	0	0.455137	2.206079	0.062797
22	8	0	-1.132755	2.444369	2.377592
23	8	0	3.146313	2.895232	0.213700
24	8	0	5.505884	1.836598	-0.847699
25	8	0	-1.759338	3.994048	-0.223240
26	1	0	-5.536873	0.446067	-0.033944
27	1	0	-1.674122	1.814300	-1.372829
28	1	0	-3.413734	3.173016	-0.840913
29	1	0	-4.167551	-2.837087	0.340527
30	1	0	-0.129068	-3.701018	-0.007041
31	1	0	-0.219678	-0.931909	1.274759
32	1	0	1.801453	0.043705	1.841013
33	1	0	4.255075	0.313125	1.575132
34	1	0	4.256413	-2.753942	-1.442440
35	1	0	1.813638	-3.029131	-1.168643
36	1	0	6.135904	-1.541904	-0.751523
37	1	0	0.304293	1.291629	-0.278072
38	1	0	-0.912913	3.497869	-0.256490
39	1	0	-1.538574	4.926106	-0.347435
40	1	0	1.422946	2.372726	0.071261
41	1	0	3.934518	2.455439	-0.176152
42	1	0	3.270585	3.839519	0.050685
43	1	0	5.579063	1.919178	-1.808062
44	1	0	5.730258	0.909117	-0.644196
45	1	0	-0.470577	2.262683	1.678329
46	1	0	-1.772159	3.011249	1.921365

INT2-5wh

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.393114	-0.652788	1.173503
2	6	0	1.571017	-1.471156	0.387402
3	6	0	2.160898	-2.239780	-0.624143
4	6	0	3.533833	-2.173182	-0.869720
5	6	0	4.326745	-1.323841	-0.091308
6	6	0	3.765826	-0.577344	0.946690

7	6	0	0.075725	-1.401467	0.558300
8	6	0	-0.696864	-2.679067	0.416666
9	6	0	-2.057258	-2.597403	0.240477
10	8	0	-2.923793	-3.588844	0.275208
11	8	0	5.675883	-1.141926	-0.324943
12	6	0	-2.597733	-1.243083	-0.056971
13	6	0	-1.734354	-0.204604	-0.437043
14	6	0	-2.203669	1.040692	-0.837324
15	6	0	-3.576478	1.300210	-0.760027
16	6	0	-4.482088	0.294026	-0.407047
17	6	0	-3.989067	-0.982507	-0.093355
18	8	0	-0.374030	-0.401660	-0.453377
19	8	0	-4.847190	-1.992666	0.188240
20	8	0	-4.049607	2.561200	-1.017272
21	8	0	0.590921	2.264874	0.131739
22	8	0	3.290306	2.834063	0.313578
23	8	0	5.565677	1.692563	-0.839278
24	8	0	-1.073603	2.697031	2.386461
25	8	0	-1.659684	4.060941	-0.303961
26	1	0	-5.547542	0.493983	-0.370664
27	1	0	-1.511600	1.804045	-1.156879
28	1	0	-3.299787	3.187360	-0.950124
29	1	0	-4.221963	-2.818856	0.265308
30	1	0	-0.201603	-3.625251	0.609882
31	1	0	-0.136374	-0.900413	1.519416
32	1	0	1.951584	-0.046442	1.959677
33	1	0	4.398695	0.070060	1.544508
34	1	0	3.979319	-2.758097	-1.669833
35	1	0	1.536296	-2.880060	-1.239520
36	1	0	5.981125	-1.713691	-1.044785
37	1	0	0.450104	1.332600	-0.125654
38	1	0	-0.795722	3.600339	-0.309071
39	1	0	-1.475068	4.992045	-0.484307
40	1	0	1.563325	2.416487	0.157227
41	1	0	4.042725	2.362781	-0.109590
42	1	0	3.473190	3.775120	0.192349
43	1	0	5.655931	1.863706	-1.786297
44	1	0	5.739323	0.739052	-0.724076
45	1	0	-0.387622	2.458136	1.730675
46	1	0	-1.691242	3.230250	1.864000

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.232270	-0.631421	1.037542
2	6	0	1.563367	-1.507550	0.157543
3	6	0	2.351651	-2.318343	-0.684527
4	6	0	3.741959	-2.258341	-0.650605
5	6	0	4.376102	-1.377620	0.235035
6	6	0	3.623060	-0.564764	1.085759
7	6	0	0.100031	-1.508156	0.138971
8	6	0	-0.716118	-2.419972	-0.423623
9	6	0	-2.186753	-2.374379	-0.266153
10	8	0	-2.749965	-3.495214	-0.045934
11	8	0	5.745545	-1.257855	0.301695
12	6	0	-2.933809	-1.134948	-0.235002
13	6	0	-2.499020	0.094867	-0.897734
14	6	0	-3.257573	1.267564	-0.629393
15	6	0	-4.297120	1.283235	0.284547
16	6	0	-4.799535	0.092744	0.845465
17	6	0	-4.149307	-1.097225	0.539119
18	8	0	-1.491015	0.165010	-1.697113
19	8	0	-4.660158	-2.242675	1.064116
20	8	0	-4.868663	2.470356	0.656408
21	8	0	6.552952	1.459959	0.389170
22	8	0	4.287371	3.029108	0.543941
23	8	0	2.258779	1.988456	-1.016165
24	8	0	-0.490405	2.642958	-1.032863
25	8	0	-2.528794	4.147034	0.257179
26	1	0	-5.653653	0.099088	1.512765
27	1	0	-2.968798	2.180091	-1.131403
28	1	0	-4.217144	3.179854	0.467086

29	1	0	-4.089876	-2.981391	0.707302
30	1	0	-0.332431	-3.329205	-0.880584
31	1	0	-0.363183	-0.664669	0.645939
32	1	0	1.650941	0.010795	1.693274
33	1	0	4.125840	0.117610	1.762679
34	1	0	4.332592	-2.880015	-1.317664
35	1	0	1.876013	-2.990603	-1.391186
36	1	0	6.178758	-1.844947	-0.335471
37	1	0	-0.808474	1.747992	-1.327656
38	1	0	-1.760085	3.639652	-0.093583
39	1	0	-2.192054	4.680180	0.988514
40	1	0	0.480701	2.555742	-0.952566
41	1	0	2.237134	1.056690	-0.754163
42	1	0	2.974352	2.386120	-0.467662
43	1	0	7.172158	1.585484	1.120832
44	1	0	6.359549	0.502235	0.363876
45	1	0	4.548317	3.931039	0.315395
46	1	0	5.108931	2.487014	0.489146

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.707906	-2.525917	-0.732367
2	6	0	1.159535	-1.688347	0.253157
3	6	0	2.029922	-0.859425	0.981478
4	6	0	3.401336	-0.859222	0.744154
5	6	0	3.918615	-1.690074	-0.253165
6	6	0	3.078402	-2.534805	-0.987684
7	6	0	-0.295623	-1.578379	0.475974
8	6	0	-1.198690	-2.649159	0.235354
9	6	0	-2.574389	-2.364600	0.239659
10	8	0	-3.502236	-3.268275	0.255759
11	8	0	5.274639	-1.607443	-0.491012
12	6	0	-2.973272	-0.941325	0.105180
13	6	0	-4.326789	-0.555535	0.314022
14	6	0	-4.768070	0.757710	0.117852
15	6	0	-3.862929	1.689250	-0.404307
16	6	0	-2.571620	1.310649	-0.773162
17	6	0	-2.082440	0.035814	-0.451539
18	8	0	-5.224428	-1.485837	0.734128
19	8	0	-0.784971	-0.198852	-0.673522
20	8	0	-4.253917	2.995659	-0.533988
21	8	0	0.264753	2.317192	0.178122
22	8	0	3.009755	2.709283	-0.150479
23	8	0	5.573702	1.199332	-0.780952
24	8	0	-1.713233	4.269833	-0.251328
25	1	0	-5.786358	1.038927	0.362493
26	1	0	-1.899136	2.027962	-1.221044
27	1	0	-3.441974	3.550146	-0.550042
28	1	0	-4.736454	-2.369605	0.614967
29	1	0	-0.850327	-3.638090	-0.044072
30	1	0	-0.539015	-0.919754	1.310540
31	1	0	1.623743	-0.190610	1.734964
32	1	0	4.063613	-0.206755	1.302622
33	1	0	3.489018	-3.176084	-1.762784
34	1	0	1.055978	-3.160034	-1.324540
35	1	0	5.539837	-2.219248	-1.193589
36	1	0	0.026955	1.414592	-0.125906
37	1	0	-0.992164	3.622789	-0.062528
38	1	0	-1.637549	4.962745	0.417166
39	1	0	1.231202	2.418701	0.040502
40	1	0	3.525045	2.153832	-0.757068
41	1	0	3.527444	2.656967	0.678875
42	1	0	6.279777	1.532671	-1.350404
43	1	0	5.639247	0.224494	-0.800329
44	8	0	4.985140	2.116479	1.764450
45	1	0	5.539402	2.790579	2.178862
46	1	0	5.456729	1.827000	0.954262

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.094729	0.030193	-0.283080
2	6	0	-3.031370	-0.936111	0.114308
3	6	0	-4.392778	-0.548548	0.156728
4	6	0	-4.780522	0.776805	-0.096889
5	6	0	-3.804368	1.706780	-0.472007
6	6	0	-2.467833	1.323291	-0.630950
7	6	0	-2.604668	-2.342830	0.341648
8	8	0	-3.557877	-3.250119	0.403225
9	8	0	-5.326137	-1.484666	0.456688
10	8	0	-4.165850	3.014021	-0.667677
11	8	0	-0.760250	-0.281924	-0.372640
12	6	0	-1.250518	-2.558000	0.427850
13	6	0	-0.346070	-1.367487	0.558479
14	6	0	1.118462	-1.583723	0.271782
15	6	0	1.548125	-2.373209	-0.802638
16	6	0	2.900883	-2.456950	-1.138169
17	6	0	3.837830	-1.740193	-0.386690
18	6	0	3.436068	-0.967949	0.705040
19	6	0	2.080212	-0.892576	1.020359
20	8	0	5.185458	-1.730084	-0.694186
21	8	0	5.584834	1.074763	-0.852245
22	8	0	5.121524	1.928003	1.740304
23	8	0	3.110366	2.688793	-0.066502
24	8	0	0.378991	2.408642	0.329899
25	8	0	-1.649610	4.326515	-0.215205
26	1	0	-5.819509	1.072088	0.002772
27	1	0	-1.724275	2.025846	-0.974077
28	1	0	-3.354724	3.565443	-0.608858
29	1	0	-4.776118	-2.366395	0.480256
30	1	0	-0.839776	-3.553416	0.564032
31	1	0	-0.433682	-0.895934	1.553858
32	1	0	1.765153	-0.269202	1.852962
33	1	0	4.172909	-0.415842	1.278314
34	1	0	3.222047	-3.058914	-1.983938
35	1	0	0.814891	-2.914289	-1.392909
36	1	0	5.370633	-2.305141	-1.451231
37	1	0	0.150022	1.486824	0.115033
38	1	0	-0.914334	3.716751	0.022247
39	1	0	-1.634399	5.036251	0.439757
40	1	0	1.346543	2.493416	0.174140
41	1	0	3.564438	2.130141	-0.717378
42	1	0	3.659139	2.572284	0.736648
43	1	0	6.289292	1.407611	-1.424014
44	1	0	5.611060	0.099952	-0.920200
45	1	0	5.723858	2.568192	2.141271
46	1	0	5.542896	1.635822	0.903409

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.904010	-2.348358	0.237877
2	6	0	-1.693073	-1.869468	-0.373477
3	6	0	-1.644977	-0.473774	-0.796758
4	6	0	-2.717032	0.369893	-0.394097
5	6	0	-3.807040	-0.121937	0.317923
6	6	0	-3.933509	-1.492479	0.610551
7	6	0	-0.582181	-2.792910	-0.504837
8	8	0	-0.771773	-4.052613	-0.503110
9	8	0	-0.690766	-0.002986	-1.531100
10	8	0	-4.813481	0.699388	0.732912
11	8	0	-3.053206	-3.667766	0.522529
12	6	0	0.830264	-2.362565	-0.528813
13	6	0	1.295437	-1.296123	0.152266
14	6	0	2.679595	-0.842386	0.268213
15	6	0	2.975112	0.218150	1.150289
16	6	0	4.269454	0.717193	1.287943
17	6	0	5.309785	0.157314	0.534318
18	6	0	5.041732	-0.897234	-0.352223

19	6	0	3.744797	-1.384696	-0.479235
20	8	0	6.558733	0.682682	0.702774
21	8	0	-0.098485	2.400573	-0.805418
22	8	0	-1.202153	2.380752	1.666878
23	8	0	-3.642837	3.224521	0.830334
24	8	0	2.700820	2.715797	-1.031460
25	8	0	-2.217781	4.062305	-1.586656
26	1	0	-4.808709	-1.874768	1.123052
27	1	0	-2.692491	1.406866	-0.705186
28	1	0	-4.513419	1.636747	0.687787
29	1	0	-2.246061	-4.118088	0.139142
30	1	0	1.500822	-3.060910	-1.023890
31	1	0	0.571155	-0.681104	0.680347
32	1	0	2.173655	0.662681	1.734266
33	1	0	4.485809	1.531741	1.971495
34	1	0	5.845823	-1.326241	-0.943969
35	1	0	3.560879	-2.191345	-1.181419
36	1	0	7.200858	0.227869	0.138624
37	1	0	-1.376806	1.439621	1.813539
38	1	0	-2.774935	2.991733	1.256340
39	1	0	-4.059975	3.894819	1.388228
40	1	0	-0.711769	2.404366	0.801564
41	1	0	0.865409	2.537575	-0.904768
42	1	0	-0.307025	1.463025	-1.149065
43	1	0	3.053088	2.539722	-1.914861
44	1	0	3.122808	2.061792	-0.450976
45	1	0	-2.814662	3.890436	-0.836605
46	1	0	-1.413150	3.538517	-1.384737

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.976503	-0.395725	-1.324388
2	6	0	-2.329542	-1.084649	-0.285613
3	6	0	-3.050802	-1.332708	0.895264
4	6	0	-4.376881	-0.930255	1.031726
5	6	0	-5.013830	-0.267652	-0.028329
6	6	0	-4.308714	0.005523	-1.209568
7	6	0	-0.926174	-1.521702	-0.441866
8	6	0	-0.488573	-2.769213	0.086339
9	6	0	0.887373	-3.035827	0.122578
10	8	0	1.389166	-4.203451	0.376518
11	8	0	-6.313655	0.147817	0.033598
12	6	0	1.811231	-1.883837	-0.029616
13	6	0	1.377761	-0.537320	0.201816
14	6	0	2.321581	0.501591	0.252450
15	6	0	3.680110	0.238172	0.034090
16	6	0	4.136839	-1.067871	-0.174811
17	6	0	3.208704	-2.112219	-0.167159
18	8	0	0.086038	-0.227222	0.397264
19	8	0	3.667249	-3.384869	-0.281570
20	8	0	4.602946	1.241924	0.017951
21	8	0	1.228142	3.360709	-1.756607
22	8	0	3.273372	3.662106	-0.026858
23	8	0	-0.463779	2.376837	0.110440
24	8	0	1.159360	3.745949	1.989175
25	8	0	-3.205688	2.825473	0.056812
26	1	0	5.193332	-1.273301	-0.306575
27	1	0	1.985427	1.512137	0.437835
28	1	0	4.157139	2.120957	0.053111
29	1	0	2.862147	-3.958550	-0.030786
30	1	0	-1.187839	-3.465835	0.536796
31	1	0	-0.493224	-1.211111	-1.394014
32	1	0	-2.434651	-0.175125	-2.239936
33	1	0	-4.813613	0.514692	-2.024519
34	1	0	-4.917774	-1.127143	1.953187
35	1	0	-2.562709	-1.839729	1.721546
36	1	0	-6.703176	-0.072398	0.892318
37	1	0	1.382216	2.692228	-2.437607
38	1	0	2.599487	3.617404	-0.756804
39	1	0	3.807299	4.452768	-0.182688
40	1	0	0.532871	2.984982	-1.156759
41	1	0	-1.430487	2.547190	0.097325

42	1	0	-0.336147	1.394670	0.215460
43	1	0	-3.602836	2.983397	0.924683
44	1	0	-3.618573	2.009477	-0.271928
45	1	0	1.964993	3.807907	1.445234
46	1	0	0.515422	3.285347	1.412851

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.312033	-2.032017	-0.013608
2	6	0	1.906708	-1.860534	-0.051126
3	6	0	1.408657	-0.553041	0.051377
4	6	0	2.242777	0.557738	0.161143
5	6	0	3.633162	0.357729	0.155829
6	6	0	4.173785	-0.930177	0.069040
7	6	0	0.980512	-3.023097	-0.053988
8	8	0	1.515804	-4.213181	0.131522
9	8	0	0.048641	-0.338351	0.110627
10	8	0	4.500599	1.408597	0.232253
11	8	0	3.817121	-3.287981	-0.038568
12	6	0	-0.352401	-2.741304	-0.213939
13	6	0	-0.768822	-1.350356	-0.600974
14	6	0	-2.211202	-1.025205	-0.295584
15	6	0	-3.105227	-0.686208	-1.316612
16	6	0	-4.446940	-0.399571	-1.039217
17	6	0	-4.903226	-0.443315	0.284196
18	6	0	-4.016323	-0.768357	1.321113
19	6	0	-2.686772	-1.062457	1.023219
20	8	0	-6.222850	-0.151839	0.503990
21	8	0	-0.649432	2.340204	-0.102821
22	8	0	1.161459	3.486817	-1.784706
23	8	0	3.059650	3.763894	0.109879
24	8	0	-3.362145	2.673391	-0.484411
25	8	0	0.803415	3.660797	1.968821
26	1	0	5.248397	-1.076701	0.083401
27	1	0	1.823230	1.549650	0.247085
28	1	0	4.010093	2.263644	0.214703
29	1	0	2.964695	-3.885818	0.032360
30	1	0	-1.104816	-3.523253	-0.196302
31	1	0	-0.583558	-1.140467	-1.669383
32	1	0	-2.756706	-0.640992	-2.344926
33	1	0	-5.142902	-0.152041	-1.834558
34	1	0	-4.368112	-0.795328	2.348991
35	1	0	-2.002529	-1.321844	1.825134
36	1	0	-6.425215	-0.188648	1.449893
37	1	0	1.379971	2.878602	-2.503480
38	1	0	2.450369	3.739220	-0.674644
39	1	0	3.566997	4.584561	0.048405
40	1	0	0.433269	3.055526	-1.272203
41	1	0	-1.616384	2.479755	-0.220260
42	1	0	-0.508063	1.370674	-0.031374
43	1	0	-3.845912	3.038378	0.269613
44	1	0	-3.751257	1.796540	-0.643004
45	1	0	1.639985	3.772695	1.482332
46	1	0	0.210027	3.218118	1.330310

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.319539	-0.576421	0.931306
2	6	0	1.723821	-1.699123	0.323031
3	6	0	2.566837	-2.623031	-0.326820
4	6	0	3.940546	-2.409507	-0.407304
5	6	0	4.495532	-1.260466	0.172055
6	6	0	3.689984	-0.356731	0.867815
7	6	0	0.266969	-1.774920	0.311291
8	6	0	-0.530960	-2.739276	-0.186253
9	6	0	-2.002123	-2.628113	-0.140716

10	8	0	-2.642407	-3.696438	0.125822
11	8	0	5.825639	-0.928681	0.044145
12	6	0	-2.687135	-1.358164	-0.303520
13	6	0	-2.136276	-0.213905	-1.032817
14	6	0	-2.883139	0.993914	-0.990532
15	6	0	-4.032371	1.131750	-0.230534
16	6	0	-4.629077	0.023430	0.399284
17	6	0	-3.982264	-1.204677	0.311412
18	8	0	-1.031379	-0.238215	-1.700427
19	8	0	-4.591368	-2.271401	0.893287
20	8	0	-4.624819	2.356889	-0.089039
21	8	0	-0.047969	2.138430	-0.887613
22	8	0	-0.332031	1.957192	1.808961
23	8	0	2.670524	2.682747	-0.567520
24	8	0	2.247121	2.755900	2.206743
25	8	0	5.252352	1.649535	-1.287965
26	8	0	-2.259120	4.017140	-0.451254
27	1	0	-5.561178	0.117248	0.944480
28	1	0	-2.502474	1.837409	-1.548358
29	1	0	-3.965480	3.039333	-0.337290
30	1	0	-4.015863	-3.060785	0.678343
31	1	0	-0.142860	-3.685745	-0.555137
32	1	0	-0.223173	-0.894112	0.716455
33	1	0	1.689800	0.154392	1.428487
34	1	0	4.137424	0.524627	1.314439
35	1	0	4.574235	-3.112510	-0.941024
36	1	0	2.145968	-3.500812	-0.806908
37	1	0	6.309007	-1.613015	-0.442038
38	1	0	-0.303260	1.258791	-1.293362
39	1	0	-1.469252	3.470718	-0.644578
40	1	0	-2.165529	4.819191	-0.981243
41	1	0	0.928496	2.239568	-0.937905
42	1	0	3.496242	2.237847	-0.841747
43	1	0	2.670076	2.679424	0.413013
44	1	0	5.465194	1.631715	-2.230451
45	1	0	5.594216	0.813752	-0.924212
46	1	0	-0.330570	1.942463	0.817646
47	1	0	-0.854493	1.202051	2.106182
48	1	0	1.325376	2.408590	2.237854
49	1	0	2.746448	2.276509	2.880045

TS2-6w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.968651	-0.193102	-0.627848
2	6	0	-2.832786	-1.122191	0.037264
3	6	0	-4.193204	-0.745931	0.211535
4	6	0	-4.664674	0.528328	-0.125247
5	6	0	-3.782637	1.416852	-0.749856
6	6	0	-2.481972	1.030612	-1.077729
7	6	0	-2.398005	-2.512760	0.327296
8	8	0	-3.304264	-3.429999	0.449453
9	8	0	-5.067842	-1.644496	0.734777
10	8	0	-4.206672	2.689666	-1.026813
11	8	0	-0.666325	-0.432021	-0.838250
12	6	0	-1.015991	-2.758162	0.349800
13	6	0	-0.146065	-1.637606	0.462329
14	6	0	1.313033	-1.725321	0.257769
15	6	0	1.890063	-2.628952	-0.649651
16	6	0	3.258952	-2.607616	-0.913169
17	6	0	4.067247	-1.667664	-0.263317
18	6	0	3.521027	-0.777359	0.664195
19	6	0	2.152334	-0.805588	0.909128
20	8	0	5.412245	-1.532596	-0.531586
21	8	0	0.393398	2.085505	-0.357522
22	8	0	3.090871	2.543939	-0.304524
23	8	0	5.328913	1.222237	-1.447505
24	8	0	-1.672312	4.034010	-0.797269
25	8	0	0.295765	2.290072	2.360128
26	1	0	-5.689193	0.810818	0.089978
27	1	0	-1.830198	1.711871	-1.604866
28	1	0	-3.411732	3.255097	-1.133569
29	1	0	-4.559618	-2.524683	0.711836

30	1	0	-0.636302	-3.762041	0.190459
31	1	0	-0.413178	-0.899642	1.219844
32	1	0	1.723994	-0.084902	1.598992
33	1	0	4.164486	-0.056535	1.156515
34	1	0	3.691535	-3.295187	-1.634677
35	1	0	1.259683	-3.335889	-1.179535
36	1	0	5.707010	-2.204127	-1.164507
37	1	0	0.147407	1.157903	-0.594322
38	1	0	-0.911198	3.424458	-0.681306
39	1	0	-1.341611	4.784033	-1.308077
40	1	0	1.370733	2.179621	-0.472500
41	1	0	3.808329	2.025977	-0.722984
42	1	0	3.219961	2.464438	0.665006
43	1	0	5.394844	1.269544	-2.410535
44	1	0	5.490110	0.288970	-1.216490
45	1	0	0.214140	2.179374	1.379403
46	1	0	-0.241918	1.596400	2.763634
47	8	0	3.025314	2.443537	2.489082
48	1	0	2.051578	2.325427	2.595835
49	1	0	3.446380	1.768988	3.037104

INT2-6w

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.183584	-0.859945	0.928815
2	6	0	1.238750	-1.641688	0.251386
3	6	0	1.685852	-2.522990	-0.741700
4	6	0	3.039014	-2.602550	-1.075705
5	6	0	3.957931	-1.789760	-0.403699
6	6	0	3.539038	-0.932259	0.614863
7	6	0	-0.229544	-1.423831	0.508932
8	6	0	-1.112845	-2.635390	0.539766
9	6	0	-2.471680	-2.447931	0.451489
10	8	0	-3.412150	-3.350159	0.638881
11	8	0	5.298245	-1.751005	-0.734039
12	6	0	-2.919010	-1.082842	0.063319
13	6	0	-2.003724	-0.164889	-0.473327
14	6	0	-2.397366	1.074568	-0.962591
15	6	0	-3.734307	1.462725	-0.819993
16	6	0	-4.691399	0.577770	-0.311613
17	6	0	-4.283143	-0.703524	0.092354
18	8	0	-0.668904	-0.481789	-0.560700
19	8	0	-5.198607	-1.603284	0.526602
20	8	0	-4.115548	2.732728	-1.167282
21	8	0	0.533020	2.135870	-0.277126
22	8	0	0.495346	2.302050	2.466418
23	8	0	3.228675	2.472275	-0.273831
24	8	0	3.238117	2.344611	2.514190
25	8	0	5.344579	1.045103	-1.510953
26	8	0	-1.565485	4.082363	-0.819886
27	1	0	-5.731290	0.873749	-0.224804
28	1	0	-1.673578	1.740728	-1.405551
29	1	0	-3.310111	3.289710	-1.215576
30	1	0	-4.640281	-2.471752	0.641197
31	1	0	-0.683540	-3.601087	0.786755
32	1	0	-0.330785	-0.823788	1.431029
33	1	0	1.855071	-0.162719	1.693910
34	1	0	4.268135	-0.312693	1.126241
35	1	0	3.374575	-3.271667	-1.863486
36	1	0	0.964789	-3.135586	-1.274246
37	1	0	5.501721	-2.402770	-1.421098
38	1	0	0.288713	1.208726	-0.470948
39	1	0	-0.790670	3.503827	-0.660828
40	1	0	-1.236642	4.840459	-1.320149
41	1	0	1.514204	2.209585	-0.401645
42	1	0	3.897989	1.915038	-0.721454
43	1	0	3.382315	2.373030	0.690852
44	1	0	5.406194	1.136840	-2.471072
45	1	0	5.458534	0.094234	-1.327443
46	1	0	0.386131	2.227343	1.487267
47	1	0	-0.035721	1.594465	2.854879
48	1	0	2.264111	2.265364	2.647773
49	1	0	3.644921	1.634078	3.026433

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.322909	0.721825	0.797662
2	6	0	3.071328	-0.379815	-0.047830
3	6	0	4.160699	-0.919103	-0.765241
4	6	0	5.438868	-0.385862	-0.644589
5	6	0	5.661112	0.708809	0.207291
6	6	0	4.598138	1.263584	0.930090
7	6	0	1.709572	-0.895844	-0.139480
8	6	0	1.288427	-1.969885	-0.845762
9	6	0	-0.064120	-2.539734	-0.786365
10	8	0	-0.128530	-3.806505	-0.929883
11	8	0	6.896667	1.274868	0.366726
12	6	0	-1.268861	-1.777665	-0.480659
13	6	0	-1.442315	-0.365847	-0.777700
14	6	0	-2.592572	0.283935	-0.274809
15	6	0	-3.580987	-0.408628	0.418307
16	6	0	-3.494231	-1.798414	0.611854
17	6	0	-2.374179	-2.467048	0.132158
18	8	0	-0.598385	0.312939	-1.512441
19	8	0	-2.333062	-3.813892	0.310058
20	8	0	-4.679276	0.227001	0.908675
21	8	0	-1.908796	2.052638	-3.075511
22	8	0	-2.317104	3.769788	-0.888429
23	8	0	-4.541647	2.938851	0.522879
24	8	0	0.039782	2.544399	-0.037936
25	8	0	-0.846563	-0.975494	2.653945
26	8	0	-0.075353	1.688626	2.624681
27	1	0	-4.289819	-2.345041	1.105119
28	1	0	-2.703360	1.340907	-0.467034
29	1	0	-4.622003	1.201734	0.733763
30	1	0	-1.514931	-4.124263	-0.174028
31	1	0	1.993958	-2.589524	-1.393611
32	1	0	0.979624	-0.337057	0.438619
33	1	0	2.499886	1.158997	1.354943
34	1	0	4.780559	2.111210	1.582610
35	1	0	6.265126	-0.812345	-1.205859
36	1	0	4.012087	-1.763628	-1.429659
37	1	0	7.551985	0.823496	-0.187139
38	1	0	-1.396445	1.397645	-2.516704
39	1	0	-1.499370	3.443132	-0.443320
41	1	0	-5.316614	3.270592	0.047652
42	1	0	0.023798	2.235664	0.894534
43	1	0	-0.140458	1.735372	-0.580863
44	1	0	-1.816899	-0.984751	2.648191
45	1	0	-0.617540	-1.323485	1.775098
46	1	0	-2.295125	3.282660	-1.742879
47	1	0	-1.267593	2.422953	-3.697889
48	1	0	-0.325752	0.735212	2.643495
49	1	0	0.789722	1.738903	3.054792

TS2-6wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.158589	-0.048330	1.253763
2	6	0	2.610416	-0.812584	0.208246
3	6	0	3.400503	-1.046401	-0.931537
4	6	0	4.699783	-0.553778	-1.020012
5	6	0	5.230451	0.194045	0.041901
6	6	0	4.458197	0.446753	1.182710
7	6	0	1.221929	-1.299518	0.304645
8	6	0	0.816973	-2.523386	-0.317644
9	6	0	-0.540621	-2.798729	-0.475916
10	8	0	-1.000799	-3.962071	-0.848010
11	8	0	6.499926	0.706263	0.013993
12	6	0	-1.502512	-1.676697	-0.336306

13	6	0	-1.078731	-0.314186	-0.459337
14	6	0	-2.022800	0.713624	-0.563277
15	6	0	-3.391153	0.423595	-0.518777
16	6	0	-3.845940	-0.897553	-0.417976
17	6	0	-2.905855	-1.926978	-0.369451
18	8	0	0.222276	0.031146	-0.486817
19	8	0	-3.349677	-3.211681	-0.360223
20	8	0	-4.321917	1.416054	-0.568185
21	8	0	0.830953	2.004830	-2.310282
22	8	0	-0.439305	3.913688	-0.635780
23	8	0	-3.193856	3.900870	-0.794854
24	8	0	0.406036	2.170212	1.365327
25	8	0	-1.796089	-1.268101	2.798923
26	8	0	-1.723557	1.493549	3.037988
27	1	0	-4.906598	-1.123187	-0.420470
28	1	0	-1.677279	1.733899	-0.637063
29	1	0	-3.884244	2.301599	-0.659177
30	1	0	-2.514757	-3.761481	-0.559976
31	1	0	1.553133	-3.199295	-0.740897
32	1	0	0.755444	-1.054739	1.258443
33	1	0	2.558075	0.159136	2.134438
34	1	0	4.880172	1.029907	1.994739
35	1	0	5.299742	-0.739810	-1.906058
36	1	0	2.991619	-1.610678	-1.763526
37	1	0	6.940607	0.473267	-0.817486
38	1	0	0.654955	1.257481	-1.688960
39	1	0	-0.186647	3.414730	0.176775
40	1	0	-2.203630	3.919219	-0.765489
41	1	0	-3.438142	4.303770	-1.640289
42	1	0	-0.339462	1.954270	1.970378
43	1	0	0.444829	1.411753	0.742737
44	1	0	-2.689581	-1.602653	2.966304
45	1	0	-1.646724	-1.428082	1.846622
46	1	0	-0.028277	3.377684	-1.348724
47	1	0	1.786652	2.150241	-2.264862
48	1	0	-1.775243	0.510193	2.979452
49	1	0	-1.501955	1.685444	3.960273

INT2-6wb

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.220473	-0.281498	1.353779
2	6	0	2.484271	-0.817459	0.290024
3	6	0	3.101770	-0.925239	-0.964340
4	6	0	4.418599	-0.506928	-1.157786
5	6	0	5.140318	0.022167	-0.078305
6	6	0	4.542979	0.131479	1.181744
7	6	0	1.039391	-1.204917	0.477513
8	6	0	0.652096	-2.559502	-0.043657
9	6	0	-0.658952	-2.827703	-0.328802
10	8	0	-1.163807	-4.012758	-0.641548
11	8	0	6.439625	0.450248	-0.199469
12	6	0	-1.595291	-1.674233	-0.334579
13	6	0	-1.098444	-0.359677	-0.316218
14	6	0	-1.917517	0.753328	-0.461552
15	6	0	-3.295872	0.556156	-0.628197
16	6	0	-3.841312	-0.733512	-0.653587
17	6	0	-2.989342	-1.836408	-0.530992
18	8	0	0.253684	-0.132092	-0.199664
19	8	0	-3.495934	-3.093545	-0.620373
20	8	0	-4.144033	1.615301	-0.765174
21	8	0	1.177378	1.675744	-2.154743
22	8	0	-0.043337	3.801015	-0.708929
23	8	0	-2.786471	3.989136	-0.976048
24	8	0	0.520865	2.212696	1.514556
25	8	0	-2.104790	-0.990806	2.796286
26	8	0	-1.812245	1.767799	2.961355
27	1	0	-4.906272	-0.878962	-0.798971
28	1	0	-1.491505	1.744913	-0.434899
29	1	0	-3.632995	2.462851	-0.825215
30	1	0	-2.652902	-3.690130	-0.646929
31	1	0	1.405396	-3.341142	-0.058557

32	1	0	0.776063	-1.085521	1.540356
33	1	0	2.755211	-0.179302	2.330151
34	1	0	5.112080	0.542664	2.009396
35	1	0	4.884232	-0.590142	-2.136041
36	1	0	2.543843	-1.333671	-1.801557
37	1	0	6.751892	0.325681	-1.108166
38	1	0	0.925194	0.977606	-1.514774
39	1	0	0.130526	3.381514	0.165630
40	1	0	-1.799717	3.928591	-0.917629
41	1	0	-2.973534	4.386312	-1.838544
42	1	0	-0.299238	2.084937	2.045760
43	1	0	0.570330	1.414490	0.955064
44	1	0	-3.029509	-1.251775	2.918497
45	1	0	-1.904233	-1.211718	1.867875
46	1	0	0.366205	3.168398	-1.337909
47	1	0	2.144017	1.707878	-2.109910
48	1	0	-1.945296	0.791601	2.917413
49	1	0	-1.676272	1.966698	3.898704

TS2-6wc

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.896069	3.890135	0.195460
2	6	0	-0.113463	2.899344	0.050771
3	6	0	0.304980	1.581455	-0.312367
4	6	0	1.666605	1.290810	-0.469092
5	6	0	2.634141	2.277554	-0.230897
6	6	0	2.257048	3.586125	0.093060
7	6	0	-1.546939	3.291035	0.049589
8	8	0	-1.841771	4.546543	-0.086268
9	8	0	-0.581642	0.591348	-0.533770
10	8	0	3.963286	1.992793	-0.309307
11	8	0	0.534873	5.177191	0.432334
12	6	0	-2.497130	2.262823	0.096565
13	6	0	-2.067362	0.957498	0.479624
14	6	0	-2.923823	-0.232176	0.298699
15	6	0	-2.788653	-1.328980	1.169042
16	6	0	-3.549664	-2.483775	1.005706
17	6	0	-4.463315	-2.562419	-0.053006
18	6	0	-4.606670	-1.485954	-0.940351
19	6	0	-3.838610	-0.337448	-0.762412
20	8	0	-5.185062	-3.717919	-0.173972
21	8	0	0.422160	-1.790432	-0.108898
22	8	0	2.467144	-1.755745	1.678437
23	8	0	4.298278	-0.697547	-0.239532
24	8	0	2.627110	-2.208955	-1.859670
25	8	0	3.549577	-4.284760	1.565175
26	1	0	3.003315	4.359070	0.240215
27	1	0	1.967353	0.289377	-0.743785
28	1	0	4.099766	1.010102	-0.365582
29	1	0	-0.470266	5.184991	0.260158
30	1	0	-3.511184	2.446351	-0.242370
31	1	0	-1.450604	0.893109	1.378010
32	1	0	-2.076726	-1.274630	1.988512
33	1	0	-3.446462	-3.325248	1.683075
34	1	0	-5.308909	-1.553681	-1.766917
35	1	0	-3.943117	0.483112	-1.464972
36	1	0	-5.785444	-3.666018	-0.931794
37	1	0	-0.013870	-0.897271	-0.272264
38	1	0	2.238122	-1.342836	2.521553
39	1	0	3.833265	-0.968792	0.577004
40	1	0	3.812635	-1.200174	-0.936187
41	1	0	1.785266	-2.125180	-1.367275
42	1	0	2.929891	-3.130322	-1.692048
43	1	0	1.648990	-1.742175	1.119456
44	1	0	-0.292599	-2.430443	0.010677
45	1	0	4.422644	-4.279586	1.979606
46	1	0	3.180431	-3.379781	1.691640
47	8	0	3.569548	-4.710943	-1.138494
48	1	0	3.579438	-4.632571	-0.153625
49	1	0	3.030780	-5.486162	-1.343712

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.731910	-1.809585	0.369188
2	6	0	-2.445358	-1.697190	-0.264998
3	6	0	-2.028554	-0.382442	-0.756845
4	6	0	-2.816099	0.739662	-0.368644
5	6	0	-4.003356	0.582259	0.340387
6	6	0	-4.491526	-0.695664	0.691517
7	6	0	-1.617482	-2.874001	-0.356568
8	8	0	-2.101040	-4.049168	-0.272250
9	8	0	-1.019021	-0.239268	-1.542528
10	8	0	-4.768688	1.645093	0.702850
11	8	0	-4.216137	-3.031907	0.713057
12	6	0	-0.139714	-2.774622	-0.438048
13	6	0	0.557835	-1.937255	0.350020
14	6	0	2.006424	-1.724575	0.369045
15	6	0	2.582126	-1.002998	1.435380
16	6	0	3.935984	-0.669556	1.443747
17	6	0	4.739773	-1.044432	0.364464
18	6	0	4.204667	-1.791570	-0.691968
19	6	0	2.853091	-2.124895	-0.684115
20	8	0	6.038680	-0.585218	0.364401
21	8	0	-3.616252	4.034759	0.177554
22	8	0	-1.013528	4.078393	-0.461432
23	8	0	0.127520	2.084993	-1.926121
24	8	0	1.092512	3.772624	1.373336
25	8	0	2.436929	1.900268	-0.183012
26	8	0	5.198774	2.161241	-0.263249
27	1	0	-5.440395	-0.803496	1.204392
28	1	0	-2.498869	1.723712	-0.692317
29	1	0	-4.327736	2.500084	0.459785
30	1	0	-3.553716	-3.694094	0.363519
31	1	0	0.347990	-3.496005	-1.089799
32	1	0	-0.007148	-1.299355	1.027868
33	1	0	1.954948	-0.685384	2.264050
34	1	0	4.366041	-0.094372	2.256985
35	1	0	4.832214	-2.074782	-1.532182
36	1	0	2.444577	-2.665563	-1.531599
37	1	0	6.544671	-0.982500	-0.360435
38	1	0	-0.339648	1.203062	-1.773490
39	1	0	-0.379686	4.066563	0.286798
40	1	0	-2.648665	4.047948	-0.061344
41	1	0	-4.065088	4.583002	-0.479125
42	1	0	5.665730	1.327607	-0.071363
43	1	0	5.603996	2.512688	-1.067466
44	1	0	2.339660	1.016773	0.206152
45	1	0	3.410192	2.026459	-0.276326
46	1	0	-0.679347	3.357761	-1.055707
47	1	0	0.989077	2.011619	-1.475729
48	1	0	0.908555	3.384028	2.238620
49	1	0	1.619259	3.100951	0.882495

TS2-6wd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.382083	-1.388227	1.423192
2	6	0	1.575754	-1.813813	0.353444
3	6	0	2.190727	-2.071090	-0.882742
4	6	0	3.564480	-1.911270	-1.052342
5	6	0	4.346042	-1.489944	0.028874
6	6	0	3.761360	-1.236126	1.273689
7	6	0	0.111336	-1.925441	0.522880
8	6	0	-0.633506	-2.945460	-0.124218
9	6	0	-2.034660	-2.840356	-0.146361
10	8	0	-2.817192	-3.810680	-0.499902
11	8	0	5.700012	-1.258168	-0.086541
12	6	0	-2.629316	-1.509625	0.128593
13	6	0	-1.860584	-0.301227	0.018707

14	6	0	-2.507065	0.947677	0.032439
15	6	0	-3.897245	1.024833	0.187226
16	6	0	-4.675144	-0.135691	0.297842
17	6	0	-4.044093	-1.378806	0.232686
18	8	0	-0.531243	-0.309124	-0.118331
19	8	0	-4.816777	-2.495560	0.241451
20	8	0	-4.543039	2.221014	0.242365
21	8	0	5.636704	1.621643	-0.118192
22	8	0	0.743805	1.563239	-1.610712
23	8	0	-0.353529	3.956096	-0.785308
24	8	0	-2.939447	4.354140	-0.203169
25	8	0	2.916140	1.819105	0.213714
26	1	0	-5.754562	-0.073447	0.380531
27	1	0	-1.906336	1.846585	-0.038405
28	1	0	-3.918636	2.972938	0.074857
29	1	0	-4.181281	-3.234061	-0.060287
30	1	0	-0.143029	-3.733321	-0.686571
31	1	0	-0.224261	-1.622533	1.515240
32	1	0	1.926120	-1.176437	2.386464
33	1	0	4.384622	-0.912426	2.100896
34	1	0	4.023529	-2.091018	-2.020468
35	1	0	1.582639	-2.373837	-1.729016
36	1	0	6.033878	-1.598316	-0.930446
37	1	0	0.266008	0.854129	-1.112127
38	1	0	0.274495	4.116110	-0.047724
39	1	0	-1.982371	4.202124	-0.431742
40	1	0	-3.286596	4.952226	-0.877876
41	1	0	5.854743	0.670260	-0.132919
42	1	0	6.029372	1.997970	-0.917458
43	1	0	2.751112	1.021576	0.740530
44	1	0	3.888527	1.812271	0.042104
45	1	0	-0.054158	3.094893	-1.165336
46	1	0	1.597925	1.648653	-1.143419
47	8	0	1.671105	4.108971	1.139545
48	1	0	1.433573	4.011989	2.071026
49	1	0	2.171366	3.295666	0.899342

INT2-6wd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.137600	-1.258727	-0.045684
2	6	0	2.735283	-1.446123	-0.106031
3	6	0	1.926523	-0.299132	-0.111312
4	6	0	2.452653	0.992058	-0.081677
5	6	0	3.850314	1.144016	-0.045934
6	6	0	4.694268	0.026086	-0.032878
7	6	0	2.127069	-2.799439	-0.016998
8	8	0	2.937873	-3.800984	0.262350
9	8	0	0.556411	-0.424792	-0.081327
10	8	0	4.435027	2.373679	-0.030672
11	8	0	4.939990	-2.347400	0.028814
12	6	0	0.769440	-2.873939	-0.197450
13	6	0	0.028095	-1.666070	-0.695038
14	6	0	-1.454722	-1.675551	-0.407730
15	6	0	-2.388847	-1.476114	-1.432134
16	6	0	-3.761528	-1.452585	-1.163724
17	6	0	-4.202642	-1.613192	0.151776
18	6	0	-3.287562	-1.820834	1.189088
19	6	0	-1.924104	-1.857925	0.900190
20	8	0	-5.561691	-1.509956	0.377229
21	8	0	2.684508	4.425907	0.083406
22	8	0	0.132407	3.905072	0.692272
23	8	0	-0.870100	1.447666	1.477349
24	8	0	-1.944804	4.071415	-1.166710
25	8	0	-3.061478	1.698099	-0.296323
26	8	0	-5.738736	1.351741	0.189998
27	1	0	5.770436	0.154636	0.012417
28	1	0	1.789818	1.848862	-0.097281
29	1	0	3.756743	3.095462	0.016739
30	1	0	4.260842	-3.131811	0.141975
31	1	0	0.236979	-3.816336	-0.117662
32	1	0	0.170636	-1.504482	-1.778020
33	1	0	-2.045729	-1.337148	-2.453892

34	1	0	-4.486564	-1.298806	-1.956327
35	1	0	-3.636929	-1.937039	2.211418
36	1	0	-1.209876	-2.014627	1.702338
37	1	0	-5.779654	-1.797110	1.276687
38	1	0	-0.387936	0.737739	1.007662
39	1	0	-0.522845	4.068459	-0.020988
40	1	0	1.736812	4.233395	0.320702
41	1	0	2.975589	5.126599	0.681619
42	1	0	-5.883330	0.391341	0.291610
43	1	0	-6.126889	1.765495	0.972764
44	1	0	-2.893833	0.925663	-0.858758
45	1	0	-4.021393	1.641829	-0.069436
46	1	0	-0.121934	3.022785	1.051239
47	1	0	-1.726037	1.509328	1.005833
48	1	0	-1.733651	4.027063	-2.108475
49	1	0	-2.407552	3.229940	-0.950053

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.669759	-1.740244	0.181704
2	6	0	-2.382134	-1.590672	-0.437451
3	6	0	-1.977726	-0.258399	-0.871297
4	6	0	-2.782174	0.834985	-0.451268
5	6	0	-3.949967	0.646161	0.284444
6	6	0	-4.434731	-0.645492	0.568184
7	6	0	-1.523283	-2.754258	-0.529685
8	8	0	-1.998179	-3.933407	-0.529507
9	8	0	-0.944689	-0.054685	-1.620685
10	8	0	-4.678779	1.706711	0.730662
11	8	0	-4.149211	-2.978675	0.468763
12	6	0	-0.048754	-2.632130	-0.498823
13	6	0	0.574017	-1.713078	0.264106
14	6	0	2.007534	-1.472424	0.413694
15	6	0	2.434862	-0.530602	1.372133
16	6	0	3.776146	-0.189747	1.511247
17	6	0	4.724010	-0.782524	0.673145
18	6	0	4.334979	-1.735689	-0.277381
19	6	0	2.988859	-2.074500	-0.400173
20	8	0	6.022009	-0.339710	0.790644
21	8	0	0.307488	2.060611	-0.801012
22	8	0	-2.875976	3.769364	0.980865
23	8	0	-1.342993	4.153487	-1.329262
24	8	0	2.951807	1.437407	-1.510809
25	8	0	-0.757764	2.002608	1.746665
26	8	0	5.292320	2.287802	-0.213147
27	1	0	-5.370138	-0.786180	1.097392
28	1	0	-2.488660	1.830645	-0.757508
29	1	0	-4.112074	2.520539	0.720834
30	1	0	-3.483997	-3.622001	0.095931
31	1	0	0.495567	-3.402969	-1.039160
32	1	0	-0.054293	-1.027191	0.827554
33	1	0	1.696526	-0.040697	2.000530
34	1	0	4.094332	0.551728	2.236361
35	1	0	5.074861	-2.188697	-0.931198
36	1	0	2.700105	-2.794643	-1.158802
37	1	0	6.613695	-0.846649	0.214694
38	1	0	-0.159297	1.239767	-1.183085
39	1	0	-1.325861	1.225127	1.633891
40	1	0	-2.161999	3.256580	1.417881
41	1	0	-2.451600	4.047993	0.139141
42	1	0	5.780132	1.517776	0.131342
43	1	0	5.915193	2.767912	-0.775133
44	1	0	2.965139	0.476807	-1.390459
45	1	0	3.755404	1.762630	-1.048521
46	1	0	-0.263570	2.046495	0.891474
47	1	0	1.262997	1.949485	-0.994042
48	1	0	-0.878536	4.991940	-1.448678
49	1	0	-0.643468	3.463175	-1.201338

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.503042	-0.938483	1.238274
2	6	0	1.762363	-1.678420	0.301546
3	6	0	2.433505	-2.202842	-0.816041
4	6	0	3.799279	-1.995509	-0.997724
5	6	0	4.510920	-1.251494	-0.049918
6	6	0	3.870347	-0.732040	1.077477
7	6	0	0.302210	-1.822837	0.469674
8	6	0	-0.394925	-2.976769	0.016120
9	6	0	-1.795744	-2.932015	-0.034297
10	8	0	-2.543290	-3.974179	-0.222521
11	8	0	5.849827	-0.956189	-0.196661
12	6	0	-2.440763	-1.595524	0.017782
13	6	0	-1.717478	-0.396778	-0.294082
14	6	0	-2.408773	0.816735	-0.444278
15	6	0	-3.794266	0.879214	-0.239215
16	6	0	-4.529486	-0.277466	0.045769
17	6	0	-3.855956	-1.498609	0.132157
18	8	0	-0.388033	-0.389923	-0.474568
19	8	0	-4.587160	-2.626895	0.321228
20	8	0	-4.468785	2.060094	-0.314440
21	8	0	5.672918	1.898589	-0.370648
22	8	0	0.655650	2.048787	0.037246
23	8	0	-1.186150	2.842529	1.930462
24	8	0	-2.719045	4.120098	-0.059571
25	8	0	3.237783	2.663478	0.717980
26	1	0	-5.606109	-0.235645	0.168213
27	1	0	-1.855782	1.709388	-0.699766
28	1	0	-3.834556	2.824911	-0.321219
29	1	0	-3.927168	-3.380821	0.130267
30	1	0	0.133349	-3.838337	-0.378539
31	1	0	-0.062855	-1.359646	1.387628
32	1	0	1.999316	-0.510289	2.100401
33	1	0	4.441537	-0.159632	1.800555
34	1	0	4.304921	-2.389121	-1.875212
35	1	0	1.877406	-2.758105	-1.564367
36	1	0	6.217737	-1.405474	-0.972229
37	1	0	0.414027	1.106030	-0.159577
38	1	0	-1.706525	2.038069	2.068548
39	1	0	-2.240779	3.807035	0.740401
40	1	0	-2.019474	4.129177	-0.750036
41	1	0	5.869919	0.942569	-0.374491
42	1	0	5.833699	2.206928	-1.272474
43	1	0	3.369487	2.565848	1.670205
44	1	0	4.070423	2.343816	0.302050
45	1	0	-0.457496	2.560287	1.326257
46	1	0	1.617356	2.117697	0.237400
47	8	0	-0.519470	3.764290	-1.741730
48	1	0	0.041358	4.520202	-1.959188
49	1	0	0.020601	3.176700	-1.158514

INT2-6we

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.959300	-1.435410	-0.024279
2	6	0	-2.551695	-1.575460	0.048672
3	6	0	-1.778937	-0.406967	-0.033737
4	6	0	-2.348396	0.857835	-0.158638
5	6	0	-3.748792	0.968463	-0.193685
6	6	0	-4.558180	-0.172454	-0.125468
7	6	0	-1.900646	-2.911700	0.062847
8	8	0	-2.679348	-3.956947	-0.138196
9	8	0	-0.404721	-0.490877	-0.058608
10	8	0	-4.360359	2.182472	-0.291328
11	8	0	-4.726924	-2.551624	-0.017173
12	6	0	-0.541475	-2.928622	0.247827
13	6	0	0.159984	-1.665506	0.655249
14	6	0	1.642548	-1.625280	0.374110
15	6	0	2.536670	-1.128333	1.329940
16	6	0	3.899658	-1.013576	1.052124

17	6	0	4.372378	-1.387471	-0.206466
18	6	0	3.501191	-1.897302	-1.174586
19	6	0	2.144347	-2.015961	-0.874948
20	8	0	5.717807	-1.189825	-0.455950
21	8	0	0.822068	2.029455	0.092705
22	8	0	-2.524470	4.180545	-0.216193
23	8	0	-0.385660	3.517413	-1.898443
24	8	0	3.410884	2.431097	0.811791
25	8	0	-0.752684	3.484696	1.843224
26	8	0	5.730341	1.668167	-0.489036
27	1	0	-5.638298	-0.082656	-0.170795
28	1	0	-1.721362	1.734591	-0.217723
29	1	0	-3.688676	2.914966	-0.290896
30	1	0	-4.023504	-3.320618	-0.070507
31	1	0	0.019994	-3.857474	0.241009
32	1	0	0.001360	-1.425427	1.721671
33	1	0	2.164712	-0.815738	2.302123
34	1	0	4.593970	-0.625828	1.790593
35	1	0	3.878006	-2.185370	-2.152351
36	1	0	1.460567	-2.405210	-1.622928
37	1	0	5.966744	-1.580191	-1.307123
38	1	0	0.554116	1.086904	0.053536
39	1	0	-1.128712	2.898426	2.513313
40	1	0	-2.004867	4.039653	0.606295
41	1	0	-1.854832	4.063978	-0.925820
42	1	0	5.863161	0.701507	-0.534125
43	1	0	5.833103	1.992793	-1.393723
44	1	0	3.538935	2.105241	1.712585
45	1	0	4.202543	2.129106	0.309024
46	1	0	-0.144672	2.923125	1.307060
47	1	0	1.788782	2.075868	0.293348
48	1	0	0.182926	4.221993	-2.235616
49	1	0	0.164416	3.000253	-1.265055

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.835864	-1.622341	-1.560071
2	6	0	-1.307662	-1.815327	-0.267921
3	6	0	-2.212235	-2.092058	0.776858
4	6	0	-3.583032	-2.153560	0.547522
5	6	0	-4.076995	-1.938186	-0.745188
6	6	0	-3.204064	-1.685385	-1.805543
7	6	0	0.130448	-1.653875	-0.066150
8	6	0	0.838290	-1.878701	1.057825
9	6	0	2.306299	-1.740068	1.131670
10	8	0	2.904055	-2.621557	1.832185
11	8	0	-5.425904	-1.905434	-1.025800
12	6	0	3.052690	-0.740459	0.391411
13	6	0	2.484357	0.531314	-0.061268
14	6	0	3.283089	1.330771	-0.935039
15	6	0	4.582904	0.967351	-1.256559
16	6	0	5.186328	-0.191573	-0.737487
17	6	0	4.434617	-1.009628	0.095795
18	8	0	1.334522	0.947048	0.332228
19	8	0	5.044720	-2.109795	0.604913
20	8	0	5.369360	1.736342	-2.076014
21	8	0	-0.321108	2.581359	-0.862072
22	8	0	-0.393780	4.621923	0.877667
23	8	0	-2.887785	1.551862	-0.127771
24	8	0	-1.934868	0.760542	2.436448
25	8	0	-2.654365	3.420665	1.971585
26	8	0	-5.277347	0.947665	-1.462417
27	1	0	6.217966	-0.433337	-0.964286
28	1	0	2.861426	2.264650	-1.296913
29	1	0	4.874512	2.513665	-2.373232
30	1	0	4.377482	-2.518997	1.231160
31	1	0	0.382388	-2.309537	1.945940
32	1	0	0.671516	-1.283358	-0.933397
33	1	0	-1.161380	-1.401322	-2.382714
34	1	0	-3.605016	-1.517081	-2.799524
35	1	0	-4.268499	-2.339046	1.369713

36	1	0	-1.848225	-2.229678	1.789172
37	1	0	-5.945154	-2.163843	-0.249607
38	1	0	0.352119	1.951970	-0.455990
39	1	0	-0.318393	3.919171	0.172528
40	1	0	-0.514542	5.461389	0.415416
41	1	0	-1.195773	2.162365	-0.740050
42	1	0	-3.698832	1.262701	-0.597854
43	1	0	-2.679336	0.883987	0.553327
44	1	0	-6.010298	1.501500	-1.161967
45	1	0	-5.580537	0.026327	-1.369073
46	1	0	-1.871083	3.950000	1.700315
47	1	0	-2.938090	2.982151	1.143986
48	1	0	-2.129776	1.718757	2.534925
49	1	0	-2.507495	0.302967	3.065374

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.810675	-0.178461	-0.238739
2	6	0	-2.763535	-1.233047	-0.053035
3	6	0	-4.131810	-0.864423	0.074129
4	6	0	-4.541629	0.472036	0.151363
5	6	0	-3.575335	1.471075	-0.014549
6	6	0	-2.249419	1.152227	-0.302123
7	6	0	-2.383707	-2.658423	-0.230014
8	8	0	-3.307520	-3.506083	-0.552756
9	8	0	-5.077401	-1.838339	0.138640
10	8	0	-3.945461	2.784423	0.128619
11	8	0	-0.496462	-0.391643	-0.339499
12	6	0	-1.016580	-2.977078	-0.143157
13	6	0	-0.152329	-2.031528	0.470864
14	6	0	1.320346	-2.082216	0.386880
15	6	0	1.990912	-2.597639	-0.734220
16	6	0	3.372769	-2.466863	-0.868454
17	6	0	4.098393	-1.803274	0.127749
18	6	0	3.459864	-1.316964	1.271520
19	6	0	2.080358	-1.452750	1.387682
20	8	0	5.449683	-1.554110	0.021827
21	8	0	0.466626	1.632833	1.358808
22	8	0	0.787363	4.540652	-0.681227
23	8	0	2.769207	2.399940	-0.021843
24	8	0	5.352185	1.335920	0.298586
25	8	0	-1.263068	3.757532	1.092620
26	1	0	-5.582368	0.719290	0.328600
27	1	0	-1.522009	1.931949	-0.477511
28	1	0	-3.137245	3.303560	0.310797
29	1	0	-4.580442	-2.681583	-0.133760
30	1	0	-0.634455	-3.866851	-0.633228
31	1	0	-0.500039	-1.604021	1.412186
32	1	0	1.577888	-1.033506	2.254097
33	1	0	4.041256	-0.809846	2.034406
34	1	0	3.878708	-2.846318	-1.751996
35	1	0	1.424431	-3.071202	-1.529730
36	1	0	5.805868	-1.926991	-0.798182
37	1	0	0.185374	0.883015	0.785944
38	1	0	-0.708796	2.959066	1.302163
39	1	0	-1.312716	4.279319	1.905059
40	1	0	1.340933	1.894152	0.994964
41	1	0	3.656477	1.997018	0.087696
42	1	0	2.467921	2.196614	-0.931044
43	1	0	6.034636	1.810652	-0.194196
44	1	0	5.523741	0.387798	0.148092
45	1	0	0.017773	4.394865	-0.090071
46	1	0	1.555939	4.222990	-0.178228
47	8	0	1.238446	2.389024	-2.366888
48	1	0	0.915112	3.216172	-1.942459
49	1	0	1.577472	2.646653	-3.234056

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.195133	-1.497789	-1.461006
2	6	0	-1.328928	-1.955465	-0.459639
3	6	0	-1.873143	-2.345437	0.770434
4	6	0	-3.244332	-2.246537	1.013886
5	6	0	-4.081875	-1.746256	0.011653
6	6	0	-3.567376	-1.395349	-1.238000
7	6	0	0.162746	-1.839871	-0.657036
8	6	0	1.028821	-2.918901	-0.075879
9	6	0	2.363055	-2.660606	0.128006
10	8	0	3.297735	-3.532471	0.448079
11	8	0	-5.431815	-1.529732	0.209693
12	6	0	2.785113	-1.237591	0.022850
13	6	0	1.821791	-0.220267	-0.009321
14	6	0	2.159727	1.126657	0.049582
15	6	0	3.510857	1.482842	0.029781
16	6	0	4.514886	0.509195	0.069189
17	6	0	4.143679	-0.845401	0.103877
18	8	0	0.485442	-0.516571	-0.061380
19	8	0	5.091084	-1.807462	0.217089
20	8	0	3.866049	2.806940	-0.041890
21	8	0	-0.589827	1.771947	-1.599180
22	8	0	1.188493	3.868955	-1.129884
23	8	0	-2.709917	2.299900	0.105062
24	8	0	-1.054293	1.984152	2.339832
25	8	0	-0.713475	4.339258	0.913640
26	8	0	-5.331995	1.345029	-0.167595
27	1	0	5.562486	0.790077	0.077019
28	1	0	1.384036	1.874987	0.078638
29	1	0	3.076661	3.321652	-0.297585
30	1	0	4.530842	-2.675858	0.336122
31	1	0	0.626043	-3.923099	0.012278
32	1	0	0.357881	-1.694954	-1.735028
33	1	0	-1.789362	-1.187088	-2.420024
34	1	0	-4.235697	-1.018872	-2.005586
35	1	0	-3.654354	-2.527509	1.980319
36	1	0	-1.212289	-2.700505	1.555397
37	1	0	-5.701837	-1.833934	1.088767
38	1	0	-0.266665	0.946094	-1.193163
39	1	0	0.617162	3.129973	-1.457449
40	1	0	1.221480	4.528595	-1.835853
41	1	0	-1.414668	1.968097	-1.098134
42	1	0	-3.618188	1.940843	0.009514
43	1	0	-2.353237	1.968677	0.955005
44	1	0	-5.987575	1.840543	0.340992
45	1	0	-5.511411	0.402657	0.009809
46	1	0	0.007065	4.299964	0.249963
47	1	0	-1.514117	4.067425	0.433451
48	1	0	-0.750023	2.859782	2.010349
49	1	0	-1.353392	2.127534	3.247211

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.817485	-1.404261	0.224760
2	6	0	-2.499180	-1.555291	-0.333458
3	6	0	-1.996321	-0.492262	-1.206784
4	6	0	-2.826305	0.652793	-1.375642
5	6	0	-4.020599	0.803453	-0.694124
6	6	0	-4.550373	-0.226181	0.105048
7	6	0	-1.752631	-2.758110	-0.000051
8	8	0	-2.346667	-3.810547	0.400475
9	8	0	-0.864887	-0.536332	-1.823496
10	8	0	-4.732979	1.972740	-0.768512
11	8	0	-4.376600	-2.409426	0.944376
12	6	0	-0.279038	-2.810947	-0.032843
13	6	0	0.478982	-1.774870	0.375426
14	6	0	1.935768	-1.662395	0.378786
15	6	0	2.516040	-0.539512	1.002622
16	6	0	3.881739	-0.292458	0.927144

17	6	0	4.696578	-1.166763	0.204829
18	6	0	4.157675	-2.313918	-0.391942
19	6	0	2.788905	-2.555283	-0.300270
20	8	0	6.019158	-0.806525	0.066545
21	8	0	0.053564	1.853138	-1.060283
22	8	0	2.697769	2.650414	-0.780160
23	8	0	-0.095404	1.508323	1.677902
24	8	0	2.118256	3.049151	1.936010
25	8	0	-2.148378	3.522027	-0.580101
26	8	0	-2.765851	2.321378	1.886586
27	8	0	5.377040	1.743282	-1.261918
28	1	0	-5.515367	-0.125052	0.587863
29	1	0	-2.468660	1.439997	-2.027778
30	1	0	-4.136313	2.672710	-1.087460
31	1	0	-3.750878	-3.185885	0.851985
32	1	0	0.147272	-3.774287	-0.303467
33	1	0	-0.037000	-0.878796	0.710344
34	1	0	1.874908	0.161650	1.525177
35	1	0	4.317758	0.589095	1.385403
36	1	0	4.797954	-2.990911	-0.950995
37	1	0	2.378134	-3.426519	-0.800734
38	1	0	6.510130	-1.476379	-0.431993
39	1	0	-0.168653	0.961919	-1.459844
40	1	0	-1.332803	3.024832	-0.826563
41	1	0	-1.904169	4.456741	-0.557269
42	1	0	1.017973	2.024416	-1.142065
43	1	0	3.565889	2.235555	-0.950841
44	1	0	2.638433	2.779852	0.191166
45	1	0	5.667004	1.770323	-2.183327
46	1	0	5.741312	0.918714	-0.893886
47	1	0	-0.090948	1.566376	0.692712
48	1	0	-1.006000	1.768373	1.932526
49	1	0	1.281866	2.521615	1.994062
50	1	0	2.698545	2.717770	2.633452
51	1	0	-2.666114	2.806060	1.037558
52	1	0	-3.322956	1.556881	1.673565

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.359682	-0.712896	0.914665
2	6	0	1.587586	-1.674457	0.241367
3	6	0	2.234371	-2.561062	-0.634454
4	6	0	3.609329	-2.477612	-0.852847
5	6	0	4.351504	-1.498530	-0.181345
6	6	0	3.734409	-0.629557	0.721968
7	6	0	0.121357	-1.662561	0.411130
8	6	0	-0.661302	-2.854032	0.451421
9	6	0	-2.053809	-2.705701	0.420117
10	8	0	-2.905417	-3.650313	0.666100
11	8	0	5.698901	-1.306308	-0.398241
12	6	0	-2.576043	-1.386071	-0.030063
13	6	0	-1.782629	-0.505977	-0.834118
14	6	0	-2.376285	0.619532	-1.425145
15	6	0	-3.691423	0.965840	-1.110922
16	6	0	-4.497764	0.132284	-0.328469
17	6	0	-3.946827	-1.065232	0.148275
18	8	0	-0.472791	-0.705288	-1.040252
19	8	0	-4.752940	-1.933594	0.808934
20	8	0	-4.214279	2.159646	-1.540891
21	8	0	0.469945	1.851201	-0.801585
22	8	0	-0.024425	1.639655	1.918898
23	8	0	3.035665	2.642154	-0.355085
24	8	0	2.408905	2.774858	2.377382
25	8	0	5.570968	1.526207	-0.995463
26	8	0	-1.735378	3.550778	-0.874273
27	1	0	-5.531488	0.385495	-0.121938
28	1	0	-1.775417	1.268844	-2.048053
29	1	0	-3.472665	2.777492	-1.684545
30	1	0	-4.198327	-2.784468	0.871551
31	1	0	-0.204974	-3.838187	0.426524
32	1	0	-0.203675	-0.854499	1.066849
33	1	0	1.870966	-0.010833	1.582223

34	1	0	4.328050	0.119090	1.235566
35	1	0	4.097412	-3.149668	-1.553237
36	1	0	1.652591	-3.302146	-1.173795
37	1	0	6.042022	-1.945914	-1.039598
38	1	0	0.310211	0.900180	-1.015524
39	1	0	-0.894095	3.038866	-0.931645
40	1	0	-1.496736	4.485781	-0.926191
41	1	0	1.441534	2.030195	-0.784466
42	1	0	3.869831	2.179431	-0.572977
43	1	0	2.969081	2.669518	0.624150
44	1	0	5.908975	1.781806	-1.863858
45	1	0	5.764157	0.575462	-0.900781
46	1	0	0.104611	1.687575	0.943779
47	1	0	-0.943823	1.952239	2.045009
48	1	0	1.491393	2.407467	2.371392
49	1	0	2.906084	2.249619	3.017877
50	8	0	-2.683507	2.541530	1.594061
51	1	0	-2.446377	2.969543	0.743106
52	1	0	-3.227449	1.779093	1.342432

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.041760	-1.042065	0.058606
2	6	0	-2.665862	-1.366107	-0.008209
3	6	0	-1.822931	-0.492768	-0.714915
4	6	0	-2.303038	0.651086	-1.345575
5	6	0	-3.647262	0.998705	-1.169017
6	6	0	-4.528803	0.162325	-0.476004
7	6	0	-2.138199	-2.651358	0.530882
8	8	0	-3.027197	-3.566905	0.854963
9	8	0	-0.479414	-0.762022	-0.812053
10	8	0	-4.120150	2.193835	-1.652314
11	8	0	-4.887357	-1.911509	0.657979
12	6	0	-0.769567	-2.752439	0.599011
13	6	0	0.018613	-1.492699	0.397467
14	6	0	1.505532	-1.617939	0.210564
15	6	0	2.360924	-0.776740	0.934150
16	6	0	3.735561	-0.779086	0.707682
17	6	0	4.263165	-1.620239	-0.273299
18	6	0	3.434023	-2.489738	-0.990675
19	6	0	2.060475	-2.485178	-0.739790
20	8	0	5.618006	-1.511980	-0.517502
21	8	0	0.601710	1.875024	-0.772238
22	8	0	3.169833	2.568830	-0.311384
23	8	0	0.080937	1.766641	1.967735
24	8	0	2.596865	2.706183	2.428502
25	8	0	-1.625425	3.589554	-0.913615
26	8	0	-2.590078	2.625926	1.564187
27	8	0	5.626699	1.339102	-1.016824
28	1	0	-5.573100	0.431551	-0.361964
29	1	0	-1.634339	1.288111	-1.906776
30	1	0	-3.363613	2.802449	-1.747844
31	1	0	-4.285120	-2.741464	0.836129
32	1	0	-0.271104	-3.654327	0.939211
33	1	0	-0.158799	-0.771003	1.210090
34	1	0	1.942344	-0.089692	1.663126
35	1	0	4.395064	-0.114738	1.256238
36	1	0	3.854218	-3.147398	-1.746930
37	1	0	1.409481	-3.145800	-1.304559
38	1	0	5.893901	-2.132319	-1.208102
39	1	0	0.457035	0.927298	-0.961759
40	1	0	-0.774971	3.095385	-0.948745
41	1	0	-1.405261	4.527851	-0.986672
42	1	0	1.578180	2.045147	-0.736446
43	1	0	3.974660	2.065857	-0.551891
44	1	0	3.122194	2.585829	0.669527
45	1	0	5.966885	1.598788	-1.883136
46	1	0	5.768591	0.376727	-0.949526
47	1	0	0.214782	1.775944	0.994143
48	1	0	-0.839855	2.079460	2.077216
49	1	0	1.652933	2.416161	2.426539
50	1	0	3.057162	2.122305	3.045430

51	1	0	-2.346016	3.034103	0.705780
52	1	0	-3.115922	1.847774	1.326160

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.773659	-2.432568	-0.201276
2	6	0	-1.539021	-1.781670	-0.577147
3	6	0	-1.580570	-0.333013	-0.746643
4	6	0	-2.766109	0.350433	-0.387669
5	6	0	-3.893262	-0.322703	0.071881
6	6	0	-3.914374	-1.726149	0.153663
7	6	0	-0.372196	-2.617406	-0.838632
8	8	0	-0.518995	-3.870088	-1.046945
9	8	0	-0.579623	0.359400	-1.214748
10	8	0	-5.020644	0.342956	0.437210
11	8	0	-2.845190	-3.786764	-0.136046
12	6	0	1.025906	-2.160666	-0.836550
13	6	0	1.534190	-1.172882	-0.068439
14	6	0	2.934173	-0.760922	0.011378
15	6	0	3.236372	0.499309	0.569518
16	6	0	4.542580	0.977233	0.626167
17	6	0	5.588039	0.187093	0.134011
18	6	0	5.317897	-1.077473	-0.412487
19	6	0	4.006803	-1.539306	-0.471937
20	8	0	6.856561	0.695049	0.216184
21	8	0	-0.772046	2.795650	-2.380059
22	8	0	-2.096869	3.846273	-0.103648
23	8	0	-4.701126	3.053296	0.335966
24	8	0	-0.045027	2.165820	0.780219
25	8	0	0.536849	0.681618	3.056933
26	8	0	-1.190176	-1.418623	2.593298
27	1	0	-4.807105	-2.253892	0.469409
28	1	0	-2.776383	1.426237	-0.495026
29	1	0	-4.884923	1.324026	0.367328
30	1	0	-1.974811	-4.116876	-0.514142
31	1	0	1.679728	-2.790541	-1.435602
32	1	0	0.853150	-0.588988	0.540022
33	1	0	2.430305	1.124190	0.938203
34	1	0	4.761614	1.953924	1.045377
35	1	0	6.132500	-1.693201	-0.782985
36	1	0	3.819265	-2.523290	-0.889021
37	1	0	7.495900	0.072819	-0.162532
38	1	0	-0.803685	1.874881	-2.002949
39	1	0	-1.475637	3.330033	0.454244
40	1	0	-3.769542	3.344418	0.166532
41	1	0	-5.228051	3.436965	-0.379569
42	1	0	0.179978	1.682308	1.607255
43	1	0	-0.232955	1.471787	0.096747
44	1	0	-2.104872	-1.145698	2.759377
45	1	0	-1.158221	-1.569244	1.630160
46	1	0	-1.788479	3.612345	-1.007467
47	1	0	0.105828	3.118927	-2.097689
48	1	0	-0.072362	-0.083104	2.922587
49	1	0	1.428424	0.316670	2.961297
50	8	0	1.694275	3.427762	-0.918756
51	1	0	1.171657	3.013227	-0.191183
52	1	0	2.394147	2.787414	-1.112266

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.346138	-1.720501	-0.318991
2	6	0	-1.928120	-1.594133	-0.369330
3	6	0	-1.392122	-0.269519	-0.461680
4	6	0	-2.243384	0.841022	-0.463259
5	6	0	-3.627860	0.668038	-0.342381
6	6	0	-4.190992	-0.612194	-0.262639

7	6	0	-1.081144	-2.785531	-0.629941
8	8	0	-1.663542	-3.880429	-1.033430
9	8	0	-0.067074	-0.040389	-0.551871
10	8	0	-4.470778	1.735742	-0.291777
11	8	0	-3.902458	-2.960859	-0.338410
12	6	0	0.302061	-2.632369	-0.539567
13	6	0	0.833041	-1.486462	0.133197
14	6	0	2.262560	-1.137077	0.017091
15	6	0	2.970950	-0.689084	1.144508
16	6	0	4.322413	-0.359071	1.064760
17	6	0	4.982648	-0.450099	-0.167885
18	6	0	4.288036	-0.873146	-1.311523
19	6	0	2.942161	-1.216847	-1.210821
20	8	0	6.306810	-0.104989	-0.200587
21	8	0	0.894183	2.068003	-2.151071
22	8	0	-0.436525	3.917439	-0.417406
23	8	0	-3.178360	4.132646	-0.458152
24	8	0	0.662228	1.929248	1.235890
25	8	0	0.080424	0.627796	3.611987
26	8	0	-1.859724	-1.203390	2.838559
27	1	0	-5.265854	-0.744119	-0.206363
28	1	0	-1.813651	1.830562	-0.521744
29	1	0	-3.968715	2.587947	-0.373478
30	1	0	-3.137276	-3.569748	-0.622010
31	1	0	0.960982	-3.332051	-1.043663
32	1	0	0.428009	-1.265044	1.120260
33	1	0	2.458173	-0.599719	2.097181
34	1	0	4.868270	-0.021447	1.939512
35	1	0	4.800910	-0.929082	-2.267124
36	1	0	2.407594	-1.535856	-2.099964
37	1	0	6.655709	-0.195765	-1.100321
38	1	0	0.505561	1.280465	-1.711469
39	1	0	-0.148194	3.378607	0.349999
40	1	0	-2.189978	4.070163	-0.468618
41	1	0	-3.421178	4.594791	-1.273148
42	1	0	0.516012	1.542661	2.129450
43	1	0	0.393364	1.213318	0.612056
44	1	0	-2.733773	-0.832291	3.029469
45	1	0	-1.856655	-1.345510	1.873082
46	1	0	-0.074522	3.409823	-1.175659
47	1	0	1.713937	2.230893	-1.636781
48	1	0	-0.591667	-0.035191	3.326546
49	1	0	0.839114	0.112216	3.920209
50	8	0	2.926939	2.525880	-0.222774
51	1	0	2.231487	2.322361	0.445171
52	1	0	3.520705	1.760264	-0.199492

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402579	-1.638263	-0.514755
2	6	0	-1.990999	-1.567634	-0.420007
3	6	0	-1.408228	-0.287968	-0.397714
4	6	0	-2.165360	0.878365	-0.445153
5	6	0	-3.564355	0.769635	-0.502869
6	6	0	-4.189639	-0.482994	-0.532083
7	6	0	-1.136233	-2.778981	-0.511862
8	8	0	-1.734901	-3.916474	-0.834022
9	8	0	-0.036964	-0.152078	-0.368699
10	8	0	-4.361699	1.874700	-0.525748
11	8	0	-3.993328	-2.857891	-0.607584
12	6	0	0.202997	-2.605681	-0.294583
13	6	0	0.705408	-1.294564	0.241394
14	6	0	2.169569	-1.035926	-0.005227
15	6	0	3.053271	-0.870464	1.066707
16	6	0	4.414942	-0.639985	0.851101
17	6	0	4.901788	-0.559840	-0.458636
18	6	0	4.028631	-0.714746	-1.545100
19	6	0	2.676154	-0.957991	-1.310079
20	8	0	6.244359	-0.323534	-0.619331
21	8	0	1.112423	2.090475	-1.874799
22	8	0	-0.285501	3.937405	-0.241786

23	8	0	-2.997448	4.223459	-0.510714
24	8	0	0.664443	1.913803	1.496974
25	8	0	0.127709	0.368029	3.721375
26	8	0	-1.979000	-1.224644	2.844130
27	1	0	-5.269929	-0.557662	-0.593964
28	1	0	-1.678847	1.843087	-0.423569
29	1	0	-3.822452	2.708259	-0.527640
30	1	0	-3.194382	-3.503691	-0.718730
31	1	0	0.903905	-3.430234	-0.381149
32	1	0	0.507861	-1.189992	1.318636
33	1	0	2.676558	-0.915193	2.084762
34	1	0	5.099257	-0.514100	1.683786
35	1	0	4.407734	-0.647450	-2.561020
36	1	0	2.003016	-1.080544	-2.153013
37	1	0	6.468574	-0.280677	-1.561050
38	1	0	0.709153	1.260031	-1.561051
39	1	0	-0.073807	3.435759	0.570795
40	1	0	-2.013775	4.131398	-0.437510
41	1	0	-3.156156	4.702810	-1.336333
42	1	0	0.514811	1.451770	2.355063
43	1	0	0.409874	1.247547	0.827875
44	1	0	-2.823056	-0.791522	3.038979
45	1	0	-1.973495	-1.336565	1.876314
46	1	0	0.122915	3.385356	-0.945618
47	1	0	1.901543	2.195350	-1.298538
48	1	0	-0.606350	-0.206656	3.400035
49	1	0	0.885787	-0.223135	3.834250
50	8	0	3.032355	2.454637	0.167528
51	1	0	2.295203	2.269975	0.793874
52	1	0	3.594267	1.665218	0.209438

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.313119	1.357429	0.320556
2	6	0	0.453331	2.593488	0.262321
3	6	0	-0.204772	3.758329	-0.272687
4	6	0	-1.458813	3.696405	-0.865597
5	6	0	-2.142966	2.467562	-0.883268
6	6	0	-1.594316	1.332156	-0.286434
7	6	0	1.826562	2.737388	0.720142
8	8	0	2.290573	3.888404	1.014289
9	8	0	0.408250	4.968833	-0.245857
10	8	0	-3.361897	2.448163	-1.477014
11	8	0	0.135179	0.304262	0.942385
12	6	0	2.811133	1.642381	0.789512
13	6	0	2.833777	0.577825	-0.039030
14	6	0	3.854453	-0.464813	-0.120738
15	6	0	5.014385	-0.490240	0.681792
16	6	0	5.946386	-1.516914	0.573814
17	6	0	5.740033	-2.554612	-0.349236
18	6	0	4.599087	-2.552724	-1.159705
19	6	0	3.675261	-1.518381	-1.041633
20	8	0	6.618279	-3.591443	-0.501602
21	8	0	-1.149593	-1.783353	0.704790
22	8	0	-4.485500	0.022174	-1.463643
23	8	0	-2.568422	-2.049277	-1.531645
24	8	0	-3.240053	-1.669059	2.383986
25	8	0	-5.440904	-0.497310	1.059005
26	8	0	-4.363750	-4.094977	-1.103192
27	8	0	-5.353223	-3.298670	1.386662
28	1	0	-1.908327	4.587847	-1.287736
29	1	0	-2.167054	0.415047	-0.247044
30	1	0	-3.759147	1.532543	-1.456515
31	1	0	1.242576	4.831460	0.293212
32	1	0	3.632431	1.845315	1.472618
33	1	0	2.003554	0.457445	-0.729238
34	1	0	2.791225	-1.525581	-1.673632
35	1	0	4.449786	-3.359398	-1.870019
36	1	0	6.833609	-1.517203	1.201628
37	1	0	5.197427	0.300924	1.401539
38	1	0	7.367665	-3.495309	0.103686

39	1	0	-0.582702	-0.862227	0.799080
40	1	0	-1.985016	-2.091462	-2.301215
41	1	0	-3.821643	-0.689916	-1.579885
42	1	0	-4.884095	-0.147009	-0.575422
43	1	0	-4.622779	-0.555446	1.591591
44	1	0	-5.729374	-1.434422	1.055344
45	1	0	-1.978452	-1.960699	-0.728116
46	1	0	-0.544492	-2.519456	0.868663
47	1	0	-5.024463	-4.084387	-1.808297
48	1	0	-3.711824	-3.392233	-1.332028
49	1	0	-5.038011	-3.635463	0.519023
50	1	0	-4.551288	-2.981387	1.846104
51	1	0	-2.424348	-1.723589	1.816340
52	1	0	-2.939285	-1.569046	3.296160

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.590310	-1.291011	-0.857668
2	6	0	-2.963428	-0.829619	0.311518
3	6	0	-2.753359	-1.745867	1.357995
4	6	0	-3.168555	-3.071566	1.256070
5	6	0	-3.800746	-3.507556	0.084359
6	6	0	-4.010394	-2.614055	-0.976081
7	6	0	-2.462719	0.555026	0.433790
8	6	0	-3.126459	1.654105	-0.189139
9	6	0	-2.456424	2.882234	-0.257217
10	8	0	-3.016445	3.996575	-0.612550
11	8	0	-4.186826	-4.818249	0.032268
12	6	0	-0.991294	2.878479	-0.006266
13	6	0	-0.288342	4.107191	0.124712
14	6	0	1.103253	4.157144	0.242900
15	6	0	1.834963	2.965846	0.163121
16	6	0	1.185585	1.738078	-0.043335
17	6	0	-0.212766	1.684612	-0.113411
18	8	0	-0.982034	5.273952	0.121675
19	8	0	-0.793727	0.483843	-0.309233
20	8	0	3.185682	3.041605	0.292192
21	8	0	0.494598	-1.672491	0.331714
22	8	0	2.670021	-1.187507	1.884327
23	8	0	4.309445	0.614992	0.431799
24	8	0	4.294929	-0.784632	-1.934504
25	8	0	4.416683	-3.493103	-1.198923
26	8	0	4.396567	-3.331056	1.589944
27	1	0	1.608210	5.109157	0.364206
28	1	0	1.757796	0.822531	-0.121435
29	1	0	3.593632	2.132138	0.307614
30	1	0	-1.916725	5.001891	-0.182820
31	1	0	-4.083943	1.528270	-0.683341
32	1	0	-2.011081	0.749344	1.408646
33	1	0	-2.259565	-1.413127	2.267450
34	1	0	-3.010950	-3.773691	2.068258
35	1	0	-4.490659	-2.956922	-1.888581
36	1	0	-3.739280	-0.610844	-1.690210
37	1	0	-4.618142	-5.013660	-0.812278
38	1	0	-0.019434	-0.830738	0.103271
39	1	0	2.403023	-0.918549	2.773714
40	1	0	3.776138	0.027532	1.006136
41	1	0	4.348786	0.149194	-0.438459
42	1	0	3.355011	-0.990858	-2.099163
43	1	0	4.645463	-1.671050	-1.699739
44	1	0	1.834690	-1.360179	1.379060
45	1	0	-0.158393	-2.307513	0.659654
46	1	0	5.249850	-3.102512	1.981921
47	1	0	3.800768	-2.570402	1.776689
48	1	0	4.447520	-3.491100	-0.216690
49	1	0	3.474383	-3.374200	-1.426948
50	8	0	1.907180	-2.344482	-1.910991
51	1	0	1.331456	-2.152112	-1.132396
52	1	0	1.318853	-2.596417	-2.634385

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.529748	1.680396	-0.123469
2	6	0	1.444188	2.735771	0.006632
3	6	0	0.919379	4.050324	0.057635
4	6	0	-0.455982	4.285213	-0.067193
5	6	0	-1.332338	3.201134	-0.206305
6	6	0	-0.844608	1.881652	-0.225426
7	6	0	2.889993	2.464004	0.225003
8	8	0	3.632907	3.478695	0.619609
9	8	0	1.770215	5.085264	0.253687
10	8	0	-2.660710	3.468801	-0.328779
11	8	0	0.986193	0.379963	-0.088557
12	6	0	3.309027	1.172060	0.028562
13	6	0	2.372394	0.190874	-0.609990
14	6	0	2.684323	-1.268092	-0.385387
15	6	0	3.041066	-1.744016	0.883318
16	6	0	3.247495	-3.104554	1.111607
17	6	0	3.095012	-4.015228	0.056903
18	6	0	2.741249	-3.559064	-1.218058
19	6	0	2.538128	-2.194189	-1.427715
20	8	0	3.280662	-5.364024	0.211496
21	8	0	-0.719199	-1.667244	-0.498755
22	8	0	-4.130023	1.232148	-0.491666
23	8	0	-2.913835	-0.889524	-1.941237
24	8	0	-2.055000	-1.967309	1.895153
25	8	0	-4.172674	-0.046475	1.937804
26	8	0	-4.927509	-2.714733	-1.379012
27	8	0	-4.759806	-2.737413	1.407819
28	1	0	-0.841254	5.298734	-0.034310
29	1	0	-1.518038	1.041137	-0.328909
30	1	0	-3.189012	2.627155	-0.399087
31	1	0	2.678995	4.609540	0.443245
32	1	0	4.340619	0.878942	0.194802
33	1	0	2.262242	0.361299	-1.695304
34	1	0	2.257088	-1.845918	-2.418532
35	1	0	2.630329	-4.273696	-2.027234
36	1	0	3.522254	-3.458909	2.101801
37	1	0	3.153954	-1.039273	1.701503
38	1	0	3.518679	-5.571043	1.126570
39	1	0	-0.070001	-0.927787	-0.375374
40	1	0	-2.682755	-0.731080	-2.866689
41	1	0	-3.744345	0.547486	-1.074836
42	1	0	-4.185093	0.804306	0.397562
43	1	0	-3.264183	-0.378687	2.066137
44	1	0	-4.663113	-0.883931	1.787660
45	1	0	-2.085021	-1.185262	-1.491860
46	1	0	-0.203026	-2.421072	-0.820236
47	1	0	-5.766619	-2.377307	-1.719682
48	1	0	-4.242224	-2.066710	-1.657815
49	1	0	-4.858911	-2.781766	0.430986
50	1	0	-3.797573	-2.765060	1.571561
51	1	0	-1.514859	-1.918254	1.073753
52	1	0	-1.462336	-2.265754	2.597091

INT1-7wd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.369545	-1.485247	-0.332984
2	6	0	0.441563	-2.701789	-0.358431
3	6	0	-0.188104	-3.932045	0.059836
4	6	0	-1.462230	-3.971782	0.610643
5	6	0	-2.190937	-2.772062	0.711972
6	6	0	-1.662903	-1.570556	0.253540
7	6	0	1.821545	-2.763322	-0.803635
8	8	0	2.341213	-3.876008	-1.156897
9	8	0	0.473333	-5.112465	-0.049592
10	8	0	-3.438433	-2.842132	1.249641

11	8	0	0.031910	-0.366832	-0.847312
12	6	0	2.763192	-1.627907	-0.809125
13	6	0	2.752940	-0.611958	0.077869
14	6	0	3.740286	0.457659	0.214341
15	6	0	4.894936	0.564295	-0.589053
16	6	0	5.793827	1.613593	-0.429059
17	6	0	5.558399	2.593105	0.548716
18	6	0	4.422808	2.509689	1.362189
19	6	0	3.532318	1.453361	1.191693
20	8	0	6.403280	3.649037	0.752842
21	8	0	-1.731797	1.466002	-0.634591
22	8	0	-2.872825	1.736609	1.739497
23	8	0	-4.668390	-0.403983	1.168099
24	8	0	-2.093657	3.857806	-2.021918
25	8	0	-4.723253	3.694284	1.304243
26	8	0	-4.780766	3.471176	-1.383486
27	8	0	-4.291596	0.670427	-1.363070
28	1	0	-1.891177	-4.914757	0.929622
29	1	0	-2.263023	-0.675075	0.303827
30	1	0	-3.878322	-1.951695	1.226793
31	1	0	1.318907	-4.895268	-0.547794
32	1	0	3.589827	-1.762267	-1.502872
33	1	0	1.920860	-0.557121	0.773834
34	1	0	2.651826	1.397909	1.826235
35	1	0	4.250929	3.271805	2.115357
36	1	0	6.677891	1.675824	-1.058171
37	1	0	5.099799	-0.180586	-1.351111
38	1	0	7.147323	3.614154	0.134486
39	1	0	-0.976181	0.775932	-0.761191
40	1	0	-2.243052	1.798801	2.469485
41	1	0	-4.104170	0.262485	1.608841
42	1	0	-4.691558	-0.083298	0.235015
43	1	0	-3.336096	0.858918	-1.210611
44	1	0	-4.676068	1.562680	-1.467536
45	1	0	-2.341349	1.676384	0.893074
46	1	0	-1.590472	2.271920	-1.171846
47	1	0	-5.537496	3.462156	1.770399
48	1	0	-4.057995	3.007174	1.553660
49	1	0	-4.851180	3.624651	-0.404649
50	1	0	-5.483696	3.984255	-1.803343
51	1	0	-1.948557	3.890228	-2.976517
52	1	0	-3.067690	3.803224	-1.895714

TS2-7wd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.758477	3.436800	-0.663941
2	6	0	-1.287533	2.557728	0.326126
3	6	0	-2.235070	1.859386	1.096091
4	6	0	-3.602132	2.039117	0.904644
5	6	0	-4.048733	2.928036	-0.080788
6	6	0	-3.123088	3.629414	-0.867285
7	6	0	0.151968	2.294783	0.523655
8	6	0	1.151140	3.264498	0.220480
9	6	0	2.489978	2.852915	0.168348
10	8	0	3.494744	3.670440	0.102643
11	8	0	-5.401353	3.065449	-0.234810
12	6	0	2.759467	1.394966	0.074182
13	6	0	4.089932	0.908574	0.203113
14	6	0	4.412431	-0.438364	0.011985
15	6	0	3.403739	-1.322735	-0.388150
16	6	0	2.098503	-0.866846	-0.616069
17	6	0	1.758703	0.472003	-0.368744
18	8	0	5.087830	1.775238	0.514492
19	8	0	0.485097	0.848782	-0.578394
20	8	0	3.729290	-2.635798	-0.551971
21	8	0	-1.065074	-1.229976	-0.030641
22	8	0	-0.042404	-3.029914	1.646416
23	8	0	1.476217	-4.159835	-0.462269
24	8	0	-0.754064	-3.273887	-1.888150
25	8	0	-3.194677	-4.142588	-0.695267
26	8	0	-2.012700	-4.928941	1.603334
27	1	0	5.431186	-0.782873	0.151351

28	1	0	1.333251	-1.556143	-0.944781
29	1	0	2.907617	-3.187472	-0.628175
30	1	0	4.658941	2.693552	0.397966
31	1	0	0.889067	4.278470	-0.062707
32	1	0	0.344478	1.649553	1.382587
33	1	0	-1.894049	1.158745	1.853404
34	1	0	-4.328317	1.495490	1.499922
35	1	0	-3.470964	4.312220	-1.637735
36	1	0	-1.051159	3.967987	-1.292648
37	1	0	-5.601405	3.700676	-0.937540
38	1	0	-0.590435	-0.375854	-0.227659
39	1	0	0.310854	-2.667416	2.469317
40	1	0	1.094524	-3.876991	0.393996
41	1	0	0.747423	-3.969081	-1.096695
42	1	0	-0.849755	-2.459742	-1.343921
43	1	0	-1.571326	-3.766051	-1.678199
44	1	0	-0.402566	-2.266503	1.116432
45	1	0	-2.035975	-1.084695	0.022543
46	1	0	-1.598801	-5.802364	1.596429
47	1	0	-1.277348	-4.278154	1.705933
48	1	0	-2.824606	-4.525691	0.142764
49	1	0	-3.866283	-4.759309	-1.015228
50	8	0	-3.784085	-1.519589	0.042399
51	1	0	-4.338063	-1.031430	-0.580795
52	1	0	-3.731814	-2.443639	-0.290710

INT2-7wd

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.877024	0.072062	-0.071467
2	6	0	-3.148584	-0.505434	0.059218
3	6	0	-4.269791	0.356461	-0.020982
4	6	0	-4.110882	1.740919	-0.173691
5	6	0	-2.821488	2.275959	-0.284185
6	6	0	-1.691964	1.441803	-0.245060
7	6	0	-3.302278	-1.982029	0.140935
8	8	0	-4.521355	-2.462222	-0.011843
9	8	0	-5.511208	-0.182566	0.032184
10	8	0	-2.695366	3.625951	-0.427910
11	8	0	-0.759460	-0.732741	-0.096151
12	6	0	-2.156023	-2.710160	0.335902
13	6	0	-0.882047	-1.996235	0.681641
14	6	0	0.400075	-2.747036	0.412256
15	6	0	0.554088	-3.543897	-0.729805
16	6	0	1.770689	-4.163177	-1.018836
17	6	0	2.861580	-3.983124	-0.157900
18	6	0	2.726676	-3.194087	0.989638
19	6	0	1.502349	-2.584379	1.263326
20	8	0	4.086155	-4.556488	-0.386901
21	8	0	1.514152	0.804735	0.112643
22	8	0	1.267295	2.937687	1.729838
23	8	0	-0.073926	4.371661	-0.327949
24	8	0	4.164398	0.269804	-0.140706
25	8	0	3.696941	4.154570	1.351297
26	8	0	4.322677	2.920051	-0.965245
27	8	0	1.628577	2.789239	-1.869550
28	1	0	-4.980184	2.387978	-0.222340
29	1	0	-0.698392	1.854396	-0.336732
30	1	0	-1.738346	3.888504	-0.433044
31	1	0	-5.321759	-1.209434	0.017588
32	1	0	-2.178004	-3.794112	0.386271
33	1	0	-0.868685	-1.654500	1.732181
34	1	0	1.406198	-1.964067	2.150923
35	1	0	3.578784	-3.062689	1.648833
36	1	0	1.874939	-4.780336	-1.907541
37	1	0	-0.288012	-3.677784	-1.401973
38	1	0	4.070396	-5.069509	-1.207528
39	1	0	0.822159	0.110564	0.061809
40	1	0	0.931259	2.747389	2.615639
41	1	0	0.283269	4.041151	0.520647
42	1	0	0.509657	3.941608	-0.995253
43	1	0	1.512821	1.995439	-1.304571
44	1	0	2.575961	2.999844	-1.752138

45	1	0	1.331250	2.071899	1.248005
46	1	0	2.409847	0.395066	0.066674
47	1	0	3.564094	5.110946	1.306415
48	1	0	2.817298	3.765578	1.571405
49	1	0	4.185150	3.443169	-0.132188
50	1	0	5.101780	3.285703	-1.404734
51	1	0	4.453349	-0.371374	-0.803541
52	1	0	4.361889	1.161258	-0.508398

INT1-7we

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.845151	-2.386876	0.626350
2	6	0	-1.983479	-1.847882	-0.349543
3	6	0	-2.550852	-1.019513	-1.339814
4	6	0	-3.912359	-0.717113	-1.346137
5	6	0	-4.732754	-1.232524	-0.338774
6	6	0	-4.204198	-2.085508	0.637460
7	6	0	-0.532274	-2.034708	-0.323522
8	6	0	0.169953	-2.926682	0.399356
9	6	0	1.647780	-3.004993	0.336542
10	8	0	2.145847	-4.172271	0.239944
11	8	0	-6.044262	-0.811967	-0.323187
12	6	0	2.472011	-1.818801	0.278236
13	6	0	3.759660	-1.911161	-0.358451
14	6	0	4.511812	-0.786532	-0.668920
15	6	0	4.019734	0.479352	-0.288979
16	6	0	2.849796	0.606903	0.453211
17	6	0	2.050941	-0.517794	0.791171
18	8	0	4.251679	-3.122769	-0.727600
19	8	0	1.013090	-0.375268	1.550777
20	8	0	4.751412	1.568157	-0.648874
21	8	0	0.011967	1.961383	1.220478
22	8	0	3.162926	3.773508	-0.467661
23	8	0	1.745449	3.920477	1.961386
24	8	0	0.757726	2.734689	-1.371250
25	8	0	-2.705178	1.893687	0.296283
26	8	0	-5.444283	1.870992	0.714334
27	8	0	-1.839689	3.837352	-1.504595
28	1	0	5.450733	-0.881638	-1.202240
29	1	0	2.545570	1.579348	0.815327
30	1	0	4.216371	2.395748	-0.513332
31	1	0	3.595998	-3.796643	-0.389038
32	1	0	-0.314496	-3.710513	0.977008
33	1	0	0.028987	-1.330444	-0.934753
34	1	0	-1.912081	-0.596339	-2.110560
35	1	0	-4.338138	-0.064498	-2.101248
36	1	0	-4.845226	-2.481171	1.420015
37	1	0	-2.445648	-3.017286	1.413998
38	1	0	-6.558382	-1.312265	0.328700
39	1	0	0.358801	1.014077	1.402773
40	1	0	-0.053476	3.233304	-1.597523
41	1	0	2.349064	3.496494	-0.950666
42	1	0	2.828600	3.924627	0.442959
43	1	0	-5.819579	1.037206	0.376023
44	1	0	-5.791076	1.971075	1.611195
45	1	0	-2.618469	1.039170	-0.156460
46	1	0	-3.658224	1.939318	0.543942
47	1	0	0.540542	2.346412	-0.493223
48	1	0	-0.960320	1.942825	1.167349
49	1	0	-2.359086	3.783644	-2.317458
50	1	0	-2.231925	3.175919	-0.890168
51	1	0	2.163569	3.674010	2.796604
52	1	0	1.050698	3.236856	1.791367

TS2-7we

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

1	6	0	-4.168317	-1.183369	0.326145
2	6	0	-2.791047	-1.496449	0.153183
3	6	0	-1.908480	-0.419617	-0.188599
4	6	0	-2.407334	0.886381	-0.306428
5	6	0	-3.757195	1.159700	-0.050373
6	6	0	-4.649959	0.127492	0.265689
7	6	0	-2.355152	-2.914447	0.077591
8	8	0	-3.255858	-3.830186	-0.088239
9	8	0	-0.603755	-0.619687	-0.423536
10	8	0	-4.239046	2.432012	-0.100267
11	8	0	-5.055795	-2.188644	0.543344
12	6	0	-0.973004	-3.168294	0.084784
13	6	0	-0.106042	-2.129892	0.520703
14	6	0	1.356387	-2.176119	0.317426
15	6	0	2.213640	-1.604542	1.272634
16	6	0	3.590423	-1.552354	1.068437
17	6	0	4.123328	-2.050207	-0.123735
18	6	0	3.294018	-2.635961	-1.086599
19	6	0	1.920248	-2.697479	-0.858423
20	8	0	5.480476	-1.894850	-0.311952
21	8	0	5.705449	0.972681	-0.414664
22	8	0	0.815381	1.626843	-0.505841
23	8	0	-0.197808	3.494856	1.313380
24	8	0	2.466570	4.450606	1.183717
25	8	0	3.342260	1.842603	0.657285
26	8	0	-2.211876	4.218911	-0.456402
27	1	0	-5.702944	0.331783	0.425285
28	1	0	-1.732663	1.688551	-0.567207
29	1	0	-3.501384	3.079357	-0.258898
30	1	0	-4.529269	-3.032007	0.324981
31	1	0	-0.586336	-4.089470	-0.339044
32	1	0	-0.383632	-1.619693	1.444220
33	1	0	1.795201	-1.189010	2.185390
34	1	0	4.255049	-1.121769	1.810711
35	1	0	3.715904	-3.018621	-2.011828
36	1	0	1.273733	-3.126489	-1.617312
37	1	0	5.768568	-2.342289	-1.121779
38	1	0	0.390121	0.727382	-0.458284
39	1	0	0.627329	4.016440	1.386732
40	1	0	-1.565547	4.105445	0.279032
41	1	0	-1.678984	3.987875	-1.247929
42	1	0	5.758322	-0.002461	-0.434485
43	1	0	5.910620	1.269045	-1.311734
44	1	0	3.271953	1.312107	1.463185
45	1	0	4.188232	1.559389	0.230128
46	1	0	0.081968	2.734336	0.756815
47	1	0	1.751867	1.558424	-0.228030
48	1	0	2.928860	4.835211	1.939752
49	1	0	2.896101	3.583583	1.016536
50	8	0	-0.338615	3.298789	-2.349132
51	1	0	-0.643887	2.781496	-3.105891
52	1	0	0.162663	2.670850	-1.776500

INT2-7we

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.552462	-2.651605	0.850567
2	6	0	-1.145045	-2.159712	-0.396644
3	6	0	-2.126633	-1.758367	-1.311518
4	6	0	-3.483142	-1.825634	-0.991150
5	6	0	-3.863645	-2.287053	0.270261
6	6	0	-2.903601	-2.716937	1.192084
7	6	0	0.316794	-1.941534	-0.704623
8	6	0	1.257817	-3.044869	-0.318246
9	6	0	2.593169	-2.760782	-0.171368
10	8	0	3.568133	-3.632186	-0.002112
11	8	0	-5.213525	-2.261353	0.565393
12	6	0	2.971246	-1.322138	-0.164272
13	6	0	4.324320	-0.904958	-0.127001
14	6	0	4.663315	0.451825	-0.024774
15	6	0	3.645661	1.408941	0.080598
16	6	0	2.295430	1.022634	0.074874
17	6	0	1.987358	-0.329288	-0.049340

18	8	0	5.297286	-1.847043	-0.165272
19	8	0	0.660757	-0.686352	0.010686
20	8	0	4.001233	2.720827	0.183223
21	8	0	-1.028973	1.474447	0.284406
22	8	0	1.795434	4.286918	0.530424
23	8	0	0.035769	3.009052	2.319458
24	8	0	-0.196369	3.638716	-1.305752
25	8	0	-3.601122	1.654987	-0.717464
26	8	0	-5.775915	0.541930	0.491968
27	8	0	-2.909379	4.363274	-0.955753
28	1	0	5.705147	0.753230	-0.001643
29	1	0	1.508793	1.757155	0.160498
30	1	0	3.195968	3.292874	0.290085
31	1	0	4.762503	-2.739480	-0.100676
32	1	0	0.890303	-4.066147	-0.307457
33	1	0	0.409340	-1.670371	-1.771360
34	1	0	-1.829111	-1.371370	-2.282592
35	1	0	-4.244589	-1.511653	-1.697951
36	1	0	-3.208086	-3.081813	2.169260
37	1	0	-0.801011	-2.967157	1.567796
38	1	0	-5.383522	-2.674933	1.425024
39	1	0	-0.578809	0.612183	0.155406
40	1	0	-1.058443	4.102589	-1.279418
41	1	0	1.156886	4.216461	-0.215926
42	1	0	1.283957	3.926980	1.287607
43	1	0	-5.696863	-0.428515	0.579919
44	1	0	-6.001392	0.873362	1.371692
45	1	0	-3.595258	1.234116	-1.588553
46	1	0	-4.383848	1.276161	-0.243842
47	1	0	-0.403637	2.788170	-0.862940
48	1	0	-1.970857	1.382250	0.022788
49	1	0	-3.429851	4.806796	-1.638156
50	1	0	-3.277734	3.456347	-0.881139
51	1	0	0.421066	2.429621	2.989954
52	1	0	-0.421064	2.414268	1.681322

1-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.336904	2.321566	-0.579662
2	6	0	-1.260112	1.577428	0.007316
3	6	0	-1.487269	0.180061	0.195389
4	6	0	-2.643675	-0.437152	-0.277080
5	6	0	-3.630577	0.320719	-0.925937
6	6	0	-3.483128	1.705394	-1.071296
7	6	0	-0.040882	2.298801	0.391903
8	8	0	-0.109358	3.541961	0.647385
9	8	0	-0.586227	-0.550105	0.899409
10	8	0	-4.761318	-0.249902	-1.396411
11	8	0	-2.263280	3.671952	-0.699617
12	6	0	1.298442	1.708854	0.432637
13	6	0	1.720259	0.682479	-0.341893
14	6	0	3.068940	0.133858	-0.413397
15	6	0	3.320644	-0.938714	-1.295797
16	6	0	4.582267	-1.516589	-1.400081
17	6	0	5.631945	-1.025998	-0.613938
18	6	0	5.410045	0.040769	0.272854
19	6	0	4.145103	0.608148	0.367902
20	8	0	6.854371	-1.623599	-0.750016
21	8	0	-1.205637	-3.058755	1.223748
22	8	0	-3.679439	-3.538427	1.151658
23	8	0	-4.799708	-2.854503	-1.001444
24	8	0	0.167431	0.573787	3.366587
25	1	0	-4.264633	2.300279	-1.530139
26	1	0	-2.795571	-1.492904	-0.101158
27	1	0	-4.772711	-1.242958	-1.224438
28	1	0	-1.464729	3.950616	-0.172655
29	1	0	1.996077	2.265873	1.052934
30	1	0	0.998448	0.202005	-0.997159
31	1	0	2.509258	-1.324837	-1.906359
32	1	0	4.765041	-2.342335	-2.079896
33	1	0	6.226772	0.417753	0.881275
34	1	0	3.996107	1.429011	1.061180

35	1	0	7.501937	-1.216273	-0.154303
36	1	0	-0.069263	0.192551	2.495059
37	1	0	-2.240650	-3.265879	1.187840
38	1	0	-4.358414	-3.142575	-0.088242
39	1	0	-5.705684	-3.193121	-0.988524
40	1	0	-0.793752	-3.592379	0.529674
41	1	0	-0.871456	-1.518477	0.989247
42	1	0	-4.077088	-3.025144	1.869356
43	1	0	0.715052	1.341789	3.152395

TS1-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.219934	2.436650	-0.457790
2	6	0	-1.173277	1.651631	0.129933
3	6	0	-1.382777	0.239489	0.163461
4	6	0	-2.488063	-0.337480	-0.458366
5	6	0	-3.450549	0.466091	-1.082110
6	6	0	-3.321850	1.859653	-1.083511
7	6	0	0.013141	2.344017	0.649596
8	8	0	-0.086582	3.555276	1.020086
9	8	0	-0.546815	-0.549031	0.883616
10	8	0	-4.547174	-0.079897	-1.660849
11	8	0	-2.162550	3.793383	-0.443251
12	6	0	1.355471	1.760899	0.695104
13	6	0	1.810290	0.812679	-0.157422
14	6	0	3.159741	0.269031	-0.240741
15	6	0	3.427982	-0.726057	-1.205329
16	6	0	4.687051	-1.305746	-1.324435
17	6	0	5.717889	-0.894968	-0.470583
18	6	0	5.481452	0.098074	0.494536
19	6	0	4.218267	0.666999	0.604755
20	8	0	6.937775	-1.493671	-0.621822
21	8	0	-0.827499	-3.040719	0.411438
22	8	0	-3.191379	-3.417519	0.878023
23	8	0	-4.643746	-2.727610	-1.174463
24	8	0	-2.299801	-1.122855	3.161748
25	1	0	-4.086501	2.488885	-1.524507
26	1	0	-2.629026	-1.405108	-0.394677
27	1	0	-4.581504	-1.064049	-1.490147
28	1	0	-1.402023	4.029136	0.154120
29	1	0	2.025247	2.261496	1.389488
30	1	0	1.109076	0.395475	-0.875687
31	1	0	2.630664	-1.050992	-1.867824
32	1	0	4.881844	-2.073321	-2.066265
33	1	0	6.285592	0.415436	1.151813
34	1	0	4.056658	1.428769	1.360122
35	1	0	7.568518	-1.151965	0.030464
36	1	0	-1.653888	-0.884360	2.470315
37	1	0	-1.955308	-3.245280	0.615333
38	1	0	-4.106231	-3.008344	-0.350746
39	1	0	-5.551342	-3.027478	-1.022929
40	1	0	-0.667575	-3.223920	-0.525671
41	1	0	-0.663676	-1.548700	0.643902
42	1	0	-3.367215	-2.774962	1.582551
43	1	0	-1.960151	-1.945352	3.541568

INT1-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.391978	-1.600253	-0.098893
2	6	0	2.361541	-0.821590	0.470711
3	6	0	2.732918	0.330872	1.195165
4	6	0	4.065719	0.701867	1.340801
5	6	0	5.068114	-0.083804	0.758876
6	6	0	4.728251	-1.240198	0.038998
7	6	0	0.942195	-1.117457	0.303257
8	6	0	0.392497	-2.117102	-0.420817

9	6	0	-1.048995	-2.400380	-0.441799
10	8	0	-1.374875	-3.632063	-0.484867
11	8	0	6.363422	0.324788	0.922960
12	6	0	-2.068702	-1.369529	-0.312562
13	6	0	-3.302463	-1.719797	0.337184
14	6	0	-4.246968	-0.769907	0.712160
15	6	0	-4.018793	0.566562	0.347191
16	6	0	-2.936599	0.920330	-0.446098
17	6	0	-1.911578	-0.000238	-0.772337
18	8	0	-3.560391	-3.013308	0.677038
19	8	0	-0.905226	0.430865	-1.482229
20	8	0	-4.900395	1.519903	0.779436
21	8	0	-0.520617	2.824012	-0.018689
22	8	0	2.088404	3.227562	-1.054741
23	8	0	1.636102	0.784663	-2.274787
24	8	0	-3.097814	3.754281	0.975874
25	1	0	-5.123471	-1.058536	1.280963
26	1	0	-2.840942	1.936721	-0.803430
27	1	0	-4.446503	2.391118	0.736584
28	1	0	-2.830936	-3.554226	0.267604
29	1	0	1.006922	-2.867762	-0.911338
30	1	0	0.269477	-0.429240	0.809484
31	1	0	1.958603	0.952734	1.635205
32	1	0	4.340082	1.595196	1.892265
33	1	0	5.508950	-1.848679	-0.408293
34	1	0	3.151499	-2.497241	-0.659580
35	1	0	6.972217	-0.289749	0.485818
36	1	0	-0.619841	2.012854	-0.570709
37	1	0	-2.212698	3.490523	0.645706
38	1	0	-3.301329	4.587179	0.527401
39	1	0	0.364718	3.163296	-0.261397
40	1	0	1.977479	2.368188	-1.531076
41	1	0	2.099121	3.906233	-1.744216
42	1	0	0.744325	0.523422	-1.931279
43	1	0	2.258757	0.176083	-1.850696

INT1'-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.109840	0.854465	0.551174
2	6	0	3.029122	0.351212	-0.204493
3	6	0	3.285580	-0.728443	-1.076190
4	6	0	4.555519	-1.286342	-1.194108
5	6	0	5.609465	-0.767202	-0.433023
6	6	0	5.383403	0.307526	0.442487
7	6	0	1.671793	0.881984	-0.123545
8	6	0	1.236618	1.904290	0.646535
9	6	0	-0.111206	2.485015	0.575882
10	8	0	-0.170811	3.746192	0.768318
11	8	0	6.840962	-1.345770	-0.581626
12	6	0	-1.311852	1.741179	0.221288
13	6	0	-2.405128	2.459384	-0.376397
14	6	0	-3.533940	1.821026	-0.876674
15	6	0	-3.634729	0.427115	-0.736365
16	6	0	-2.646035	-0.301703	-0.080206
17	6	0	-1.490199	0.319056	0.445056
18	8	0	-2.354807	3.813204	-0.503721
19	8	0	-0.646988	-0.402992	1.145429
20	8	0	-4.745287	-0.178686	-1.239040
21	8	0	0.012167	-2.568069	-0.315511
22	8	0	-2.409713	-3.804312	0.434603
23	8	0	-4.648900	-2.906550	-0.921654
24	8	0	-1.976780	-2.164530	2.666279
25	1	0	-4.324901	2.394488	-1.346645
26	1	0	-2.765345	-1.364425	0.071636
27	1	0	-4.701534	-1.158129	-1.091839
28	1	0	-1.540638	4.100786	0.000631
29	1	0	1.925253	2.474956	1.264854
30	1	0	0.950255	0.386364	-0.767889
31	1	0	2.470573	-1.138385	-1.665832
32	1	0	4.740678	-2.118299	-1.865760
33	1	0	6.203380	0.708201	1.031277
34	1	0	3.959186	1.683526	1.234370

35	1	0	7.489645	-0.920141	-0.000240
36	1	0	-1.458712	-1.496573	2.128288
37	1	0	-1.592082	-3.486949	-0.009198
38	1	0	-3.859642	-3.245399	-0.428856
39	1	0	-5.420564	-3.233765	-0.437938
40	1	0	0.141228	-2.260779	-1.223393
41	1	0	-0.196097	-1.747166	0.213623
42	1	0	-2.369679	-3.339454	1.301602
43	1	0	-1.339257	-2.558119	3.278155

INT2-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.474722	1.341637	1.797836
2	6	0	-0.656915	1.188428	0.655741
3	6	0	-0.612927	-0.079320	0.047766
4	6	0	-1.328534	-1.164580	0.551153
5	6	0	-2.149045	-0.970368	1.672720
6	6	0	-2.213468	0.271948	2.313949
7	6	0	0.056932	2.330407	0.043539
8	6	0	0.851233	2.057654	-1.043967
9	6	0	1.200423	0.639968	-1.410207
10	8	0	0.084042	-0.281240	-1.112026
11	6	0	2.463628	0.076749	-0.774213
12	6	0	2.807216	0.339642	0.559787
13	6	0	3.939812	-0.233598	1.141435
14	6	0	4.758814	-1.076227	0.377659
15	6	0	4.439014	-1.344903	-0.957442
16	6	0	3.296126	-0.772262	-1.518126
17	8	0	5.895738	-1.661015	0.882772
18	8	0	-0.161914	3.531425	0.547961
19	8	0	-2.908260	-1.988808	2.179986
20	8	0	-1.568834	2.565456	2.387483
21	8	0	-1.676556	2.037916	-2.720772
22	8	0	-3.626908	0.454792	-1.554917
23	8	0	-3.384892	-3.751749	0.159792
24	8	0	-3.146562	-2.202999	-2.107864
25	1	0	-2.857313	0.415219	3.175061
26	1	0	-1.261983	-2.127674	0.060987
27	1	0	-3.042851	-2.685544	1.487534
28	1	0	-1.027704	3.176616	1.761492
29	1	0	1.423081	2.848891	-1.521289
30	1	0	1.302859	0.543095	-2.494478
31	1	0	3.050299	-0.988236	-2.554989
32	1	0	5.085460	-1.992556	-1.541521
33	1	0	4.189296	-0.024681	2.178405
34	1	0	2.186243	1.003541	1.152143
35	1	0	6.027416	-1.401995	1.807000
36	1	0	-3.356796	-3.197028	-0.659659
37	1	0	-4.285584	-4.101641	0.213195
38	1	0	-3.297541	-1.249233	-1.893888
39	1	0	-2.204671	-2.263334	-2.323398
40	1	0	-2.008599	2.944435	-2.795622
41	1	0	-0.877771	2.103050	-2.138232
42	1	0	-2.917284	1.021309	-1.944660
43	1	0	-4.438916	0.714493	-2.013177

TS3-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.979947	-0.577415	-0.256615
2	6	0	2.348024	-0.043825	0.873116
3	6	0	2.895380	1.114959	1.450346
4	6	0	4.020866	1.735767	0.912199
5	6	0	4.628677	1.192006	-0.226852
6	6	0	4.112708	0.029390	-0.808568
7	6	0	1.080241	-0.630800	1.476762
8	8	0	-0.038963	0.288394	1.179693

9	6	0	-0.638841	0.162348	-0.036499
10	6	0	-0.541690	-1.029193	-0.790419
11	6	0	0.161522	-2.188818	-0.239584
12	6	0	0.691509	-2.040780	1.080603
13	6	0	-1.396950	1.242963	-0.475452
14	6	0	-2.108993	1.128852	-1.679108
15	6	0	-2.010232	-0.018873	-2.476588
16	6	0	-1.235424	-1.087176	-2.026904
17	8	0	0.174246	-3.294141	-0.890618
18	8	0	-2.916511	2.136451	-2.114398
19	8	0	-1.177264	-2.218878	-2.776820
20	8	0	5.733350	1.841881	-0.722417
21	8	0	-1.441053	-2.403946	2.595104
22	8	0	-3.412272	-0.997701	1.526105
23	8	0	-3.778777	3.421420	0.116153
24	8	0	-3.344062	1.658920	2.203193
25	1	0	-2.563405	-0.093916	-3.406067
26	1	0	-1.442877	2.143609	0.122704
27	1	0	-3.195660	2.694626	-1.341891
28	1	0	-0.644525	-2.870889	-2.224909
29	1	0	1.423778	-2.797706	1.366380
30	1	0	1.154438	-0.559865	2.564888
31	1	0	2.426800	1.542592	2.333171
32	1	0	4.435924	2.631815	1.363209
33	1	0	4.590851	-0.398925	-1.685103
34	1	0	2.597906	-1.481131	-0.718331
35	1	0	6.062820	1.390295	-1.513901
36	1	0	-3.674323	2.767800	0.852204
37	1	0	-4.726966	3.606065	0.057669
38	1	0	-3.339175	0.703562	1.937048
39	1	0	-2.432337	1.847279	2.468372
40	1	0	-1.669589	-3.344034	2.538837
41	1	0	-0.432562	-2.282699	1.851560
42	1	0	-2.659354	-1.540407	1.928782
43	1	0	-4.221763	-1.353708	1.918789

2-4H2O

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.161218	-1.334875	-1.355539
2	6	0	2.565235	-0.122399	-0.969614
3	6	0	3.078549	0.533735	0.158583
4	6	0	4.146846	-0.000873	0.883012
5	6	0	4.720721	-1.212383	0.481926
6	6	0	4.226645	-1.882698	-0.643767
7	6	0	1.376348	0.377298	-1.765291
8	6	0	1.089173	1.877058	-1.710659
9	6	0	0.447044	2.317475	-0.419050
10	6	0	-0.338705	1.338935	0.283465
11	6	0	-0.459819	0.014173	-0.223683
12	8	0	0.172583	-0.372578	-1.362386
13	6	0	-1.265805	-0.926154	0.400384
14	6	0	-1.981481	-0.554142	1.554426
15	6	0	-1.868554	0.734142	2.103179
16	6	0	-1.057756	1.667701	1.473604
17	8	0	-0.967856	2.913727	1.993442
18	8	0	-2.791601	-1.424418	2.190702
19	8	0	0.570670	3.502846	-0.019323
20	8	0	5.775000	-1.786714	1.147049
21	8	0	-3.275853	-3.551790	0.667178
22	8	0	-3.842440	-2.255709	-1.581246
23	8	0	-4.761636	-0.077457	-0.777586
24	8	0	-3.129112	1.762736	-1.661498
25	1	0	-2.423594	0.999537	2.995463
26	1	0	-1.334191	-1.928056	-0.003079
27	1	0	-2.936249	-2.253784	1.649391
28	1	0	-0.375924	3.433863	1.386766
29	1	0	2.001733	2.451968	-1.883000
30	1	0	1.500982	0.076942	-2.806135
31	1	0	2.786756	-1.860106	-2.230260
32	1	0	4.684133	-2.817091	-0.953043
33	1	0	4.531347	0.523224	1.753447
34	1	0	2.661919	1.477719	0.490045

35	1	0	6.038148	-1.235946	1.899844
36	1	0	-3.522907	-3.106974	-0.199472
37	1	0	-4.069550	-4.017163	0.967423
38	1	0	-4.242491	-1.317976	-1.256608
39	1	0	-2.988447	-2.051702	-1.987928
40	1	0	-2.346869	1.725806	-1.092137
41	1	0	0.379614	2.130768	-2.508504
42	1	0	-3.758649	1.045347	-1.305755
43	1	0	-5.621767	0.076550	-1.192976

wB97XD(PCM,solvent=n-octanol)/6-311+G(d,p)

1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.979565	-1.444565	-0.182550
2	6	0	-4.167048	-0.210280	-0.792298
3	6	0	-3.247203	0.806334	-0.556400
4	6	0	-2.077766	0.591240	0.228019
5	6	0	-1.969075	-0.659277	0.881402
6	6	0	-2.898440	-1.672272	0.674373
7	8	0	-4.904798	-2.399648	-0.429919
8	8	0	-3.496996	1.997406	-1.121931
9	8	0	-0.954855	-0.834920	1.760038
10	6	0	-1.086603	1.682257	0.317174
11	6	0	0.359049	1.449836	0.434531
12	6	0	0.973023	0.359664	-0.055804
13	6	0	2.862921	-1.078347	-0.714651
14	6	0	2.411930	0.102778	-0.109838
15	6	0	3.374620	0.978256	0.422453
16	6	0	4.726318	0.686468	0.351457
17	6	0	5.152555	-0.498314	-0.259231
18	6	0	4.216411	-1.384523	-0.793709
19	8	0	6.489367	-0.729927	-0.299230
20	8	0	-1.467029	2.863980	0.194707
21	1	0	-5.032688	-0.025517	-1.416410
22	1	0	-2.795563	-2.621117	1.193126
23	1	0	-4.694802	-3.211245	0.044852
24	1	0	-2.857859	2.638878	-0.735353
25	1	0	-1.009183	-1.709771	2.159528
26	1	0	0.912764	2.304815	0.811713
27	1	0	0.353333	-0.428893	-0.478643
28	1	0	2.140748	-1.773644	-1.133485
29	1	0	3.068703	1.902111	0.902261
30	1	0	5.465478	1.364713	0.763932
31	1	0	4.541315	-2.305983	-1.268038
32	1	0	6.675480	-1.565006	-0.742376

2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.055831	-0.756406	0.008556
2	6	0	-0.688107	0.395742	0.455703
3	6	0	-0.221613	1.642145	-0.289941
4	6	0	1.269248	1.823115	-0.161153
5	6	0	3.466787	0.640804	-0.004678
6	6	0	4.203771	-0.534465	0.027070
7	6	0	3.525810	-1.754469	0.041376
8	6	0	2.127954	-1.827997	0.040875
9	6	0	1.401855	-0.647857	0.017411
10	6	0	2.044687	0.612120	-0.014179
11	8	0	1.787956	2.948656	-0.220614
12	8	0	4.118549	1.809656	-0.041155
13	8	0	4.288831	-2.867936	0.068643
14	6	0	-2.151430	0.101122	0.264422
15	6	0	-3.046469	0.242944	1.325789

16	6	0	-4.407147	0.011287	1.153180
17	6	0	-4.886053	-0.379765	-0.096699
18	6	0	-4.002000	-0.534849	-1.167746
19	6	0	-2.646354	-0.289143	-0.982151
20	8	0	-6.224116	-0.599653	-0.215124
21	1	0	-0.478163	0.520113	1.526401
22	1	0	-0.457479	1.553780	-1.358390
23	1	0	-0.733174	2.528417	0.091710
24	1	0	5.286466	-0.505523	0.031223
25	1	0	1.607496	-2.778644	0.074485
26	1	0	3.438903	2.522488	-0.100458
27	1	0	3.738617	-3.659359	0.070052
28	1	0	-2.680776	0.539502	2.305056
29	1	0	-5.101775	0.123399	1.978707
30	1	0	-4.371707	-0.844495	-2.141231
31	1	0	-1.967328	-0.415675	-1.820255
32	1	0	-6.443116	-0.862946	-1.115425

(1,1)-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.345853	-4.060586	-0.838704
2	6	0	0.222011	-3.449198	0.288168
3	6	0	-0.584098	-3.271166	1.420998
4	6	0	-1.908277	-3.694451	1.437707
5	6	0	-2.452851	-4.278950	0.296112
6	6	0	-1.672336	-4.470342	-0.843254
7	6	0	1.604490	-2.954608	0.288393
8	8	0	2.290364	-0.578403	-1.093200
9	6	0	3.491322	-0.368090	-0.505878
10	6	0	4.327064	-1.480412	-0.219454
11	6	0	3.974123	-2.886924	-0.450466
12	6	0	2.584369	-3.379481	-0.520200
13	6	0	5.637003	-1.177107	0.271353
14	6	0	6.040327	0.124621	0.550822
15	6	0	5.169273	1.175376	0.284688
16	6	0	3.897613	0.931057	-0.242806
17	8	0	4.873612	-3.747045	-0.555829
18	8	0	6.533415	-2.147916	0.489676
19	8	0	5.600488	2.427739	0.526006
20	8	0	-3.788175	-4.594426	0.323730
21	8	0	-5.545188	-2.453416	-0.437730
22	6	0	-5.136199	-1.187633	-0.232704
23	6	0	-5.980713	-0.161963	-0.644506
24	6	0	-5.604959	1.157697	-0.418538
25	6	0	-4.342688	1.498360	0.161032
26	6	0	-3.538449	0.414634	0.602755
27	6	0	-3.920068	-0.903132	0.398057
28	6	0	-3.999801	2.917939	0.308847
29	6	0	-2.612034	3.409834	0.422213
30	6	0	-1.596468	2.926705	-0.305344
31	8	0	-2.399516	0.681689	1.282726
32	6	0	-0.213920	3.421526	-0.268636
33	6	0	0.632718	3.223745	-1.368436
34	6	0	1.954580	3.654686	-1.346785
35	6	0	2.456833	4.262531	-0.197186
36	6	0	1.634774	4.474018	0.908601
37	6	0	0.310201	4.059347	0.864344
38	8	0	-4.898653	3.783985	0.289114
39	8	0	-6.476588	2.108087	-0.781240
40	8	0	3.792478	4.576512	-0.180754
41	1	0	-1.785469	2.096551	-0.984184
42	1	0	-2.500345	4.298125	1.038363
43	1	0	-6.939558	-0.380645	-1.098267
44	1	0	-3.285778	-1.708172	0.752579
45	1	0	-6.128963	2.963741	-0.429271
46	1	0	-4.910411	-3.100029	-0.079831
47	1	0	0.249642	2.733602	-2.259289
48	1	0	2.604650	3.509391	-2.203325
49	1	0	2.032106	4.934740	1.807968
50	1	0	-0.311397	4.201319	1.742467
51	1	0	3.985448	5.183832	0.544052

52	1	0	1.824678	-2.170830	1.011155
53	1	0	2.445801	-4.224239	-1.189756
54	1	0	7.038955	0.311144	0.926401
55	1	0	3.234499	1.755960	-0.476180
56	1	0	6.151547	-2.978236	0.111190
57	1	0	4.951081	3.090492	0.229280
58	1	0	-0.167433	-2.800141	2.306836
59	1	0	-2.526192	-3.565765	2.320371
60	1	0	-2.103440	-4.912374	-1.736459
61	1	0	0.241829	-4.186893	-1.742131
62	1	0	-4.005312	-5.198999	-0.396536
63	1	0	1.855207	0.267518	-1.250628
64	1	0	-1.976975	-0.142754	1.548049

(1,1)-b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.738669	-2.712214	-0.752688
2	6	0	3.887182	-2.666985	0.626170
3	6	0	2.927451	-2.010165	1.389416
4	6	0	1.751792	-1.455022	0.804428
5	6	0	1.679596	-1.476359	-0.608595
6	6	0	2.646560	-2.107846	-1.380155
7	8	0	4.707522	-3.340670	-1.457616
8	8	0	3.147735	-1.942493	2.709895
9	8	0	0.656056	-0.827230	-1.217837
10	6	0	0.737424	-0.875647	1.707201
11	6	0	-0.704611	-0.868139	1.425960
12	6	0	-1.334876	-1.768701	0.656379
13	6	0	-3.257479	-2.620487	-0.628732
14	6	0	-2.779878	-1.858526	0.444648
15	6	0	-3.717260	-1.181121	1.241544
16	6	0	-5.071563	-1.240696	0.961369
17	6	0	-5.522748	-1.979431	-0.136378
18	6	0	-4.613463	-2.679784	-0.929479
19	8	0	-6.860388	-1.974563	-0.383553
20	8	0	1.090470	-0.437207	2.820027
21	1	0	4.760835	-3.091841	1.104861
22	1	0	2.571073	-2.096923	-2.463962
23	1	0	4.547852	-3.257540	-2.403888
24	1	0	2.499230	-1.293849	3.071565
25	1	0	0.795688	-0.824087	-2.170852
26	1	0	-1.253418	-0.130645	2.004427
27	1	0	-0.738746	-2.497032	0.110817
28	1	0	-2.553953	-3.164154	-1.253321
29	1	0	-3.388004	-0.594145	2.092628
30	1	0	-5.791142	-0.706577	1.572355
31	1	0	-4.960220	-3.265775	-1.775754
32	1	0	-7.067554	-2.544172	-1.132598
33	6	0	4.255478	0.825643	-1.613790
34	6	0	4.461440	0.770249	-0.243671
35	6	0	3.574976	1.431705	0.600288
36	6	0	2.426216	2.112097	0.101122
37	6	0	2.307074	2.204241	-1.305556
38	6	0	3.196272	1.558855	-2.157138
39	8	0	5.138202	0.165612	-2.400204
40	8	0	3.841526	1.382751	1.912321
41	8	0	1.326078	2.984792	-1.820252
42	6	0	1.477665	2.692294	1.076063
43	6	0	0.033922	2.802427	0.835046
44	6	0	-0.640847	1.982876	0.010936
45	6	0	-2.587612	1.096813	-1.204793
46	6	0	-2.088330	1.915936	-0.183024
47	6	0	-3.012473	2.621254	0.605366
48	6	0	-4.375248	2.513321	0.380269
49	6	0	-4.847704	1.691133	-0.647424
50	6	0	-3.949577	0.989708	-1.451318
51	8	0	-6.194276	1.603897	-0.803349
52	8	0	1.896076	3.034147	2.201042
53	1	0	5.299256	0.224388	0.171440
54	1	0	3.084228	1.651568	-3.233984
55	1	0	4.925111	0.293310	-3.330860

56	1	0	3.216441	1.999775	2.356955
57	1	0	1.394881	3.009253	-2.780639
58	1	0	-0.469143	3.505668	1.493057
59	1	0	-0.075449	1.262505	-0.574230
60	1	0	-1.893178	0.519826	-1.808579
61	1	0	-2.667820	3.251545	1.419001
62	1	0	-5.087392	3.044450	1.002728
63	1	0	-4.313657	0.336655	-2.239137
64	1	0	-6.415215	0.930926	-1.456609

(1,1)-g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.837068	-1.001847	1.157323
2	6	0	1.391284	-1.905029	-0.345434
3	6	0	0.975186	-0.906917	-1.141407
4	6	0	-0.369336	-0.809550	-1.719886
5	6	0	-2.690119	-1.686887	-1.916162
6	6	0	-3.855084	-2.246892	-1.404191
7	6	0	-3.984782	-2.391727	-0.029291
8	6	0	-2.968803	-1.984265	0.837826
9	6	0	-1.795007	-1.454358	0.318673
10	6	0	-1.589029	-1.332062	-1.079975
11	8	0	-0.447602	-0.298452	-2.859857
12	8	0	-2.644093	-1.496392	-3.243337
13	8	0	-5.141698	-2.917355	0.430643
14	6	0	2.748886	-2.102584	0.162277
15	6	0	3.030692	-3.245152	0.927109
16	6	0	4.297054	-3.477825	1.445285
17	6	0	5.317088	-2.555605	1.206212
18	6	0	5.059726	-1.407205	0.450135
19	6	0	3.790520	-1.189527	-0.063220
20	8	0	6.539312	-2.821149	1.735080
21	1	0	0.670052	-2.658821	-0.037340
22	1	0	1.668148	-0.168618	-1.533771
23	1	0	-4.663633	-2.520816	-2.070757
24	1	0	-3.105256	-2.050131	1.913320
25	1	0	-1.829317	-0.965392	-3.422527
26	1	0	-5.152719	-2.925603	1.394181
27	1	0	2.240510	-3.965609	1.120002
28	1	0	4.506771	-4.363421	2.035301
29	1	0	5.848766	-0.682386	0.269192
30	1	0	3.615605	-0.286644	-0.639080
31	1	0	7.162780	-2.121910	1.510256
32	8	0	-1.986988	2.098916	-1.419949
33	6	0	1.305173	2.352377	0.949029
34	6	0	0.068958	2.139341	0.463724
35	6	0	-1.092504	2.132861	1.370241
36	6	0	-3.452237	1.511149	1.879612
37	6	0	-4.725335	1.076981	1.523252
38	6	0	-5.046966	0.954696	0.179224
39	6	0	-4.126788	1.295692	-0.814969
40	6	0	-2.859094	1.727213	-0.454854
41	6	0	-2.453206	1.824267	0.903054
42	8	0	-0.899966	2.334704	2.592725
43	8	0	-3.188763	1.594578	3.188362
44	8	0	-6.287116	0.513049	-0.124080
45	6	0	2.550239	2.338364	0.181871
46	6	0	3.773694	2.318955	0.869491
47	6	0	4.985189	2.261760	0.195370
48	6	0	4.995797	2.227808	-1.199861
49	6	0	3.790234	2.267094	-1.909556
50	6	0	2.586671	2.326614	-1.221379
51	8	0	6.203973	2.161983	-1.815367
52	1	0	1.406459	2.530301	2.017915
53	1	0	-0.100331	1.925083	-0.580002
54	1	0	-5.445353	0.826792	2.292735
55	1	0	-4.398526	1.229097	-1.864425
56	1	0	-2.254303	1.939137	3.257106
57	1	0	-6.390684	0.417670	-1.077436
58	1	0	3.773733	2.334128	1.955635
59	1	0	5.925215	2.237065	0.736041

60	1	0	3.794593	2.254802	-2.995648
61	1	0	1.664849	2.369582	-1.793008
62	1	0	6.096747	2.149281	-2.772885
63	1	0	-2.325267	1.862330	-2.290657
64	1	0	-1.137366	-1.067703	2.070309

(1,1)-g'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	5.197464	0.712852	-2.032605
2	6	0	2.408275	1.110427	-1.135019
3	6	0	2.983151	2.209318	-0.613027
4	6	0	4.170769	2.182474	0.243068
5	6	0	5.598830	0.653973	1.587432
6	6	0	6.337460	-0.512666	1.763019
7	6	0	6.686114	-1.266348	0.645725
8	6	0	6.316689	-0.866005	-0.640587
9	6	0	5.536171	0.274052	-0.798383
10	6	0	5.103408	1.033858	0.309618
11	8	0	4.309291	3.114809	1.059216
12	8	0	5.337811	1.384003	2.685177
13	8	0	7.421216	-2.378905	0.864939
14	6	0	1.073424	1.019677	-1.720648
15	6	0	0.107751	2.024339	-1.557027
16	6	0	-1.185994	1.849805	-2.018469
17	6	0	-1.552610	0.650718	-2.640521
18	6	0	-0.594276	-0.337100	-2.861850
19	6	0	0.699472	-0.151599	-2.394364
20	8	0	-2.829664	0.417329	-3.041853
21	1	0	2.944747	0.166512	-1.080390
22	1	0	2.485623	3.174845	-0.629221
23	1	0	6.675088	-0.799015	2.751507
24	1	0	6.639519	-1.431193	-1.509952
25	1	0	4.970058	2.242545	2.379906
26	1	0	7.606777	-2.836557	0.037651
27	1	0	0.355575	2.943526	-1.036406
28	1	0	-1.919143	2.639538	-1.890872
29	1	0	-0.886351	-1.261986	-3.347443
30	1	0	1.427737	-0.947294	-2.521781
31	1	0	-3.433160	0.868034	-2.431971
32	8	0	-3.865671	1.316507	-0.454493
33	6	0	-2.250347	-1.026991	0.447168
34	6	0	-3.042368	-1.581916	-0.486411
35	6	0	-4.509066	-1.521277	-0.502491
36	6	0	-6.537632	-0.844407	0.772759
37	6	0	-7.268776	0.047726	1.551137
38	6	0	-6.827460	1.359069	1.673446
39	6	0	-5.679837	1.799358	1.005981

(1,1)-g''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.314836	-0.155961	2.949339
2	6	0	-0.027788	-0.507495	1.274299
3	6	0	-0.070131	0.829738	1.387679
4	6	0	-1.205048	1.648465	0.957268
5	6	0	-3.556950	1.879629	0.180763
6	6	0	-4.888211	1.479584	0.139056
7	6	0	-5.321179	0.480419	0.997963
8	6	0	-4.458697	-0.088626	1.940870
9	6	0	-3.133096	0.318020	1.985409
10	6	0	-2.612687	1.268670	1.064167
11	8	0	-0.899871	2.726624	0.374067
12	8	0	-3.194857	2.845393	-0.669429
13	8	0	-6.613024	0.098437	0.896272
14	6	0	1.158238	-1.350083	1.396813
15	6	0	2.458349	-0.833024	1.534777
16	6	0	3.561265	-1.667533	1.571312

17	6	0	3.389837	-3.052804	1.472193
18	6	0	2.108155	-3.591875	1.343695
19	6	0	1.010602	-2.740419	1.305124
20	8	0	4.507961	-3.819512	1.505103
21	1	0	-0.941519	-1.034116	1.009574
22	1	0	0.826717	1.407522	1.593335
23	1	0	-5.568591	1.941088	-0.565850
24	1	0	-4.826547	-0.827562	2.646874
25	1	0	-2.257863	3.077205	-0.458603
26	1	0	-6.815464	-0.597786	1.531330
27	1	0	2.621356	0.238662	1.588545
28	1	0	4.562948	-1.260351	1.657955
29	1	0	1.970369	-4.666375	1.265747
30	1	0	0.016360	-3.165578	1.197201
31	1	0	4.282395	-4.752443	1.421244
32	8	0	1.147267	2.102105	-1.321082
33	6	0	0.134443	-0.269131	-2.315550
34	6	0	1.288574	-0.826482	-1.933248
35	6	0	2.677278	-0.304211	-2.034041
36	6	0	4.534267	0.837445	-0.857057
37	6	0	5.005378	1.711658	0.118368
38	6	0	4.149901	2.674413	0.639676
39	6	0	2.838425	2.804774	0.173598
40	6	0	2.369303	1.926821	-0.797490
41	6	0	3.173172	0.869544	-1.300869
42	8	0	3.492640	-1.066628	-2.595149
43	8	0	5.398953	-0.071457	-1.318601
44	8	0	4.652574	3.497487	1.586835
45	6	0	-1.204692	-0.838685	-2.116724
46	6	0	-1.441360	-2.076106	-1.496440
47	6	0	-2.728273	-2.504566	-1.210238
48	6	0	-3.820881	-1.702680	-1.554469
49	6	0	-3.613654	-0.493404	-2.215119
50	6	0	-2.316566	-0.070173	-2.480706
51	8	0	-5.060244	-2.155267	-1.221985
52	1	0	0.150976	0.714586	-2.769195
53	1	0	1.306635	-1.836557	-1.527128
54	1	0	6.030318	1.636015	0.460235
55	1	0	2.199954	3.611136	0.521485
56	1	0	4.902445	-0.624412	-1.976365
57	1	0	3.985455	4.129722	1.876719
58	1	0	-0.609324	-2.713151	-1.213027
59	1	0	-2.901714	-3.453137	-0.712807
60	1	0	-4.457383	0.129375	-2.495837
61	1	0	-2.166663	0.892029	-2.961975
62	1	0	-5.727328	-1.494221	-1.438514
63	1	0	0.531737	2.527743	-0.685673
64	1	0	-2.795628	-0.760454	3.525290

(2,2)-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.561128	0.768159	-0.132651
2	6	0	2.538724	2.080760	0.459540
3	6	0	3.670606	2.937127	-0.101375
4	6	0	5.001888	2.243915	0.032303
5	6	0	6.172211	0.036735	0.011945
6	6	0	6.137335	-1.345017	-0.098429
7	6	0	4.900742	-1.987000	-0.208437
8	6	0	3.695559	-1.269199	-0.213245
9	6	0	3.742085	0.110044	-0.101092
10	6	0	4.971990	0.801012	0.015221
11	8	0	6.056661	2.894361	0.108594
12	8	0	7.360552	0.647053	0.109222
13	8	0	4.920991	-3.327675	-0.305086
14	6	0	1.179795	2.678707	0.206725
15	6	0	0.407370	3.155980	1.265182
16	6	0	-0.821295	3.769428	1.036048
17	6	0	-1.283538	3.897339	-0.269752
18	6	0	-0.537782	3.407287	-1.341181
19	6	0	0.691242	2.807155	-1.095989
20	8	0	-2.506133	4.495171	-0.450337

21	1	0	2.686646	1.952290	1.539910
22	1	0	3.505032	3.132390	-1.168587
23	1	0	3.706392	3.901685	0.409922
24	1	0	7.055264	-1.920158	-0.093282
25	1	0	2.736084	-1.765983	-0.299402
26	1	0	7.188627	1.618095	0.146195
27	1	0	4.025382	-3.703039	-0.210450
28	1	0	0.765958	3.055900	2.285555
29	1	0	-1.420827	4.146348	1.857709
30	1	0	-0.912246	3.493149	-2.357168
31	1	0	1.268628	2.426418	-1.933019
32	1	0	-2.675058	4.640698	-1.388748
33	8	0	-2.561135	-0.768162	0.132727
34	6	0	-2.538726	-2.080749	-0.459492
35	6	0	-3.670604	-2.937137	0.101402
36	6	0	-5.001892	-2.243921	-0.032196
37	6	0	-6.172210	-0.036732	-0.011993
38	6	0	-6.137334	1.345022	0.098368
39	6	0	-4.900745	1.987002	0.208424
40	6	0	-3.695564	1.269198	0.213285
41	6	0	-3.742091	-0.110046	0.101146
42	6	0	-4.971993	-0.801015	-0.015192
43	8	0	-6.056650	-2.894374	-0.108645
44	8	0	-7.360550	-0.647040	-0.109357
45	8	0	-4.920996	3.327679	0.305053
46	6	0	-1.179794	-2.678698	-0.206696
47	6	0	-0.407370	-3.155942	-1.265167
48	6	0	0.821295	-3.769396	-1.036051
49	6	0	1.283541	-3.897343	0.269745
50	6	0	0.537786	-3.407321	1.341188
51	6	0	-0.691240	-2.807182	1.096014
52	8	0	2.506136	-4.495179	0.450311
53	1	0	-2.686650	-1.952251	-1.539858
54	1	0	-3.505013	-3.132448	1.168602
55	1	0	-3.706397	-3.901673	-0.409938
56	1	0	-7.055261	1.920166	0.093167
57	1	0	-2.736091	1.765980	0.299468
58	1	0	-7.188624	-1.618080	-0.146371
59	1	0	-4.025386	3.703046	0.210435
60	1	0	-0.765959	-3.055835	-2.285536
61	1	0	1.420827	-4.146293	-1.857723
62	1	0	0.912249	-3.493212	2.357173
63	1	0	-1.268625	-2.426469	1.933055
64	1	0	2.675063	-4.640733	1.388718

(2,2)-b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.727121	-2.773813	-0.160837
2	6	0	-0.091799	-1.584731	-0.240820
3	6	0	0.330059	-0.741396	-1.435984
4	6	0	1.805633	-0.434621	-1.388748
5	6	0	4.049672	-1.254764	-0.653538
6	6	0	4.846551	-2.233221	-0.073757
7	6	0	4.238631	-3.371092	0.455941
8	6	0	2.849690	-3.549854	0.433968
9	6	0	2.063419	-2.563708	-0.139730
10	6	0	2.636461	-1.398621	-0.700782
11	8	0	2.267153	0.568856	-1.950918
12	8	0	4.639360	-0.176299	-1.181316
13	8	0	5.057564	-4.293745	1.006711
14	6	0	-1.536975	-2.003151	-0.246538
15	6	0	-2.301649	-1.847588	0.911724
16	6	0	-3.652225	-2.170250	0.930503
17	6	0	-4.256282	-2.637435	-0.233561
18	6	0	-3.503030	-2.848903	-1.386955
19	6	0	-2.148895	-2.530853	-1.385089
20	8	0	-5.616370	-2.806444	-0.208640
21	1	0	0.095763	-1.009073	0.671886
22	1	0	0.135608	-1.266367	-2.379045
23	1	0	-0.233252	0.193242	-1.450681
24	1	0	5.922698	-2.115786	-0.039233

25	1	0	2.382242	-4.429270	0.862714
26	1	0	3.928685	0.390671	-1.564024
27	1	0	4.552817	-5.047140	1.333257
28	1	0	-1.841932	-1.442021	1.808366
29	1	0	-4.252991	-2.014850	1.820127
30	1	0	-3.973494	-3.228824	-2.289337
31	1	0	-1.577114	-2.689165	-2.294336
32	1	0	-5.919602	-3.230532	-1.019528
33	8	0	-0.539234	1.575282	0.832555
34	6	0	-1.451832	2.607442	0.381275
35	6	0	-0.968006	3.206103	-0.932352
36	6	0	0.465284	3.664132	-0.833918
37	6	0	2.711300	3.161378	0.134527
38	6	0	3.536069	2.365286	0.917223
39	6	0	2.966424	1.333554	1.661168
40	6	0	1.587401	1.089841	1.655114
41	6	0	0.775263	1.884998	0.862679
42	6	0	1.307875	2.938857	0.087417
43	8	0	0.891435	4.580184	-1.553945
44	8	0	3.265446	4.133223	-0.599040
45	8	0	3.808199	0.580500	2.399390
46	6	0	-2.819442	1.977626	0.343876
47	6	0	-3.658023	2.098444	1.454418
48	6	0	-4.878035	1.433306	1.512755
49	6	0	-5.274334	0.627960	0.446203
50	6	0	-4.477570	0.548168	-0.697915
51	6	0	-3.253811	1.203344	-0.735254
52	8	0	-6.440940	-0.066589	0.566616
53	1	0	-1.438214	3.390809	1.150405
54	1	0	-1.005865	2.471061	-1.745591
55	1	0	-1.601937	4.047006	-1.221679
56	1	0	4.606600	2.527610	0.930207
57	1	0	1.150875	0.304156	2.261799
58	1	0	2.542078	4.552951	-1.123109
59	1	0	3.329404	-0.124167	2.850194
60	1	0	-3.343276	2.702146	2.301451
61	1	0	-5.510835	1.502577	2.391165
62	1	0	-4.795571	-0.059505	-1.539260
63	1	0	-2.636018	1.085343	-1.619949
64	1	0	-6.381482	-0.901623	0.076486

(2,2)-b’

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.903506	-1.223887	1.011126
2	6	0	0.174524	-1.735826	-0.112792
3	6	0	0.791683	-3.052808	-0.573506
4	6	0	2.257204	-2.868262	-0.878924
5	6	0	4.346459	-1.662613	-0.217637
6	6	0	5.008293	-0.762256	0.603354
7	6	0	4.272267	-0.043593	1.546922
8	6	0	2.889080	-0.201124	1.686440
9	6	0	2.240646	-1.096705	0.855303
10	6	0	2.943345	-1.859969	-0.104321
11	8	0	2.833258	-3.571857	-1.723562
12	8	0	5.054460	-2.354710	-1.120531
13	8	0	4.961569	0.823391	2.316827
14	6	0	-1.278480	-1.853165	0.274708
15	6	0	-2.231829	-2.029598	-0.733150
16	6	0	-3.579894	-2.146196	-0.431099
17	6	0	-3.998885	-2.071563	0.898676
18	6	0	-3.061743	-1.891879	1.913687
19	6	0	-1.707712	-1.789274	1.597763
20	8	0	-5.334852	-2.177114	1.138230
21	1	0	0.265252	-0.995733	-0.920303
22	1	0	0.696477	-3.804563	0.220530
23	1	0	0.280446	-3.433647	-1.460082
24	1	0	6.076903	-0.612687	0.509976
25	1	0	2.319909	0.384962	2.399175
26	1	0	4.427908	-2.964273	-1.577942
27	1	0	4.366784	1.301089	2.905943
28	1	0	-1.921187	-2.057738	-1.774383

29	1	0	-4.319526	-2.264488	-1.215431
30	1	0	-3.382510	-1.823107	2.949364
31	1	0	-0.986598	-1.641537	2.394015
32	1	0	-5.521483	-2.008098	2.067777
33	8	0	-0.945331	1.541113	-1.169832
34	6	0	-0.272915	2.302344	-0.157887
35	6	0	-0.593533	1.740984	1.225782
36	6	0	-2.077998	1.629536	1.443310
37	6	0	-4.288132	1.234775	0.346255
38	6	0	-5.043377	0.982527	-0.790381
39	6	0	-4.398028	0.916004	-2.024067
40	6	0	-3.018846	1.117660	-2.154764
41	6	0	-2.278846	1.379046	-1.014274
42	6	0	-2.885618	1.445918	0.259785
43	8	0	-2.561725	1.660831	2.586546
44	8	0	-4.900228	1.262356	1.536220
45	8	0	-5.173349	0.647618	-3.098032
46	6	0	1.207980	2.286678	-0.455183
47	6	0	2.054251	3.131794	0.269564
48	6	0	3.427777	3.115817	0.069112
49	6	0	3.978881	2.247008	-0.874738
50	6	0	3.147394	1.412225	-1.617289
51	6	0	1.770985	1.436794	-1.404105
52	8	0	5.331463	2.267568	-1.030168
53	1	0	-0.650743	3.332746	-0.224489
54	1	0	-0.162804	0.736903	1.325695
55	1	0	-0.160759	2.369081	2.007725
56	1	0	-6.109760	0.809540	-0.715156
57	1	0	-2.526278	1.076545	-3.120098
58	1	0	-4.201576	1.414104	2.217537
59	1	0	-4.641917	0.615093	-3.901335
60	1	0	1.638508	3.816266	1.004684
61	1	0	4.082501	3.767067	0.638294
62	1	0	3.568801	0.735628	-2.355825
63	1	0	1.134404	0.788164	-1.994783
64	1	0	5.607494	1.570548	-1.634779

(2,2)-g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.425834	0.509871	1.042501
2	6	0	-3.365572	1.468768	0.509581
3	6	0	-2.825145	2.092222	-0.772950
4	6	0	-1.442322	2.651945	-0.573307
5	6	0	0.732806	2.354719	0.617903
6	6	0	1.537747	1.652268	1.503049
7	6	0	0.992908	0.567795	2.192385
8	6	0	-0.345641	0.191862	2.045887
9	6	0	-1.144982	0.908698	1.168780
10	6	0	-0.627809	1.994645	0.423977
11	8	0	-1.024056	3.595041	-1.262349
12	8	0	1.272921	3.361962	-0.079636
13	8	0	1.827438	-0.095836	3.021512
14	6	0	-4.673832	0.750671	0.316983
15	6	0	-5.810436	1.135777	1.028476
16	6	0	-7.025731	0.482560	0.847935
17	6	0	-7.108252	-0.580734	-0.050161
18	6	0	-5.977078	-0.982923	-0.765953
19	6	0	-4.772579	-0.314623	-0.582402
20	8	0	-8.316656	-1.191778	-0.190373
21	1	0	-3.486117	2.253496	1.268147
22	1	0	-2.759420	1.332675	-1.561319
23	1	0	-3.494276	2.881739	-1.121763
24	1	0	2.576091	1.929434	1.639841
25	1	0	-0.766333	-0.642343	2.595959
26	1	0	0.571656	3.706697	-0.684099
27	1	0	1.383676	-0.858701	3.408988
28	1	0	-5.751908	1.958356	1.736067
29	1	0	-7.909818	0.784477	1.399188
30	1	0	-6.039228	-1.812062	-1.465472
31	1	0	-3.898211	-0.631296	-1.144284
32	1	0	-8.258134	-1.906788	-0.833074
33	8	0	2.591810	-1.631617	-0.037076

34	6	0	3.297079	-1.007385	-1.122948
35	6	0	2.533533	0.206181	-1.649357
36	6	0	1.090621	-0.113785	-1.935140
37	6	0	-0.880277	-1.486807	-1.250133
38	6	0	-1.459989	-2.435701	-0.423226
39	6	0	-0.658954	-3.087649	0.515098
40	6	0	0.709791	-2.825432	0.633789
41	6	0	1.277394	-1.875012	-0.200937
42	6	0	0.503928	-1.178220	-1.155756
43	8	0	0.440768	0.542276	-2.765647
44	8	0	-1.650763	-0.844363	-2.139903
45	8	0	-1.273462	-3.996677	1.302871
46	6	0	4.664655	-0.634145	-0.611191
47	6	0	5.774081	-0.681319	-1.456103
48	6	0	7.026880	-0.271806	-1.012178
49	6	0	7.179804	0.184102	0.297547
50	6	0	6.079689	0.227942	1.156523
51	6	0	4.830623	-0.176567	0.696923
52	8	0	8.428125	0.567351	0.686167
53	1	0	3.386451	-1.753103	-1.924330
54	1	0	2.551784	1.010407	-0.904457
55	1	0	3.010928	0.585622	-2.555634
56	1	0	-2.518129	-2.655946	-0.489733
57	1	0	1.331024	-3.348533	1.352594
58	1	0	-1.068852	-0.197765	-2.611211
59	1	0	-0.644592	-4.404328	1.908893
60	1	0	5.664469	-1.041321	-2.475746
61	1	0	7.890695	-0.308577	-1.667287
62	1	0	6.197366	0.575834	2.179157
63	1	0	3.973690	-0.157383	1.363212
64	1	0	8.417220	0.861283	1.603258

(2,2)-g'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.582171	0.063583	-0.144704
2	6	0	3.580133	-1.163125	-0.928567
3	6	0	4.807033	-1.992061	-0.574818
4	6	0	6.070388	-1.185696	-0.746000
5	6	0	7.091470	1.094026	-0.587268
6	6	0	6.979788	2.448464	-0.301091
7	6	0	5.730304	2.968151	0.035110
8	6	0	4.580766	2.166773	0.076125
9	6	0	4.708490	0.821205	-0.214347
10	6	0	5.953096	0.243255	-0.546043
11	8	0	7.149638	-1.734994	-1.010036
12	8	0	8.296257	0.597872	-0.889566
13	8	0	5.676260	4.287963	0.307180
14	6	0	2.258956	-1.842524	-0.698769
15	6	0	1.295760	-1.850365	-1.710828
16	6	0	0.047259	-2.424946	-1.510741
17	6	0	-0.256076	-2.996738	-0.275064
18	6	0	0.695553	-3.001824	0.746933
19	6	0	1.943355	-2.431310	0.527749
20	8	0	-1.494285	-3.536515	-0.124620
21	1	0	3.647479	-0.852898	-1.978676
22	1	0	4.856479	-2.883412	-1.203927
23	1	0	7.852598	3.089097	-0.329617
24	1	0	3.607163	2.582059	0.312581
25	1	0	8.189684	-0.373724	-1.022497
26	1	0	4.780603	4.553062	0.545487
27	1	0	1.519591	-1.393027	-2.670625
28	1	0	-0.700332	-2.427228	-2.296656
29	1	0	0.460140	-3.441211	1.712140
30	1	0	2.662813	-2.429155	1.341031
31	1	0	-1.604451	-3.884665	0.766723
32	8	0	-3.889296	1.246324	0.282872
33	6	0	-3.511366	0.196675	1.194896
34	6	0	-3.885176	-1.165739	0.618214
35	6	0	-5.338060	-1.214450	0.224745
36	6	0	-7.256118	0.103983	-0.688988
37	6	0	-7.778456	1.294298	-1.174716

38	6	0	-6.974582	2.435270	-1.165595
39	6	0	-5.666288	2.418820	-0.668674
40	6	0	-5.157437	1.226353	-0.178600
41	6	0	-5.928754	0.040481	-0.181794
42	8	0	-5.966933	-2.284480	0.217063
43	8	0	-8.020381	-0.994873	-0.717957
44	8	0	-7.527626	3.567422	-1.651013
45	6	0	-2.036121	0.325226	1.462844
46	6	0	-1.538613	0.191472	2.759578
47	6	0	-0.169556	0.224968	3.008175
48	6	0	0.720461	0.410728	1.950392
49	6	0	0.232343	0.582415	0.652177
50	6	0	-1.134084	0.521084	0.414755
51	8	0	2.050256	0.417270	2.229093
52	1	0	-3.678017	-1.953210	1.345961
53	1	0	-8.789113	1.334878	-1.561964
54	1	0	-5.056083	3.314712	-0.643804
55	1	0	-7.473737	-1.740657	-0.372820
56	1	0	-6.899948	4.297888	-1.611041
57	1	0	-2.224989	0.048592	3.590245
58	1	0	0.217736	0.102267	4.014237
59	1	0	0.924598	0.730570	-0.170123
60	1	0	-1.501761	0.631852	-0.600945
61	1	0	2.560746	0.331012	1.406022
62	1	0	-3.280794	-1.379178	-0.272881
63	1	0	-4.071399	0.359123	2.125664
64	1	0	4.765713	-2.322528	0.470247

(2,2)-g''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.816419	1.458538	0.033036
2	6	0	-3.471296	0.203041	0.312466
3	6	0	-3.296263	-0.167916	1.781076
4	6	0	-1.843804	-0.145442	2.184468
5	6	0	0.379679	0.920957	1.783847
6	6	0	1.169375	1.856050	1.132150
7	6	0	0.597548	2.628507	0.121475
8	6	0	-0.741512	2.486736	-0.256173
9	6	0	-1.521265	1.550382	0.404330
10	6	0	-0.988547	0.749717	1.440153
11	8	0	-1.432845	-0.829944	3.134830
12	8	0	0.929458	0.178020	2.754888
13	8	0	1.407975	3.521630	-0.492019
14	6	0	-4.909337	0.324907	-0.110564
15	6	0	-5.454776	-0.598207	-1.004730
16	6	0	-6.789890	-0.520479	-1.387402
17	6	0	-7.594248	0.499533	-0.880194
18	6	0	-7.061262	1.434804	0.010977
19	6	0	-5.727384	1.339127	0.392051
20	8	0	-8.892211	0.536850	-1.289917
21	1	0	-2.979465	-0.555006	-0.305459
22	1	0	-3.832203	0.543827	2.422328
23	1	0	-3.710656	-1.160796	1.971776
24	1	0	2.214747	1.972363	1.391230
25	1	0	-1.174705	3.079097	-1.054570
26	1	0	0.211699	-0.388627	3.127620
27	1	0	0.922444	4.016023	-1.162027
28	1	0	-4.826678	-1.390560	-1.403699
29	1	0	-7.214480	-1.237738	-2.081753
30	1	0	-7.685242	2.232364	0.404836
31	1	0	-5.321519	2.073939	1.081446
32	1	0	-9.350356	1.282006	-0.887005
33	8	0	2.681662	-0.184890	-0.819358
34	6	0	2.357894	-1.336320	-0.029865
35	6	0	3.353259	-2.457539	-0.322125
36	6	0	4.768534	-1.985054	-0.105450
37	6	0	6.308735	-0.016776	-0.205421
38	6	0	6.534047	1.325670	-0.477301
39	6	0	5.455322	2.124958	-0.858258
40	6	0	4.155083	1.618575	-0.970344
41	6	0	3.943106	0.279210	-0.691949

42	6	0	5.004343	-0.573104	-0.306084
43	8	0	5.672738	-2.778885	0.198293
44	8	0	7.346126	-0.787358	0.145554
45	8	0	5.722129	3.426201	-1.102571
46	6	0	0.934913	-1.737251	-0.322009
47	6	0	0.255905	-2.532892	0.600655
48	6	0	-1.034586	-2.984519	0.346276
49	6	0	-1.661710	-2.633795	-0.848967
50	6	0	-1.003491	-1.821236	-1.771865
51	6	0	0.289192	-1.381016	-1.506774
52	8	0	-2.931197	-3.031536	-1.154841
53	1	0	2.439743	-1.044126	1.026594
54	1	0	3.255295	-2.775783	-1.368218
55	1	0	3.158546	-3.325568	0.311556
56	1	0	7.529735	1.744290	-0.396548
57	1	0	3.314924	2.256056	-1.223761
58	1	0	7.002094	-1.704718	0.263560
59	1	0	4.917332	3.894517	-1.352169
60	1	0	0.731751	-2.801191	1.540095
61	1	0	-1.552623	-3.595460	1.079906
62	1	0	-1.510182	-1.540080	-2.689207
63	1	0	0.796407	-0.748051	-2.226549
64	1	0	-3.281338	-3.599567	-0.459842

(1,2)-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.204392	-2.468348	1.344583
2	6	0	-0.607054	-2.664974	0.022769
3	6	0	0.205022	-3.423220	-0.823550
4	6	0	1.388812	-3.989264	-0.360796
5	6	0	1.777339	-3.777054	0.959886
6	6	0	0.988404	-3.010769	1.814660
7	6	0	-1.942103	-2.168644	-0.474104
8	8	0	-2.255923	-0.948280	0.211594
9	6	0	-3.491726	-0.433369	0.014452
10	6	0	-4.563166	-1.232424	-0.450429
11	6	0	-4.392617	-2.654839	-0.625021
12	6	0	-3.041068	-3.205972	-0.252655
13	6	0	-5.833297	-0.614532	-0.623096
14	6	0	-6.018895	0.727657	-0.330167
15	6	0	-4.937944	1.475483	0.145007
16	6	0	-3.665776	0.908457	0.309299
17	8	0	-5.305871	-3.401154	-1.011641
18	8	0	-6.878325	-1.331470	-1.056218
19	8	0	-5.180413	2.767067	0.425980
20	8	0	2.983598	-4.302357	1.351809
21	8	0	-3.128454	4.540702	1.202642
22	6	0	-1.845361	4.153087	0.917368
23	6	0	-1.261086	3.214202	1.763290
24	6	0	0.009043	2.735512	1.469334
25	6	0	0.720343	3.190927	0.350117
26	6	0	0.115662	4.153854	-0.471811
27	6	0	-1.157281	4.632683	-0.197960
28	6	0	2.034307	2.610137	0.066324
29	8	0	2.358550	0.169640	-1.411563
30	6	0	3.544683	-0.082725	-0.809324
31	6	0	4.492336	0.965561	-0.706288
32	6	0	4.230785	2.374877	-1.040149
33	6	0	2.902556	2.990830	-0.883259
34	6	0	5.790636	0.608688	-0.235773
35	6	0	6.072179	-0.665300	0.248407
36	6	0	5.080318	-1.639642	0.204110
37	6	0	3.829200	-1.361548	-0.356598
38	8	0	5.171134	3.115971	-1.390220
39	8	0	6.787499	1.506488	-0.209870
40	8	0	5.377130	-2.864587	0.682225
41	1	0	2.309531	1.773978	0.706424
42	1	0	2.734186	3.861529	-1.510526
43	1	0	7.057218	-0.891683	0.637956
44	1	0	3.090770	-2.146462	-0.470378
45	1	0	6.471640	2.302407	-0.697222

46	1	0	4.577487	-3.418367	0.731493
47	1	0	0.455809	1.989159	2.119855
48	1	0	-1.807402	2.859737	2.631001
49	1	0	-1.620832	5.361157	-0.856557
50	1	0	0.629612	4.523390	-1.352819
51	1	0	-3.379515	5.302024	0.665447
52	1	0	-1.875810	-1.936802	-1.545896
53	1	0	-3.072866	-3.490985	0.807057
54	1	0	-2.838078	-4.107344	-0.834997
55	1	0	-6.991383	1.187972	-0.455236
56	1	0	-2.821118	1.495808	0.649870
57	1	0	-6.569689	-2.261923	-1.168159
58	1	0	-4.391267	3.233554	0.757071
59	1	0	-0.090161	-3.586802	-1.856469
60	1	0	2.018667	-4.580954	-1.016651
61	1	0	1.302602	-2.831183	2.838768
62	1	0	-0.821199	-1.877286	2.013244
63	1	0	3.075090	-4.252316	2.310816
64	1	0	1.806149	-0.620732	-1.393758

(1,2)-b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.308884	3.733688	-0.063812
2	6	0	-2.587493	1.093217	0.379380
3	6	0	-2.241767	1.488513	1.619230
4	6	0	-0.831419	1.623105	2.043028
5	6	0	1.562068	1.971218	1.460960
6	6	0	2.580747	2.499287	0.679262
7	6	0	2.248442	3.348996	-0.366908
8	6	0	0.933525	3.741941	-0.602529
9	6	0	-0.084080	3.226802	0.191128
10	6	0	0.187333	2.273989	1.212569
11	8	0	-0.526291	1.108613	3.136358
12	8	0	1.920572	1.139157	2.448009
13	8	0	3.266487	3.772772	-1.166249
14	6	0	-3.926184	0.741883	-0.088180
15	6	0	-5.017529	0.559160	0.776771
16	6	0	-6.267384	0.217233	0.287872
17	6	0	-6.453544	0.050736	-1.089217
18	6	0	-5.382772	0.226562	-1.966974
19	6	0	-4.133499	0.560426	-1.461199
20	8	0	-7.696882	-0.290912	-1.508499
21	1	0	-1.800191	1.000008	-0.369333
22	1	0	-2.962621	1.532673	2.430659
23	1	0	3.609565	2.224151	0.874199
24	1	0	0.681885	4.448394	-1.385759
25	1	0	1.110534	0.963518	2.985000
26	1	0	2.947464	4.413737	-1.812816
27	1	0	-4.890791	0.666432	1.849271
28	1	0	-7.107554	0.068882	0.957690
29	1	0	-5.521997	0.091849	-3.035616
30	1	0	-3.300136	0.680201	-2.147517
31	1	0	-7.713505	-0.401077	-2.465601
32	8	0	1.553453	-1.009968	-0.719161
33	6	0	1.087730	-1.846197	0.356857
34	6	0	1.833340	-3.178843	0.344751
35	6	0	3.325696	-2.973937	0.359470
36	6	0	5.193773	-1.474270	-0.354165
37	6	0	5.642405	-0.311070	-0.964495
38	6	0	4.703818	0.583715	-1.480699
39	6	0	3.330314	0.316215	-1.445533
40	6	0	2.890277	-0.821624	-0.793683
41	6	0	3.803532	-1.749648	-0.239554
42	8	0	4.087546	-3.833617	0.829977
43	8	0	6.094996	-2.332744	0.141088
44	8	0	5.172826	1.738469	-2.000331
45	6	0	-0.398547	-2.026239	0.204703
46	6	0	-1.233318	-1.951809	1.317401
47	6	0	-2.598699	-2.204147	1.206996
48	6	0	-3.142660	-2.521531	-0.036296
49	6	0	-2.319599	-2.589294	-1.162583

50	6	0	-0.958585	-2.348601	-1.036071
51	8	0	-4.467651	-2.774189	-0.216262
52	1	0	1.303364	-1.316501	1.294960
53	1	0	1.580263	-3.738705	-0.565197
54	1	0	1.538420	-3.788000	1.202150
55	1	0	6.700695	-0.083923	-1.005550
56	1	0	2.608875	1.011841	-1.856369
57	1	0	5.595126	-3.092408	0.524309
58	1	0	4.475716	2.414935	-1.988294
59	1	0	-0.821909	-1.685071	2.287033
60	1	0	-3.238560	-2.131826	2.081947
61	1	0	-2.759045	-2.822065	-2.126743
62	1	0	-0.324201	-2.402519	-1.915790
63	1	0	-4.968479	-2.506256	0.562038
64	1	0	-1.987840	3.286864	0.462641

(1,2)-b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.085897	2.264588	-0.114562
2	6	0	-0.819330	1.307536	0.486215
3	6	0	-0.577448	1.237291	1.983927
4	6	0	0.867009	0.900794	2.260234
5	6	0	3.222637	1.150482	1.461607
6	6	0	4.140639	1.660682	0.555271
7	6	0	3.672295	2.368603	-0.550144
8	6	0	2.306898	2.577203	-0.776655
9	6	0	1.399323	2.054049	0.129614
10	6	0	1.826801	1.341947	1.272974
11	8	0	1.200259	0.314478	3.301010
12	8	0	3.673733	0.482211	2.530063
13	8	0	4.605863	2.832084	-1.410854
14	6	0	-2.213176	1.660197	0.043349
15	6	0	-2.537669	1.494769	-1.308158
16	6	0	-3.804118	1.789053	-1.786112
17	6	0	-4.783788	2.244957	-0.900953
18	6	0	-4.482551	2.407230	0.449890
19	6	0	-3.199517	2.119512	0.911621
20	8	0	-6.015092	2.509745	-1.417308
21	1	0	-0.563983	0.333052	0.052823
22	1	0	-0.783923	2.205731	2.457601
23	1	0	-1.222185	0.488083	2.449581
24	1	0	5.201910	1.497903	0.696346
25	1	0	1.949117	3.109298	-1.651314
26	1	0	2.886587	0.235039	3.071959
27	1	0	4.190405	3.310854	-2.136741
28	1	0	-1.783942	1.120994	-1.995973
29	1	0	-4.054959	1.651989	-2.832418
30	1	0	-5.243909	2.752138	1.143965
31	1	0	-2.993011	2.244226	1.969282
32	1	0	-6.612681	2.808833	-0.723739
33	6	0	-4.193302	-1.591507	-1.054946
34	6	0	-4.166472	-1.271557	0.294894
35	6	0	-3.039726	-1.588692	1.043022
36	6	0	-1.881597	-2.177302	0.452445
37	6	0	-1.988020	-2.546981	-0.909962
38	6	0	-3.115464	-2.242911	-1.662972
39	8	0	-5.316511	-1.283133	-1.739933
40	8	0	-3.079091	-1.294887	2.353412
41	8	0	-0.977268	-3.261348	-1.460388
42	6	0	-0.701935	-2.408971	1.313230
43	6	0	0.691785	-2.369475	0.853979
44	6	0	1.127942	-1.742161	-0.252917
45	6	0	2.763181	-0.815549	-1.839312
46	6	0	2.513946	-1.528907	-0.659216
47	6	0	3.617505	-1.994011	0.076408
48	6	0	4.911856	-1.750657	-0.346389
49	6	0	5.135441	-1.027332	-1.522812
50	6	0	4.056903	-0.565612	-2.277303
51	8	0	6.426432	-0.801961	-1.875608
52	8	0	-0.875920	-2.554219	2.541691
53	1	0	-5.011368	-0.787323	0.767864

54	1	0	-3.169417	-2.542433	-2.705837
55	1	0	-5.233887	-1.535346	-2.665949
56	1	0	-2.314843	-1.760638	2.769155
57	1	0	-1.198491	-3.505568	-2.365548
58	1	0	1.385875	-2.764712	1.589973
59	1	0	0.393104	-1.325514	-0.937167
60	1	0	1.926810	-0.439302	-2.421974
61	1	0	3.468180	-2.543278	0.999894
62	1	0	5.761588	-2.099029	0.230572
63	1	0	4.227254	-0.000184	-3.188825
64	1	0	6.469049	-0.271382	-2.678679

(1,2)-g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.947022	-2.317453	-0.770995
2	6	0	-0.237922	-1.566394	-0.437396
3	6	0	-0.560798	-0.590194	-1.562323
4	6	0	0.612691	0.322652	-1.806870
5	6	0	3.104088	0.437237	-1.934623
6	6	0	4.342618	-0.177861	-1.843806
7	6	0	4.407986	-1.493770	-1.386366
8	6	0	3.264541	-2.213181	-1.020944
9	6	0	2.031110	-1.592106	-1.122676
10	6	0	1.913853	-0.260748	-1.590258
11	8	0	0.453846	1.490429	-2.202686
12	8	0	3.042661	1.702608	-2.370655
13	8	0	5.640340	-2.038905	-1.294780
14	6	0	-1.349994	-2.531810	-0.138461
15	6	0	-2.001359	-2.486815	1.095801
16	6	0	-3.061953	-3.341677	1.376041
17	6	0	-3.474745	-4.265571	0.416592
18	6	0	-2.824977	-4.330856	-0.818914
19	6	0	-1.773431	-3.462574	-1.089524
20	8	0	-4.514622	-5.082935	0.738882
21	1	0	-0.007793	-0.997203	0.470722
22	1	0	-0.762121	-1.139002	-2.491351
23	1	0	-1.451724	-0.006367	-1.323995
24	1	0	5.245695	0.363151	-2.095965
25	1	0	3.326382	-3.225660	-0.637406
26	1	0	2.090414	1.958026	-2.390724
27	1	0	5.588750	-2.945404	-0.971421
28	1	0	-1.675706	-1.778641	1.853528
29	1	0	-3.568932	-3.305626	2.334398
30	1	0	-3.140626	-5.055038	-1.564794
31	1	0	-1.274057	-3.523455	-2.052269
32	1	0	-4.711349	-5.679357	0.008673
33	6	0	3.786106	1.682913	1.088175
34	6	0	3.534688	0.404770	1.569254
35	6	0	2.274964	0.108556	2.075341
36	6	0	1.214756	1.064637	2.065181
37	6	0	1.542321	2.370376	1.621828
38	6	0	2.800860	2.674406	1.121283
39	8	0	5.028116	1.935962	0.623882
40	8	0	2.089650	-1.132140	2.552236
41	8	0	0.609175	3.342158	1.747644
42	6	0	-0.114825	0.638819	2.538704
43	6	0	-1.383458	1.179552	2.034741
44	6	0	-1.538167	1.701739	0.805983
45	6	0	-2.739272	2.550405	-1.164804
46	6	0	-2.790270	2.080237	0.155290
47	6	0	-4.046869	1.991396	0.779285
48	6	0	-5.202752	2.360081	0.112928
49	6	0	-5.128579	2.827462	-1.204622
50	6	0	-3.892305	2.922868	-1.845278
51	8	0	-6.295071	3.171202	-1.806217
52	8	0	-0.199638	-0.321499	3.335059
53	1	0	4.307601	-0.353414	1.561206
54	1	0	3.026135	3.683777	0.789292
55	1	0	5.086583	2.834074	0.279880
56	1	0	1.223666	-1.132032	3.022811
57	1	0	0.960233	4.182027	1.432231

58	1	0	-2.232634	0.954281	2.673584
59	1	0	-0.652092	1.851121	0.193658
60	1	0	-1.778305	2.610934	-1.669579
61	1	0	-4.128135	1.630793	1.799553
62	1	0	-6.171481	2.291294	0.595920
63	1	0	-3.830620	3.282894	-2.868145
64	1	0	-6.135155	3.476123	-2.706141

(1,2)-g'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-4.126952	-2.299314	1.546798
2	6	0	-1.806347	-0.876414	0.569420
3	6	0	-2.391183	0.037492	1.362833
4	6	0	-3.748127	0.545594	1.136330
5	6	0	-5.810311	0.394975	-0.253126
6	6	0	-6.770435	-0.316409	-0.963799
7	6	0	-6.812473	-1.699843	-0.842844
8	6	0	-5.922360	-2.381480	-0.006632
9	6	0	-4.947472	-1.667415	0.677883
10	6	0	-4.817093	-0.262473	0.532338
11	8	0	-3.971305	1.749720	1.408391
12	8	0	-5.843725	1.730728	-0.362088
13	8	0	-7.769359	-2.349387	-1.540573
14	6	0	-0.429714	-1.363207	0.646097
15	6	0	0.496458	-0.921853	1.607479
16	6	0	1.786614	-1.423418	1.646225
17	6	0	2.183496	-2.399163	0.724508
18	6	0	1.283708	-2.852145	-0.241999
19	6	0	-0.004930	-2.332529	-0.274283
20	8	0	3.451269	-2.866987	0.823603
21	1	0	-2.399891	-1.313185	-0.231593
22	1	0	-1.842541	0.558887	2.140100
23	1	0	-7.492665	0.209686	-1.575704
24	1	0	-6.006652	-3.455811	0.128294
25	1	0	-5.220348	2.091709	0.305155
26	1	0	-7.726046	-3.298658	-1.380652
27	1	0	0.209027	-0.173495	2.338197
28	1	0	2.500900	-1.070176	2.382120
29	1	0	1.589537	-3.600976	-0.966326
30	1	0	-0.696416	-2.688206	-1.032859
31	1	0	3.642918	-3.487501	0.111537
32	8	0	3.194811	1.621220	0.168072
33	6	0	2.405936	1.771219	-1.020271
34	6	0	2.116193	0.413761	-1.658096
35	6	0	3.362643	-0.406332	-1.839499
36	6	0	5.596997	-0.969388	-0.878564
37	6	0	6.567661	-0.799686	0.097096
38	6	0	6.369527	0.172461	1.078506
39	6	0	5.233881	0.990225	1.097105
40	6	0	4.278465	0.821906	0.106986
41	6	0	4.429207	-0.158403	-0.900356
42	8	0	3.432625	-1.281410	-2.718970
43	8	0	5.766061	-1.929011	-1.797467
44	8	0	7.339205	0.295528	2.010212
45	6	0	1.120080	2.463807	-0.643072
46	6	0	0.352983	3.082384	-1.632760
47	6	0	-0.915394	3.578012	-1.348157
48	6	0	-1.428293	3.462786	-0.055568
49	6	0	-0.641137	2.909273	0.954993
50	6	0	0.617894	2.400816	0.656039
51	8	0	-2.691146	3.911925	0.190833
52	1	0	1.620889	0.545937	-2.622539
53	1	0	7.453956	-1.422018	0.107860
54	1	0	5.096053	1.755204	1.853244
55	1	0	4.967404	-1.918560	-2.378660
56	1	0	7.117376	0.987371	2.643543
57	1	0	0.735955	3.157721	-2.647453
58	1	0	-1.523865	4.031116	-2.123722
59	1	0	-1.024127	2.864735	1.969931
60	1	0	1.215054	1.948706	1.439273
61	1	0	-3.094436	3.332629	0.861034

62	1	0	-4.332003	-3.240312	1.574106
63	1	0	1.435209	-0.155373	-1.013348
64	1	0	2.983998	2.389161	-1.720900

(1,2)-g''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.367360	2.394103	0.292791
2	6	0	-1.360505	1.846345	-0.517647
3	6	0	-1.196242	1.889915	-1.902802
4	6	0	-0.060688	2.459965	-2.467666
5	6	0	0.925911	3.001292	-1.644004
6	6	0	0.770040	2.974035	-0.258263
7	6	0	-2.589662	1.254341	0.120265
8	8	0	-3.117361	0.250711	-0.758284
9	6	0	-4.241678	-0.366312	-0.338963
10	6	0	-5.143532	0.271856	0.544721
11	6	0	-4.909341	1.635127	0.965410
12	6	0	-3.667816	2.293758	0.418549
13	6	0	-4.481677	-1.640907	-0.824815
14	6	0	-5.648039	-2.299111	-0.417711
15	6	0	-6.565810	-1.713622	0.455871
16	6	0	-6.315046	-0.434134	0.931847
17	8	0	-5.690092	2.249847	1.708958
18	8	0	-7.203971	0.133452	1.757184
19	8	0	-5.933750	-3.548380	-0.845092
20	8	0	2.025104	3.535528	-2.247803
21	8	0	-1.478914	-2.737101	-1.973471
22	6	0	-0.629589	-2.018314	-1.200591
23	6	0	-0.929755	-1.921266	0.151155
24	6	0	-0.096873	-1.170456	0.971924
25	6	0	1.107976	-0.581094	0.488268
26	6	0	1.332859	-0.656862	-0.907800
27	6	0	0.483860	-1.374184	-1.742459
28	8	0	2.378550	0.020214	-1.433636
29	6	0	1.973006	0.127389	1.447176
30	6	0	3.426018	0.272782	1.284427
31	6	0	4.199441	-0.636716	0.669010
32	6	0	5.660072	-0.641791	0.584551
33	6	0	6.470583	0.360828	1.145108
34	6	0	7.849719	0.316368	1.029502
35	6	0	8.458048	-0.741627	0.344760
36	6	0	7.675509	-1.749450	-0.220210
37	6	0	6.292200	-1.691425	-0.095566
38	8	0	-0.476624	-1.024501	2.251464
39	8	0	9.813051	-0.731204	0.264225
40	8	0	1.480494	0.576290	2.504424
41	1	0	3.711288	-1.477306	0.179916
42	1	0	3.847388	1.101862	1.846013
43	1	0	-1.832480	-2.364622	0.553460
44	1	0	0.673874	-1.406341	-2.811629
45	1	0	0.126604	-0.350333	2.648797
46	1	0	-1.192654	-2.726702	-2.893417
47	1	0	6.022378	1.190506	1.682026
48	1	0	8.471036	1.091994	1.464157
49	1	0	8.142104	-2.573222	-0.752619
50	1	0	5.690150	-2.480000	-0.538348
51	1	0	10.129364	-1.500141	-0.222603
52	1	0	-2.304367	0.752115	1.055582
53	1	0	-3.939156	2.821291	-0.505287
54	1	0	-3.303717	3.035470	1.133081
55	1	0	-7.459351	-2.247248	0.755818
56	1	0	-3.749415	-2.113053	-1.471841
57	1	0	-6.876648	1.042310	1.958441
58	1	0	-5.245066	-3.868828	-1.438450
59	1	0	-0.461058	2.346925	1.374496
60	1	0	1.542570	3.379530	0.389233
61	1	0	0.073909	2.482816	-3.544155
62	1	0	-1.954175	1.457603	-2.547497
63	1	0	2.651455	3.844476	-1.584502
64	1	0	2.334288	-0.002949	-2.395445

(2,1)-g''

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.854644	-0.449114	-1.008825
2	6	0	-3.800363	0.175677	-0.114734
3	6	0	-4.004737	1.639847	-0.486942
4	6	0	-2.687322	2.367192	-0.548905
5	6	0	-0.299283	2.194220	-1.255963
6	6	0	0.752882	1.457826	-1.781383
7	6	0	0.561482	0.098840	-2.016185
8	6	0	-0.645971	-0.548496	-1.750584
9	6	0	-1.695210	0.201114	-1.237312
10	6	0	-1.552987	1.584185	-0.984918
11	8	0	-2.605029	3.576834	-0.285209
12	8	0	-0.115703	3.497773	-1.019948
13	8	0	1.635852	-0.582079	-2.499059
14	6	0	-5.069435	-0.630907	-0.150184
15	6	0	-5.657479	-1.068090	1.037649
16	6	0	-6.851074	-1.782045	1.026514
17	6	0	-7.466315	-2.076204	-0.189968
18	6	0	-6.887591	-1.649915	-1.388410
19	6	0	-5.699351	-0.928551	-1.360433
20	8	0	-8.628139	-2.784379	-0.149116
21	1	0	-3.371580	0.128911	0.891201
22	1	0	-4.478432	1.719959	-1.474162
23	1	0	-4.659358	2.124463	0.240376
24	1	0	1.706799	1.929377	-1.982696
25	1	0	-0.772545	-1.612743	-1.914266
26	1	0	-0.965054	3.852904	-0.664629
27	1	0	1.428118	-1.515113	-2.626724
28	1	0	-5.179969	-0.849173	1.989022
29	1	0	-7.307503	-2.121528	1.950118
30	1	0	-7.362833	-1.880258	-2.337893
31	1	0	-5.254669	-0.605116	-2.297067
32	1	0	-8.959014	-2.940760	-1.040046
33	8	0	3.897885	0.594062	-1.295951
34	6	0	2.224953	-0.236155	1.097719
35	6	0	2.399407	-1.432528	0.508581
36	6	0	3.711205	-2.029343	0.199721
37	6	0	6.170300	-1.758426	0.411796
38	6	0	7.330658	-0.994725	0.402551
39	6	0	7.290284	0.287859	-0.135965
40	6	0	6.119264	0.802560	-0.694321
41	6	0	4.957058	0.041505	-0.667849
42	6	0	4.924777	-1.233847	-0.048458
43	8	0	3.787204	-3.272243	0.266654
44	8	0	6.262082	-3.003044	0.906502
45	8	0	8.445291	0.991713	-0.130866
46	6	0	0.957775	0.277144	1.621965
47	6	0	0.804628	1.654247	1.828430
48	6	0	-0.391575	2.187960	2.290730
49	6	0	-1.455822	1.333648	2.582071
50	6	0	-1.307363	-0.048239	2.432849
51	6	0	-0.118275	-0.563935	1.945482
52	8	0	-2.666161	1.782435	3.006183
53	1	0	3.083397	0.422497	1.217055
54	1	0	1.567598	-2.119528	0.375841
55	1	0	8.255484	-1.407219	0.786756
56	1	0	6.103021	1.768179	-1.188269
57	1	0	5.404015	-3.450419	0.729847
58	1	0	8.315922	1.857766	-0.533145
59	1	0	1.625678	2.325234	1.593158
60	1	0	-0.500554	3.261840	2.410824
61	1	0	-2.128255	-0.705219	2.701092
62	1	0	-0.020982	-1.639407	1.839392
63	1	0	-2.672214	2.744763	3.057385
64	1	0	3.186709	-0.039580	-1.487363