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Supporting Information

For

MOF Encapsulation of Ru Olefin Metathesis Catalysts to Block Catalyst Decomposition

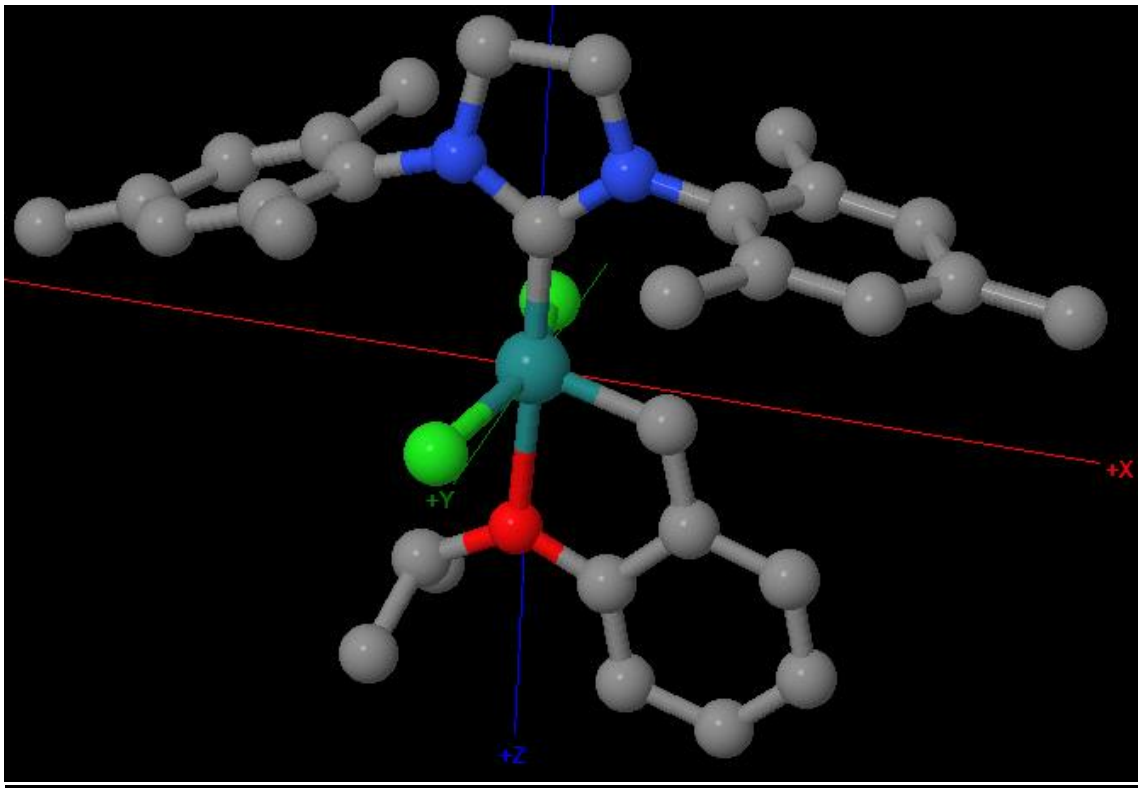
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[2] Institut de Química Computacional i Catàlisi, Departament de Química, Universitat de Girona, c/ Mª Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain; albert.poater@udg.edu

Steric maps

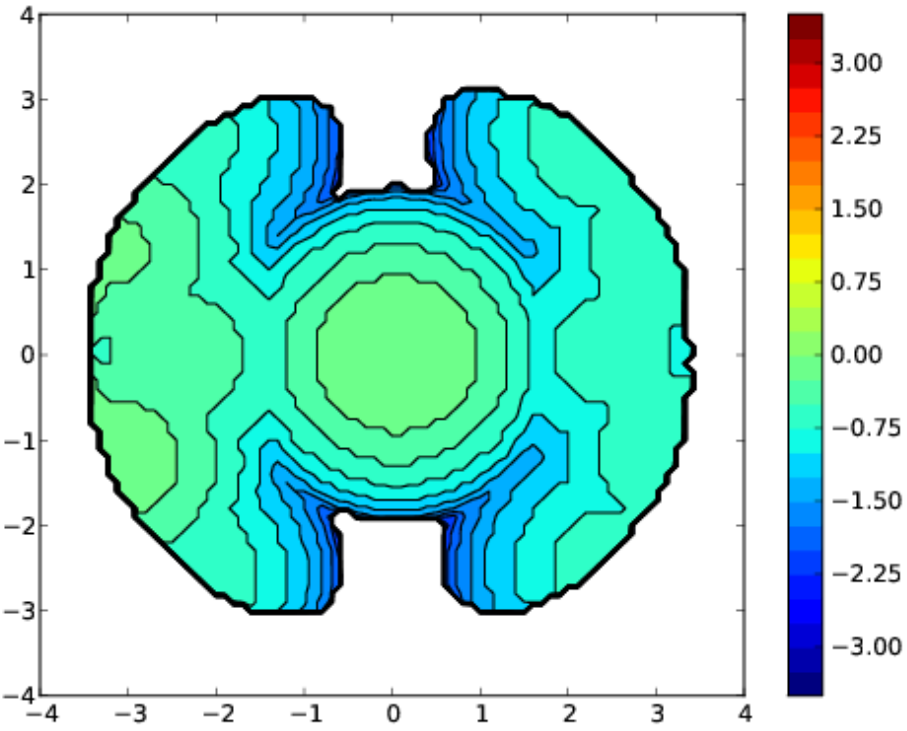
HOV



At 3.5 Å:

%V Free	%V Buried	% V Tot/V Ex
66.9	33.1	99.9

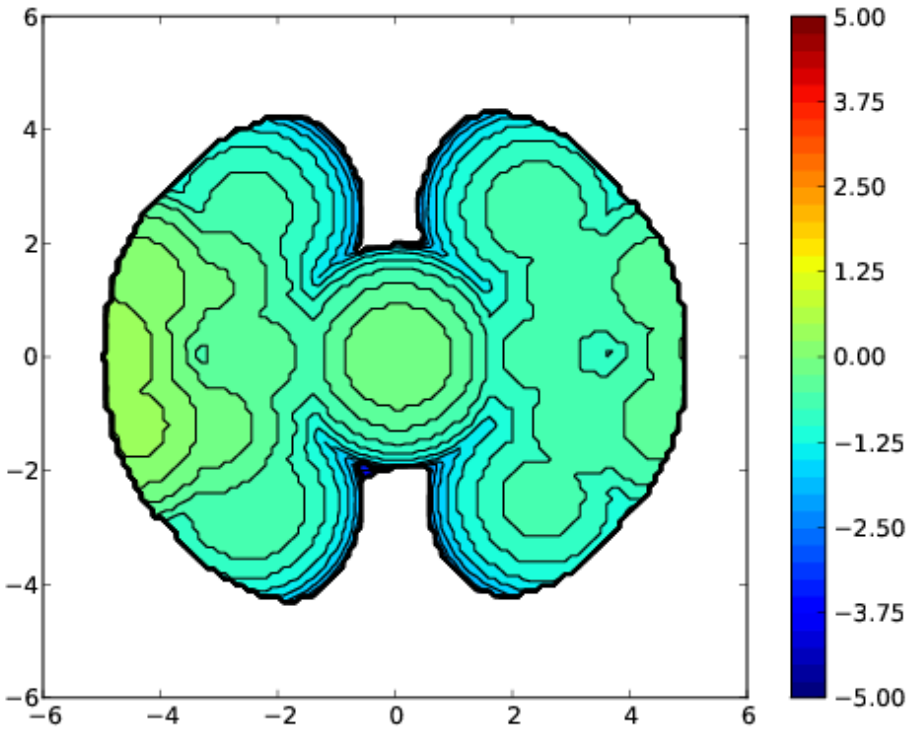
Quadrant	V f	V b	V t	%V f	%V b
SW	29.4	15.5	44.9	65.4	34.6
NW	29.7	15.2	44.9	66.2	33.8
NE	30.2	14.7	44.9	67.3	32.7
SE	30.8	14.0	44.9	68.7	31.3



At 5.0 Å:

%V Free	%V Buried	% V Tot/V Ex
64.6	35.4	99.9

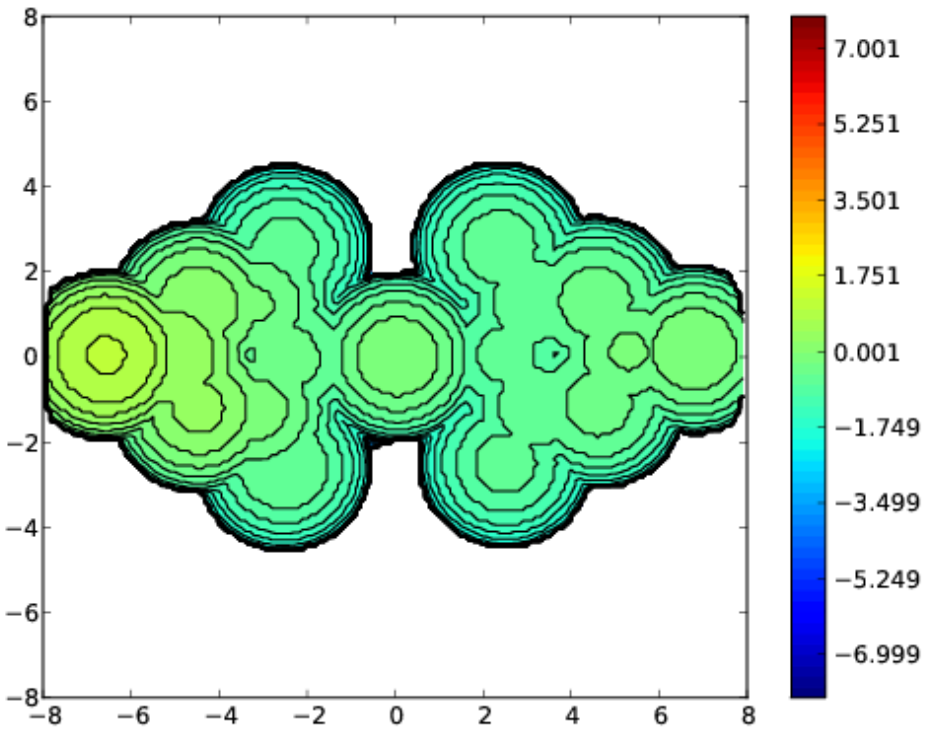
Quadrant	V f	V b	V t	%V f	%V b
SW	82.1	48.7	130.8	62.8	37.2
NW	83.6	47.2	130.8	63.9	36.1
NE	85.1	45.7	130.8	65.1	34.9
SE	87.4	43.5	130.8	66.8	33.2



At 8.0 Å:

%V Free	%V Buried	% V Tot/V Ex
83.4	16.6	100.0

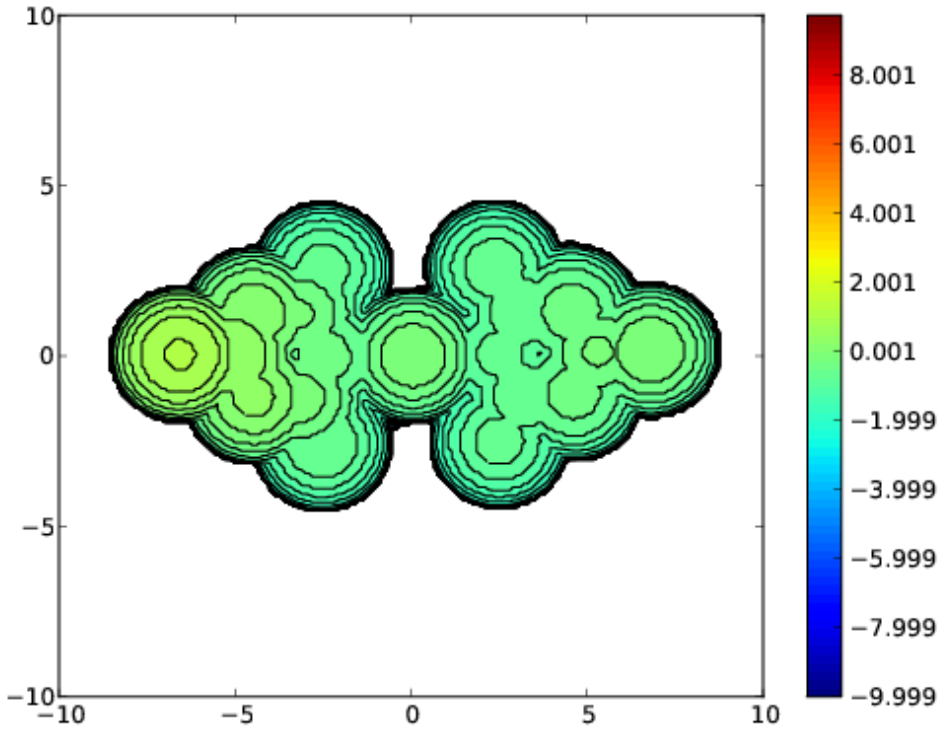
Quadrant	V f	V b	V t	%V f	%V b
SW	445.2	90.7	535.9	83.1	16.9
NW	446.4	89.5	535.9	83.3	16.7
NE	445.2	90.7	535.9	83.1	16.9
SE	451.3	84.7	535.9	84.2	15.8



At 10.0 Å:

%V Free	%V Buried	% V Tot/V Ex
91.3	8.7	100.0

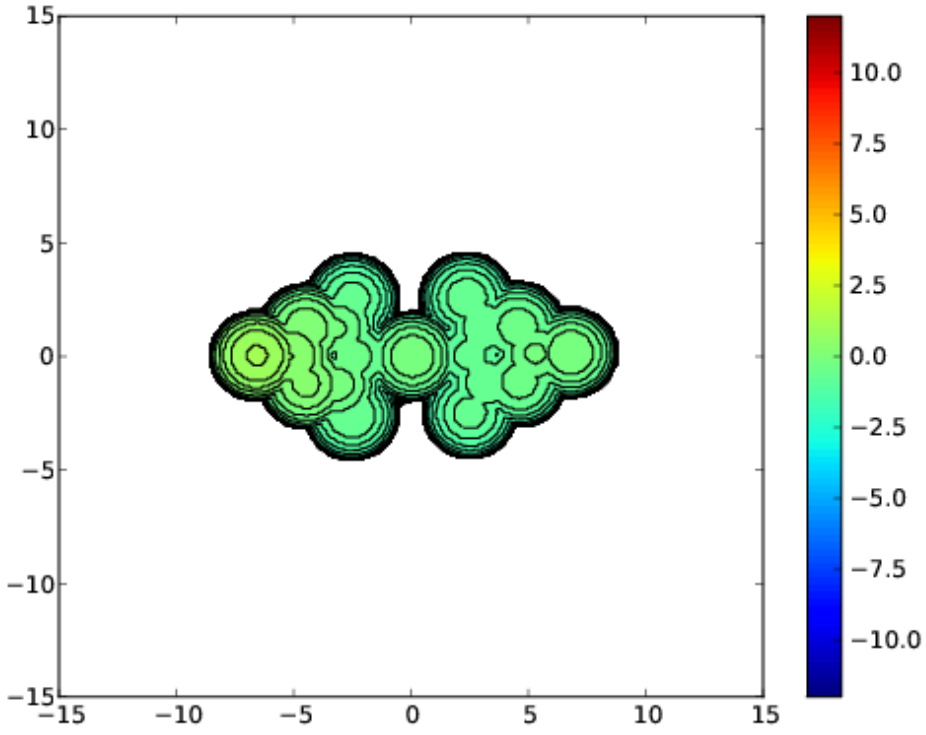
Quadrant	V f	V b	V t	%V f	%V b
SW	954.7	92.5	1047.2	91.2	8.8
NW	953.3	90.7	1044.0	91.3	8.7
NE	946.6	94.3	1040.9	90.9	9.1
SE	956.3	87.7	1044.0	91.6	8.4



At 12.0 Å:

%V Free	%V Buried	% V Tot/V Ex
95.0	5.0	100.0

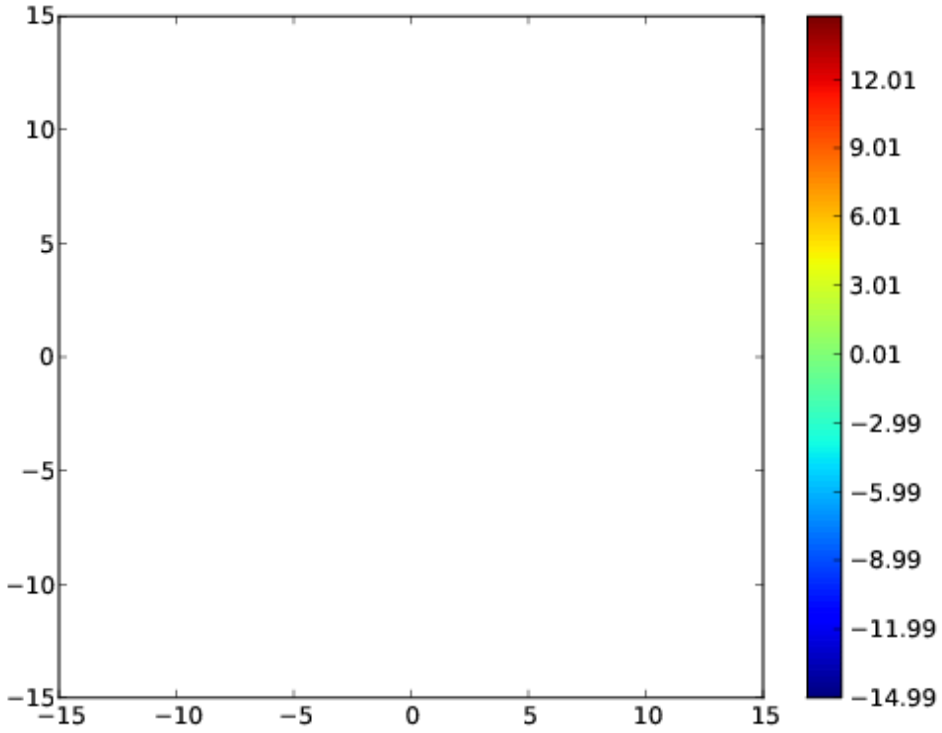
Quadrant	V f	V b	V t	%V f	%V b
SW	1717.1	92.0	1809.1	94.9	5.1
NW	1718.2	91.0	1809.1	95.0	5.0
NE	1714.4	94.7	1809.1	94.8	5.2
SE	1721.6	87.5	1809.1	95.2	4.8



At 15.0 Å:

%V Free	%V Buried	% V Tot/V Ex
100.0	0.0	100.0

Quadrant	V f	V b	V t	%V f	%V b
SW	3534.2	0.0	3534.2	100.0	0.0
NW	3527.1	0.0	3527.1	100.0	0.0
NE	3520.1	0.0	3520.1	100.0	0.0
SE	3527.1	0.0	3527.1	100.0	0.0

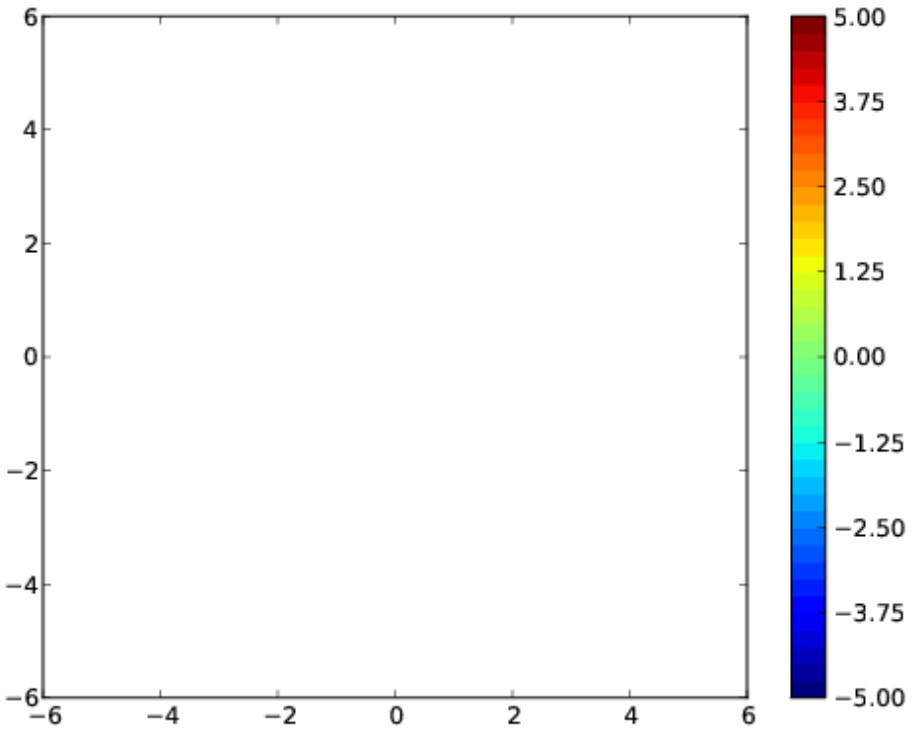


MOF without the Ru catalyst:

At 3.5 and 5.0 Å:

%V Free	%V Buried	% V Tot/V Ex
100.0	0.0	99.9

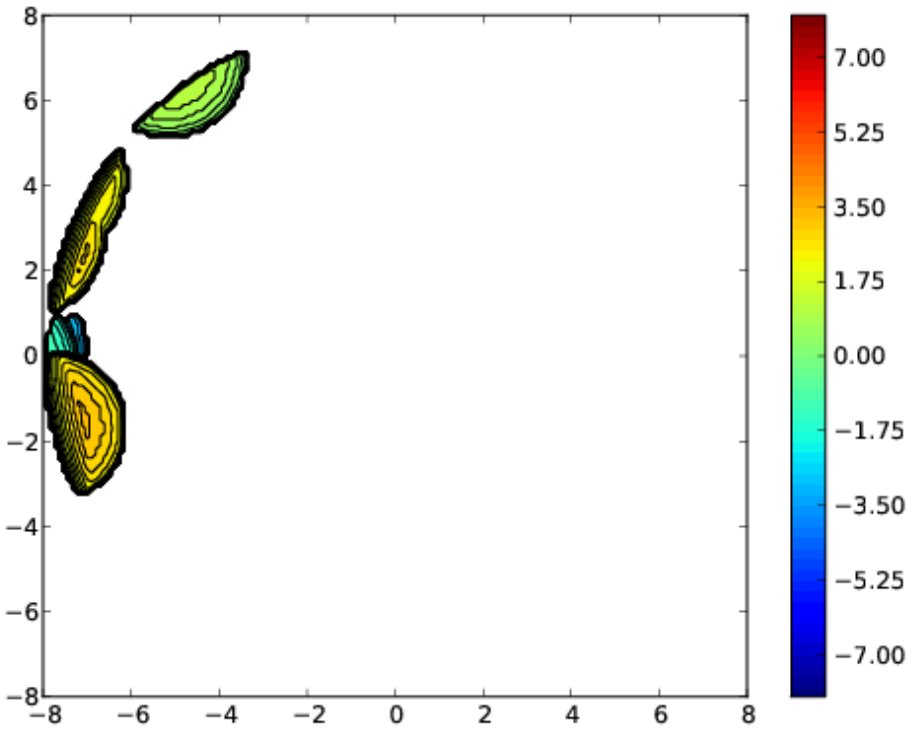
Quadrant	V f	V b	V t	%V f	%V b
SW	130.8	0.0	130.8	100.0	0.0
NW	130.8	0.0	130.8	100.0	0.0
NE	130.8	0.0	130.8	100.0	0.0
SE	130.8	0.0	130.8	100.0	0.0



At 8.0 Å:

%V Free	%V Buried	% V Tot/V Ex
99.1	0.9	100.0

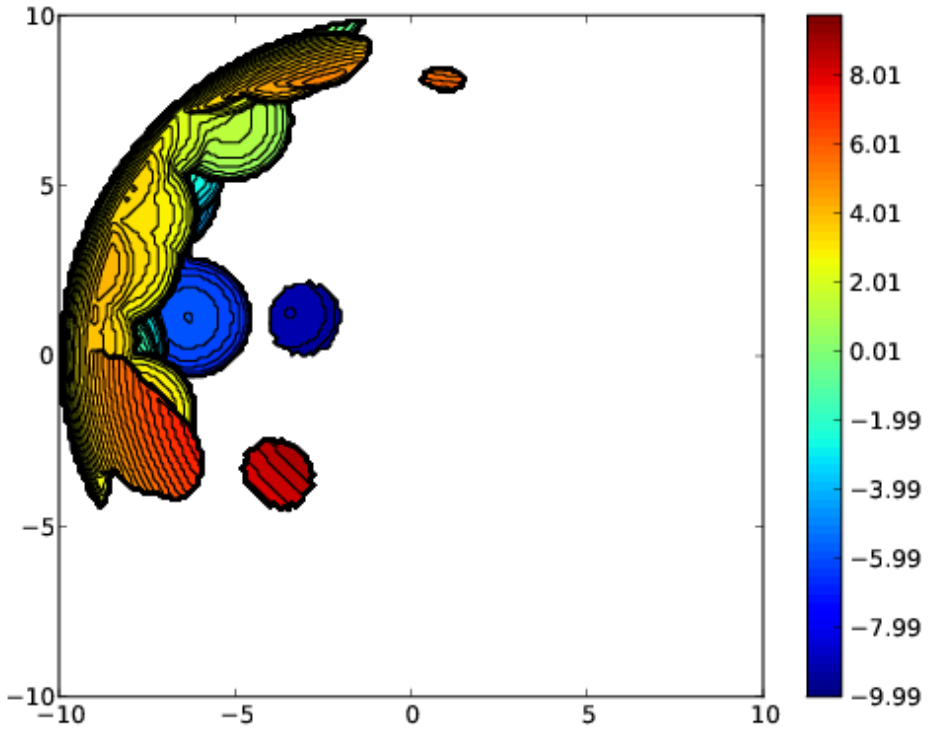
Quadrant	V f	V b	V t	%V f	%V b
SW	526.8	9.1	535.9	98.3	1.7
NW	525.2	10.7	535.9	98.0	2.0
NE	535.9	0.0	535.9	100.0	0.0
SE	535.9	0.0	535.9	100.0	0.0



At 10.0 Å:

%V Free	%V Buried	% V Tot/V Ex
95.0	5.0	100.0

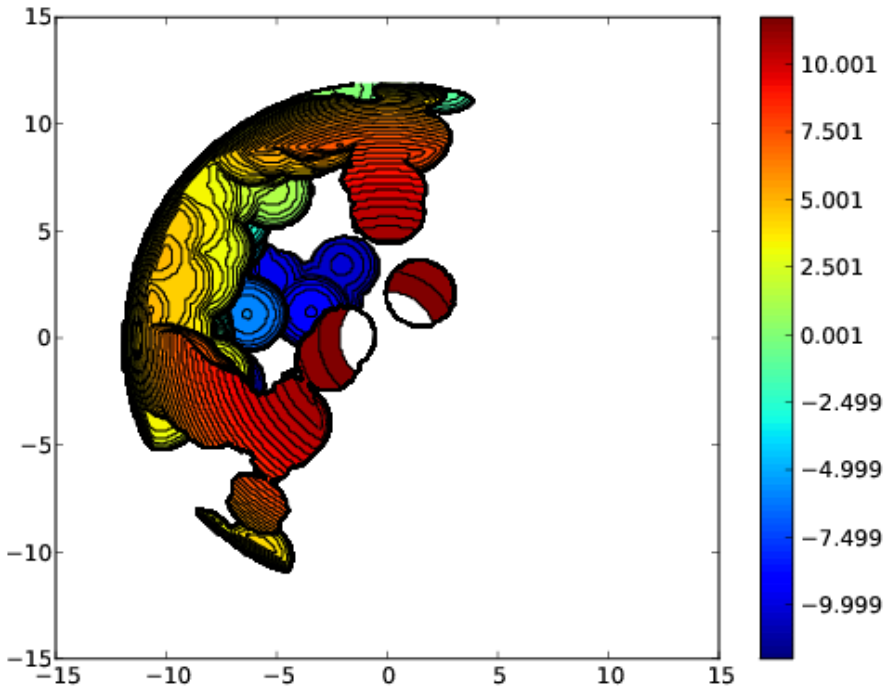
Quadrant	V f	V b	V t	%V f	%V b
SW	982.7	64.5	1047.2	93.8	6.2
NW	901.9	142.1	1044.0	86.4	13.6
NE	1040.8	0.1	1040.9	100.0	0.0
SE	1044.0	0.0	1044.0	100.0	0.0



At 12.0 Å:

%V Free	%V Buried	% V Tot/V Ex
89.8	**10.2**	100.0

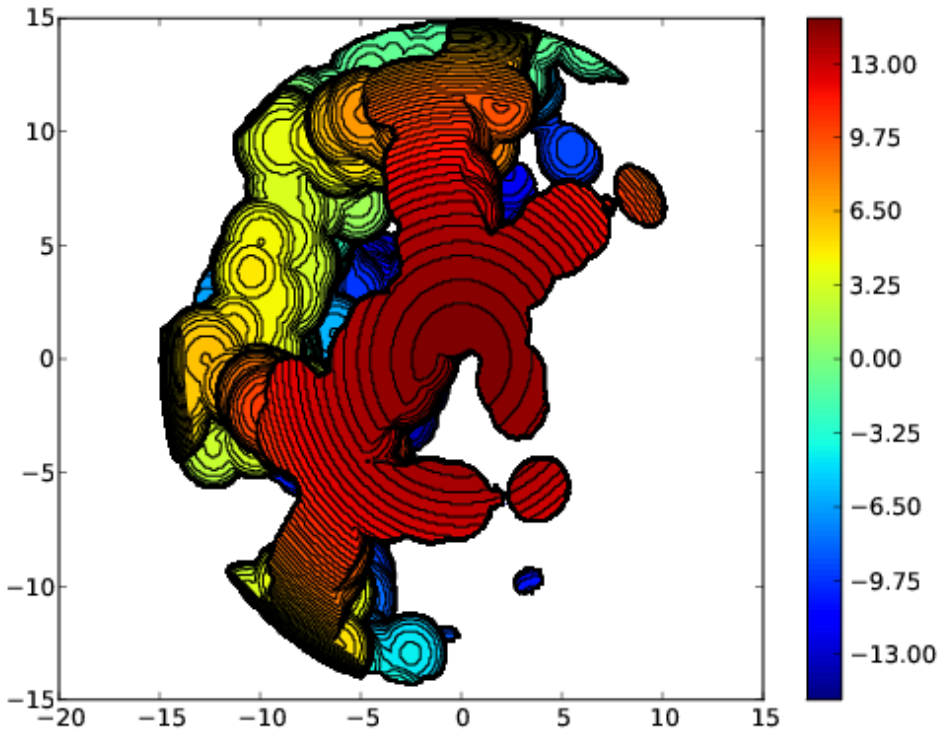
Quadrant	V f	V b	V t	%V f	%V b
SW	1578.4	230.8	1809.2	87.2	**12.8**
NW	1339.6	469.3	1808.9	74.1	**25.9**
NE	1774.2	34.4	1808.6	98.1	**1.9**
SE	1808.9	0.0	1808.9	100.0	**0.0**

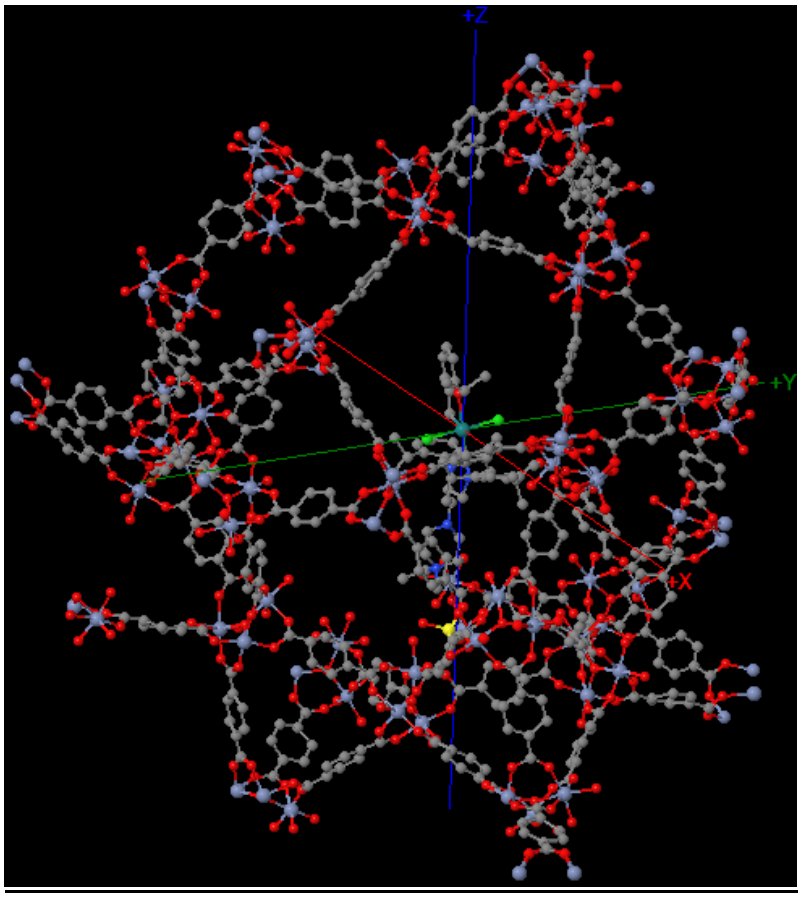


At 15.0 Å:

%V Free	%V Buried	% V Tot/V Ex
83.1	16.9	100.0

Quadrant	V f	V b	V t	%V f	%V b
SW	2638.6	895.7	3534.3	74.7	25.3
NW	2386.8	1147.5	3534.3	67.5	32.5
NE	3202.7	331.6	3534.3	90.6	9.4
SE	3519.3	15.0	3534.3	99.6	0.4

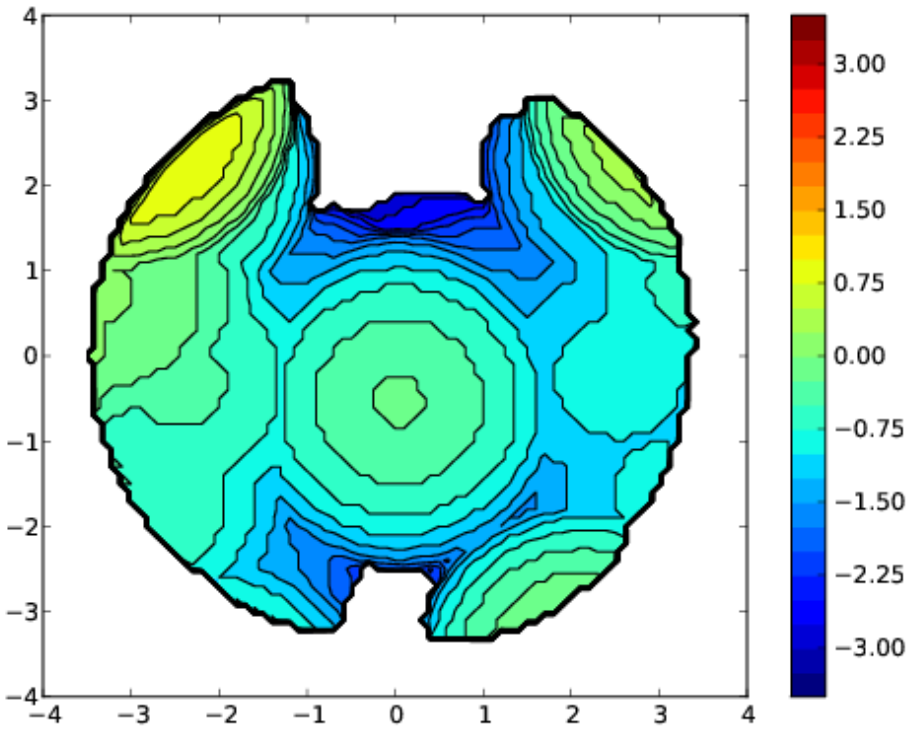



+Z
+Y
+X

At 3.5 Å:

%V Free	%V Buried	% V Tot/V Ex
67.1	32.9	99.9

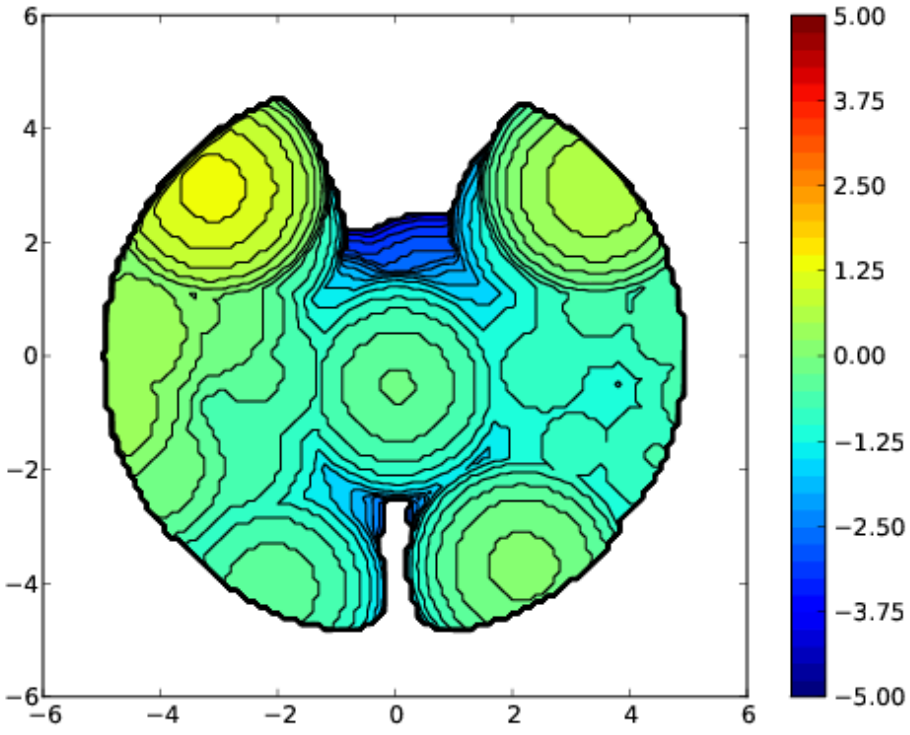
Quadrant	V f	V b	V t	%V f	%V b
SW	29.3	15.5	44.9	65.4	34.6
NW	28.3	16.6	44.9	63.1	36.9
NE	33.0	11.9	44.9	73.5	26.5
SE	29.8	15.1	44.9	66.4	33.6



At 5.0 Å:

%V Free	%V Buried	% V Tot/V Ex
60.4	39.6	99.9

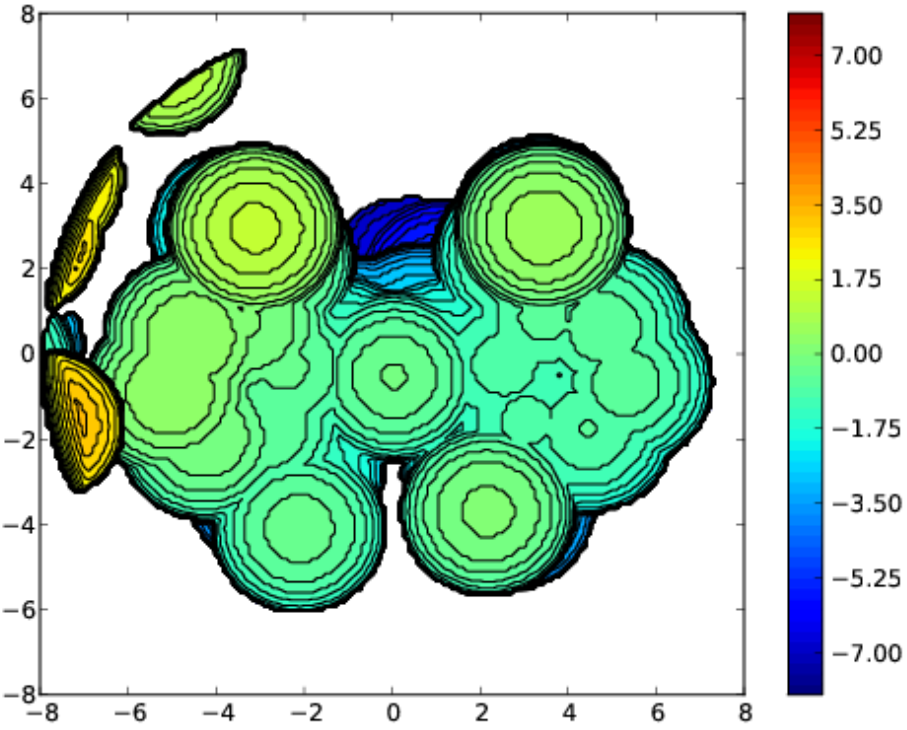
Quadrant	V f	V b	V t	%V f	%V b
SW	77.2	53.6	130.8	59.0	41.0
NW	74.6	56.2	130.8	57.0	43.0
NE	84.6	46.3	130.8	64.6	35.4
SE	79.9	50.9	130.8	61.1	38.9



At 8.0 Å:

%V Free	%V Buried	% V Tot/V Ex
75.2	24.8	100.0

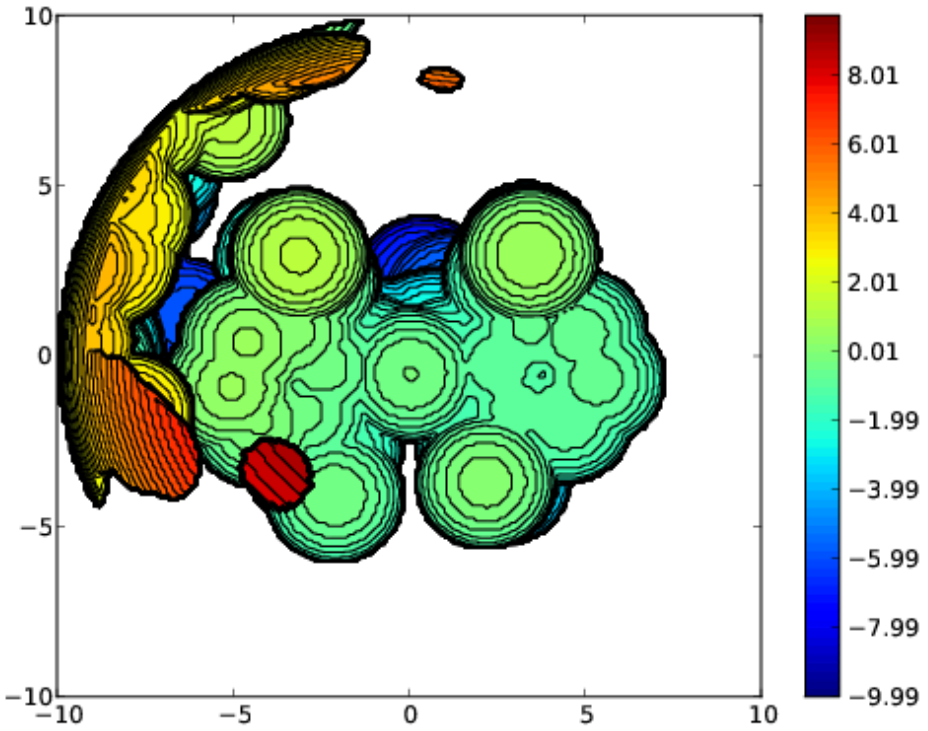
Quadrant	V f	V b	V t	%V f	%V b
SW	394.5	141.4	535.9	73.6	26.4
NW	414.1	121.8	535.9	77.3	22.7
NE	407.6	128.3	535.9	76.1	23.9
SE	395.8	140.1	535.9	73.9	26.1



At 10.0 Å:

%V Free	%V Buried	% V Tot/V Ex
81.6	18.4	100.0

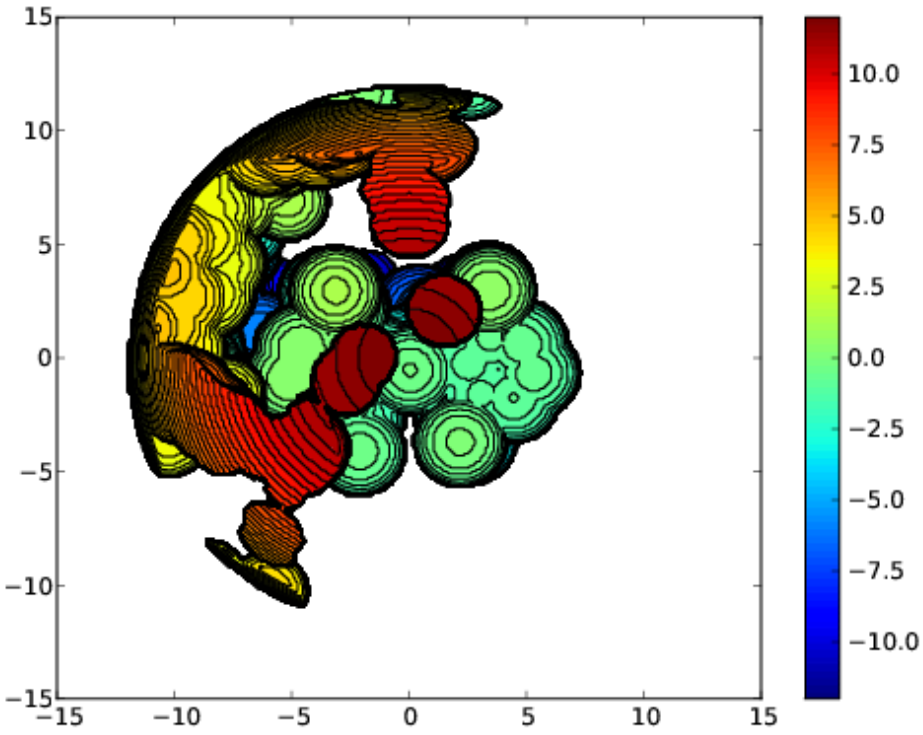
Quadrant	V f	V b	V t	%V f	%V b
SW	844.2	202.8	1046.9	80.6	19.4
NW	780.5	266.4	1046.9	74.6	25.4
NE	895.4	151.6	1046.9	85.5	14.5
SE	895.2	151.8	1046.9	85.5	14.5



At 12.0 Å:

%V Free	%V Buried	% V Tot/V Ex
81.4	18.6	100.0

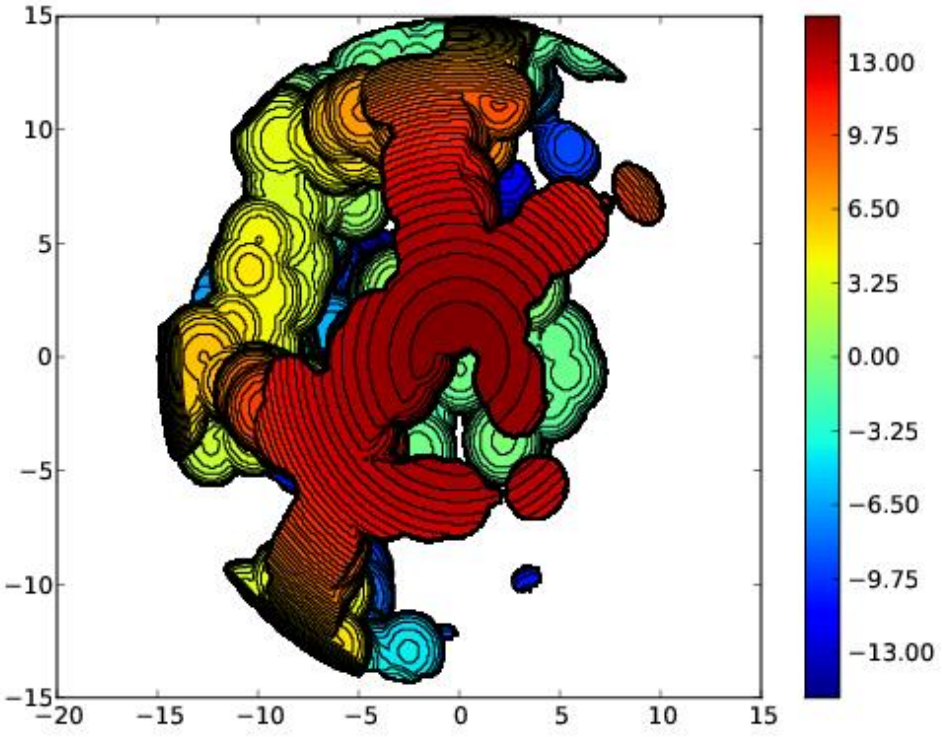
Quadrant	V f	V b	V t	%V f	%V b
SW	1439.1	370.3	1809.4	79.5	20.5
NW	1204.9	600.1	1805.0	66.8	33.2
NE	1583.8	216.7	1800.5	88.0	12.0
SE	1649.5	155.5	1805.0	91.4	8.6



At 15.0 Å:

%V Free	%V Buried	% V Tot/V Ex
78.7	21.3	100.0

Quadrant	V f	V b	V t	%V f	%V b
SW	2499.1	1035.3	3534.3	70.7	29.3
NW	2252.7	1281.6	3534.3	63.7	36.3
NE	3011.0	523.3	3534.3	85.2	14.8
SE	3364.1	170.2	3534.3	95.2	4.8

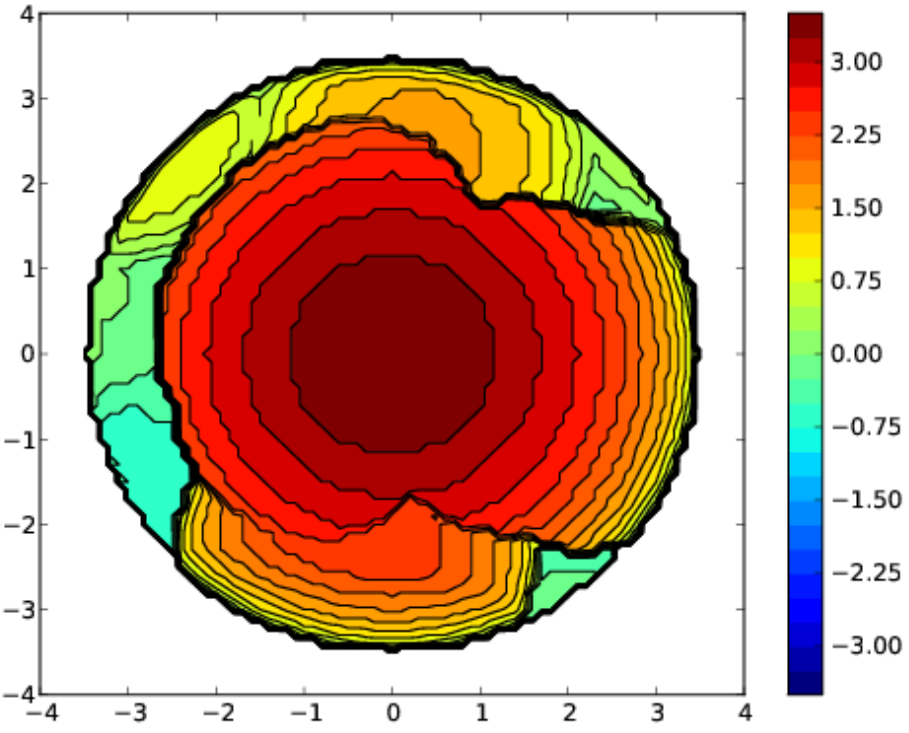


Including all the ruthenium catalyst and the MOF as well:

At 3.5 Å:

%V Free	%V Buried	% V Tot/V Ex
8.9	**91.1**	99.9

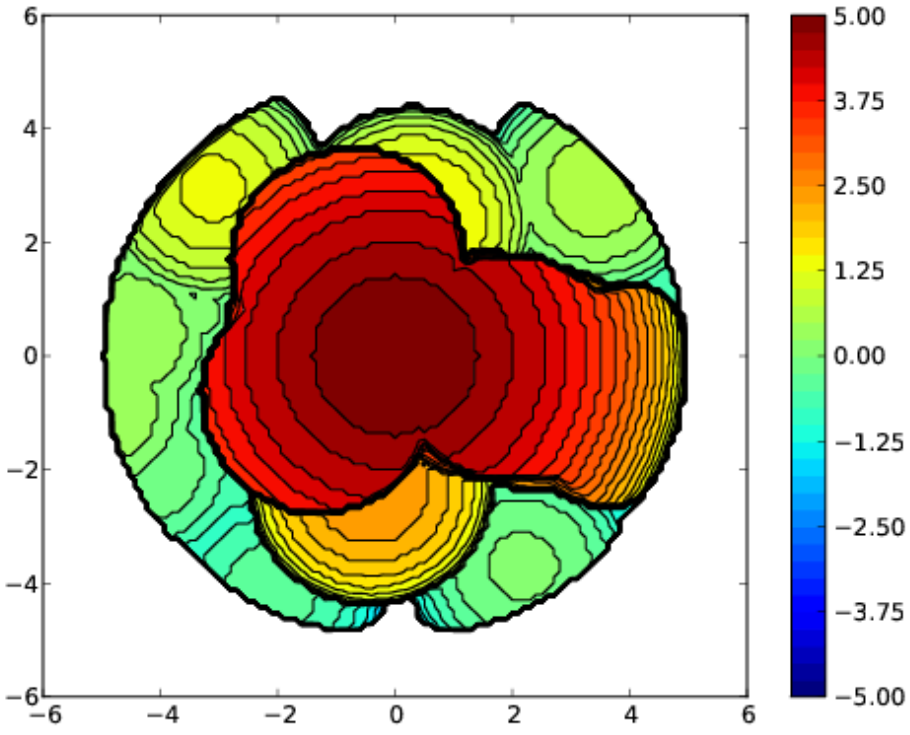
Quadrant	V f	V b	V t	%V f	%V b
SW	5.4	39.5	44.9	**11.9**	88.1
NW	5.7	39.2	44.9	**12.7**	87.3
NE	3.1	41.8	44.9	**6.9**	93.1
SE	1.9	43.0	44.9	**4.2**	95.8



At 5.0 Å:

%V Free	%V Buried	% V Tot/V Ex
25.4	74.6	99.9

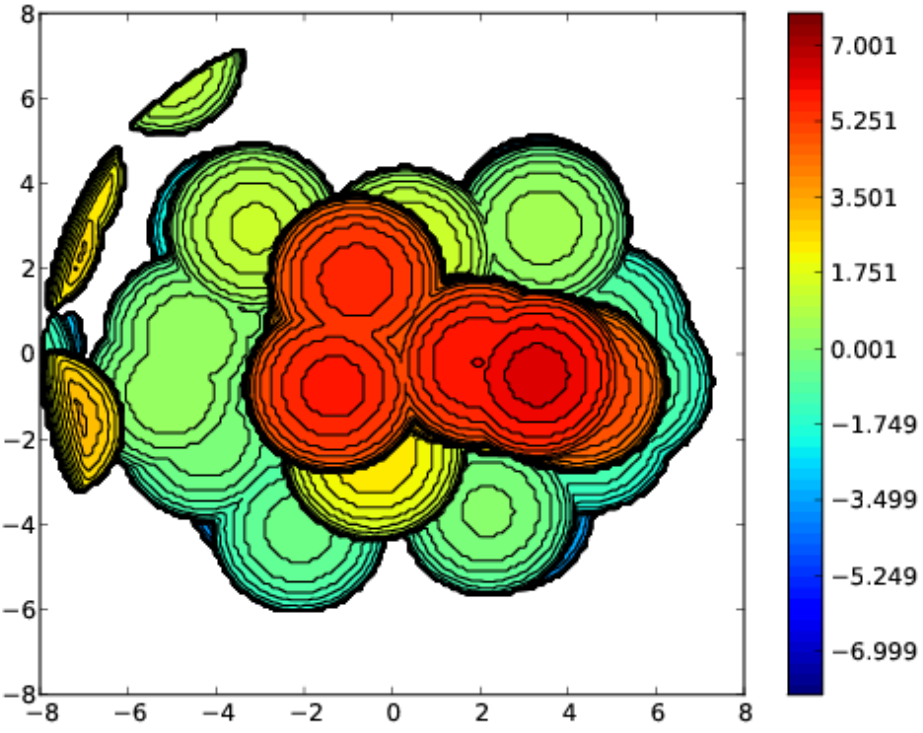
Quadrant	V f	V b	V t	%V f	%V b
SW	36.0	94.9	130.8	27.5	72.5
NW	35.1	95.7	130.8	26.8	73.2
NE	33.9	96.9	130.8	25.9	74.1
SE	28.1	102.8	130.8	21.4	78.6



At 8.0 Å:

%V Free	%V Buried	% V Tot/V Ex
63.7	36.3	100.0

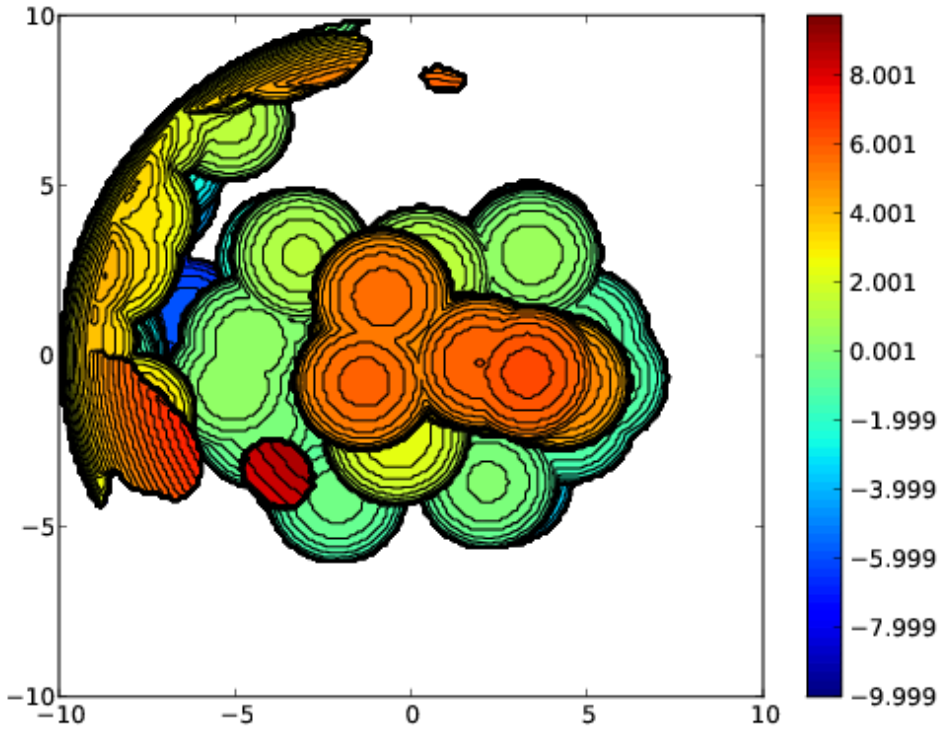
Quadrant	V f	V b	V t	%V f	%V b
SW	345.2	190.7	535.9	64.4	35.6
NW	365.3	170.5	535.8	68.2	31.8
NE	342.1	193.5	535.6	63.9	36.1
SE	312.1	223.7	535.8	58.3	41.7



At 10.0 Å:

%V Free	%V Buried	% V Tot/V Ex
75.7	24.3	100.0

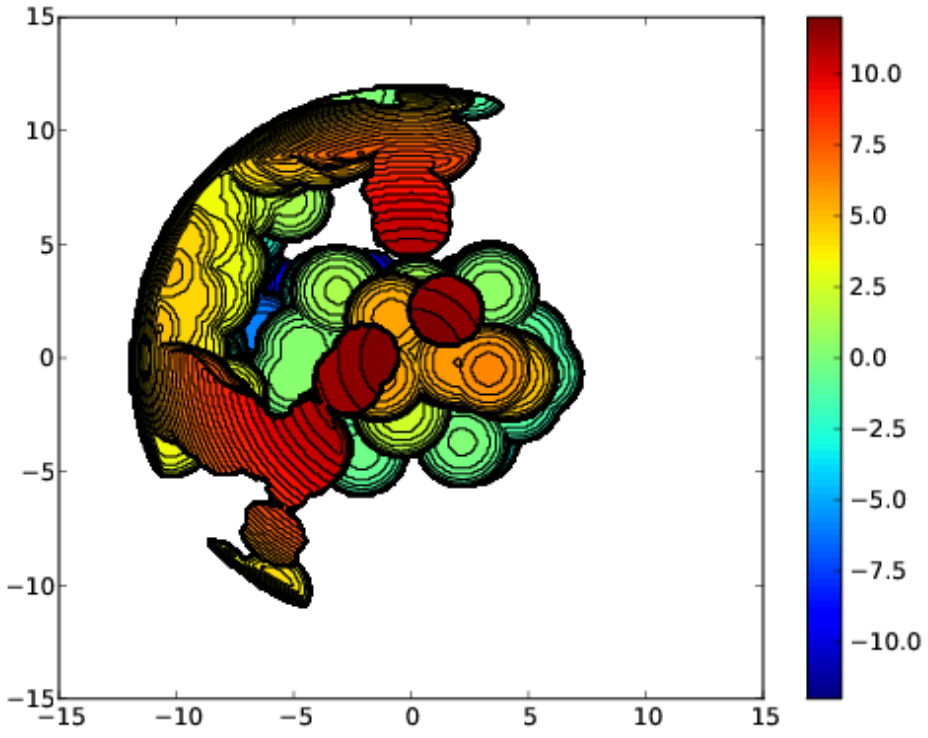
Quadrant	V f	V b	V t	%V f	%V b
SW	794.9	252.0	1046.9	75.9	24.1
NW	731.8	315.2	1046.9	69.9	30.1
NE	830.1	216.8	1046.9	79.3	20.7
SE	811.6	235.4	1046.9	77.5	22.5



At 12.0 Å:

%V Free	%V Buried	% V Tot/V Ex
78.0	22.0	100.0

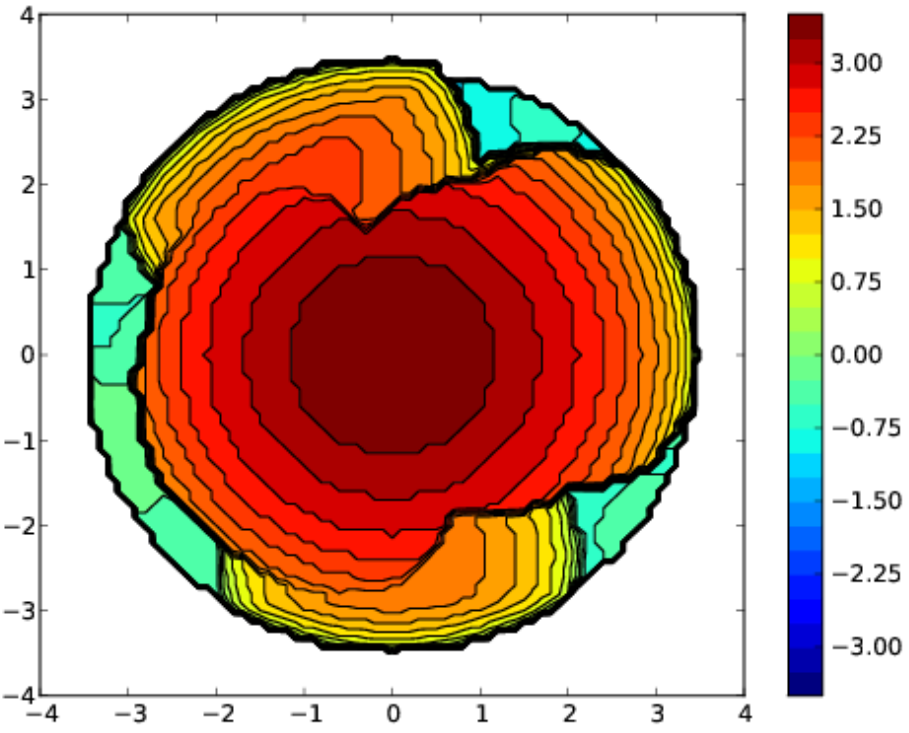
Quadrant	V f	V b	V t	%V f	%V b
SW	1389.5	419.6	1809.1	76.8	23.2
NW	1157.7	651.4	1809.1	64.0	36.0
NE	1525.7	283.5	1809.1	84.3	15.7
SE	1570.3	238.8	1809.1	86.8	13.2



AquaMet^{TM} including all atoms:

%V Free	%V Buried	% V Tot/V Ex
9.7	90.3	99.9

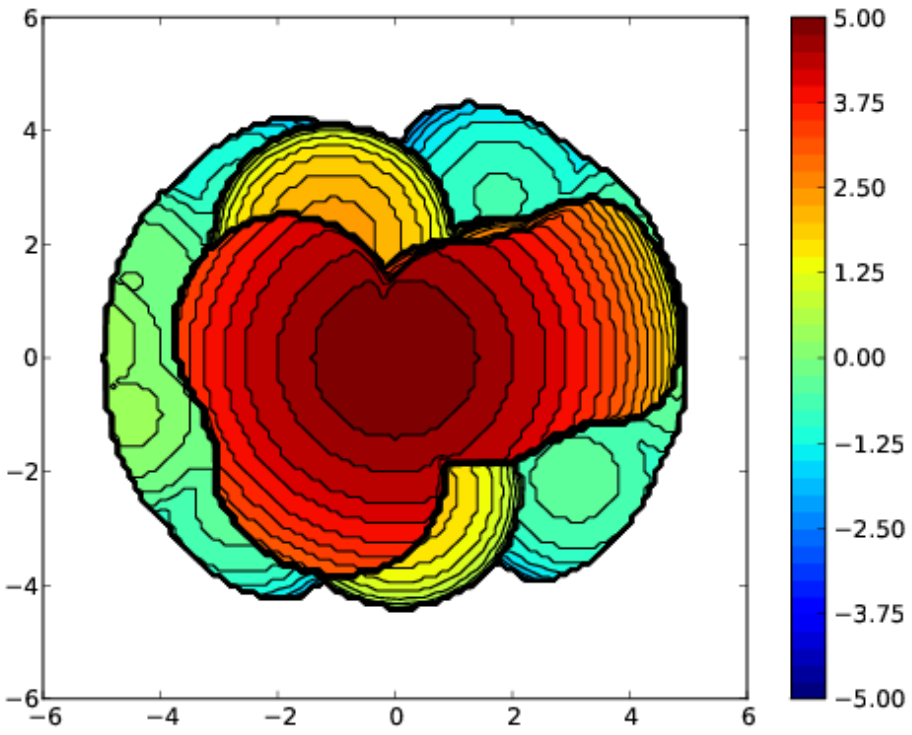
Quadrant	V f	V b	V t	%V f	%V b
SW	5.3	39.5	44.9	11.9	88.1
NW	3.6	41.3	44.9	7.9	92.1
NE	4.2	40.7	44.9	9.3	90.7
SE	4.3	40.5	44.9	9.7	90.3



At 5.0 Å:

%V Free	%V Buried	% V Tot/V Ex
30.0	70.0	99.9

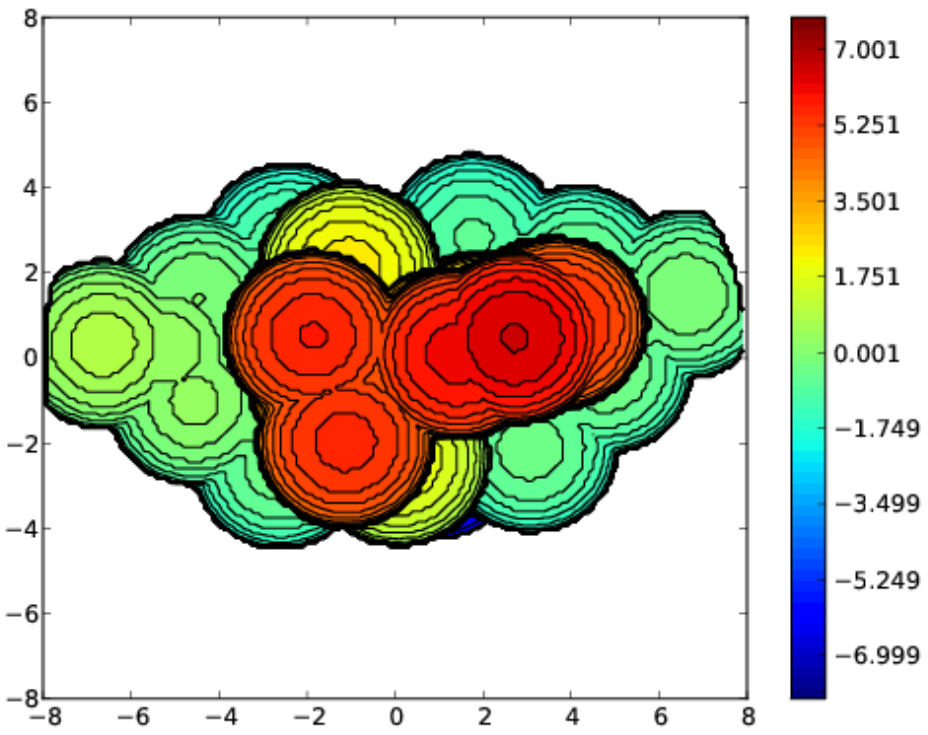
Quadrant	V f	V b	V t	%V f	%V b
SW	37.6	93.2	130.8	28.7	71.3
NW	39.1	91.8	130.8	29.9	70.1
NE	35.5	95.3	130.8	27.2	72.8
SE	44.6	86.2	130.8	34.1	65.9



At 8.0 Å:

%V Free	%V Buried	% V Tot/V Ex
70.1	29.9	100.0

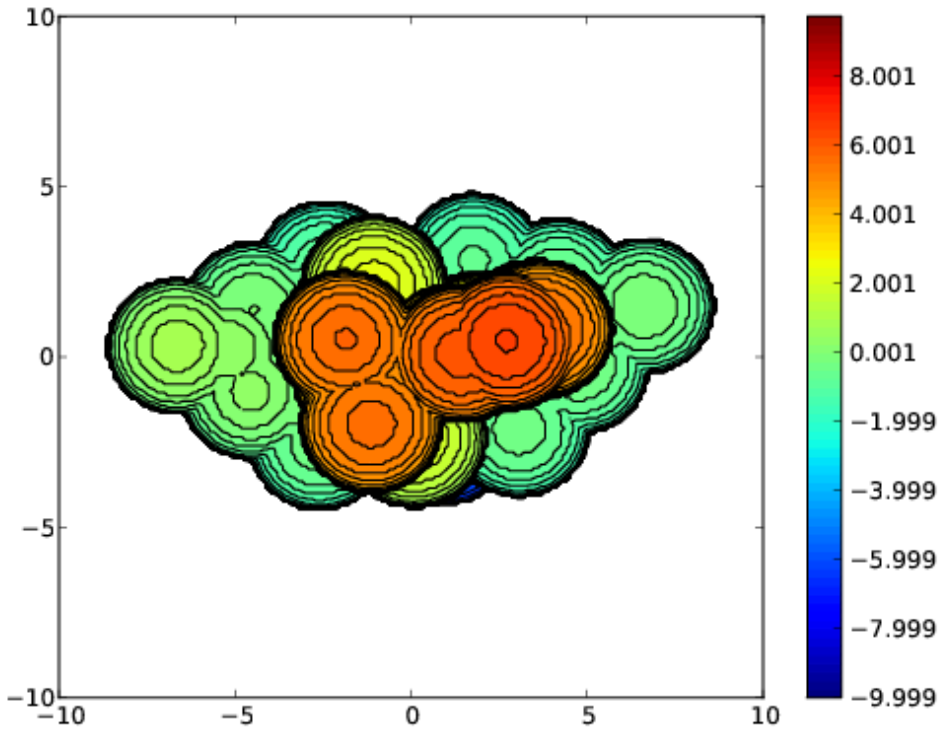
Quadrant	V f	V b	V t	%V f	%V b
SW	386.2	149.7	535.9	72.1	27.9
NW	388.6	147.2	535.8	72.5	27.5
NE	345.2	190.4	535.6	64.4	35.6
SE	381.6	154.2	535.8	71.2	28.8



At 10.0 Å:

%V Free	%V Buried	% V Tot/V Ex
83.2	**16.8**	100.0

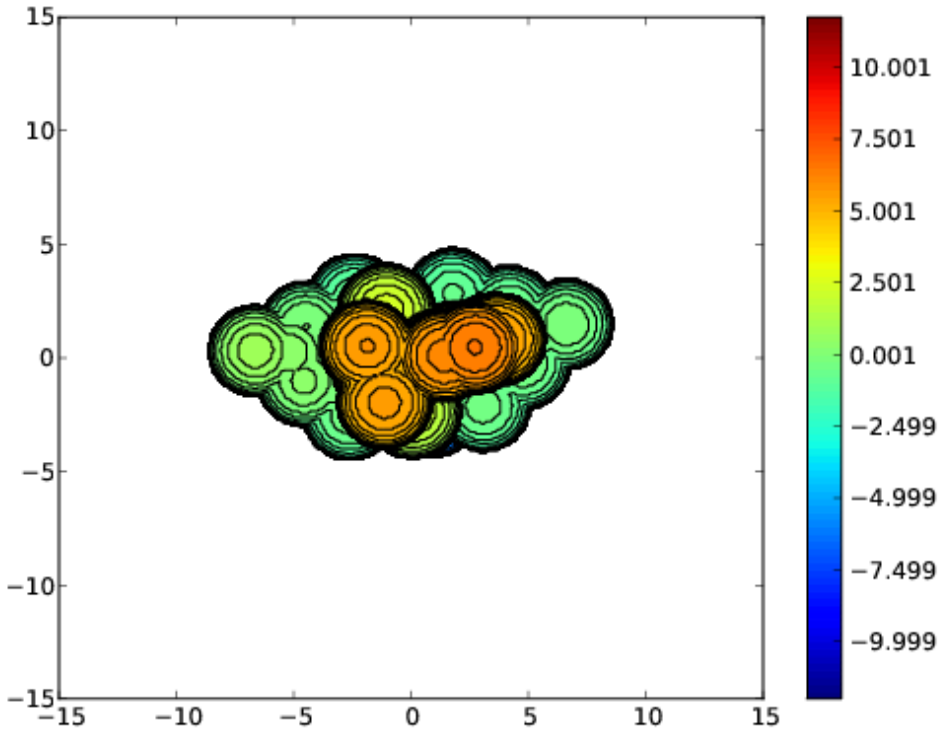
Quadrant	V f	V b	V t	%V f	%V b
SW	883.7	163.3	1047.0	84.4	**15.6**
NW	893.8	153.0	1046.8	85.4	**14.6**
NE	838.6	207.9	1046.5	80.1	**19.9**
SE	867.0	179.7	1046.8	82.8	**17.2**



At 12.0 Å:

%V Free	%V Buried	% V Tot/V Ex
89.6	**10.4**	100.0

Quadrant	V f	V b	V t	%V f	%V b
SW	1633.9	175.3	1809.2	90.3	**9.7**
NW	1653.6	155.3	1808.9	91.4	**8.6**
NE	1591.8	216.8	1808.6	88.0	**12.0**
SE	1601.5	207.4	1808.9	88.5	**11.5**

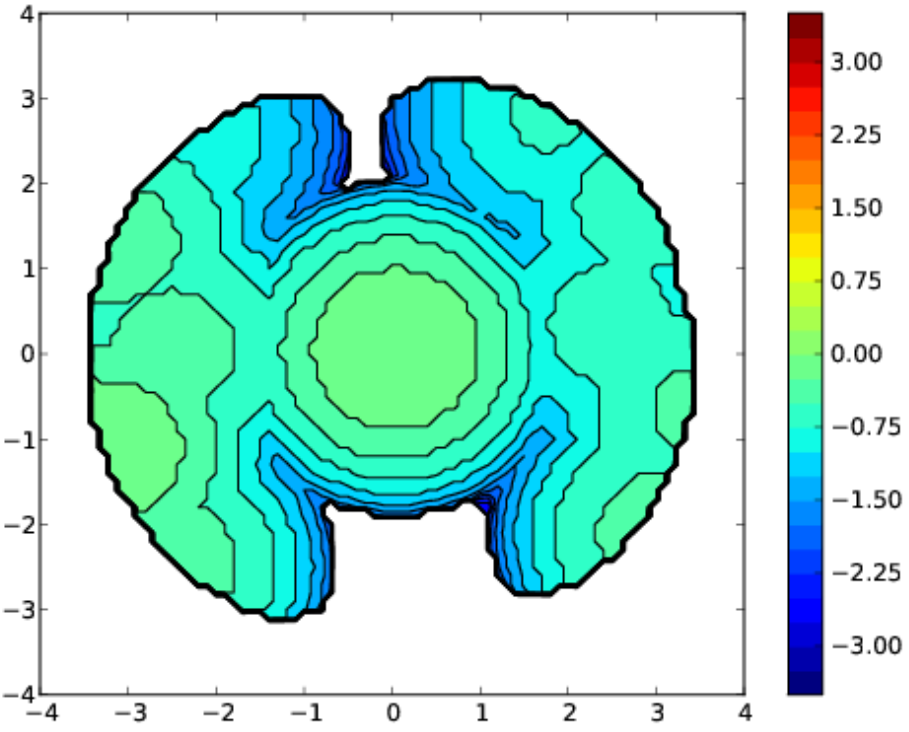


AquaMet™

At 3.5 Å:

%V Free	%V Buried	% V Tot/V Ex
66.7	33.3	99.9

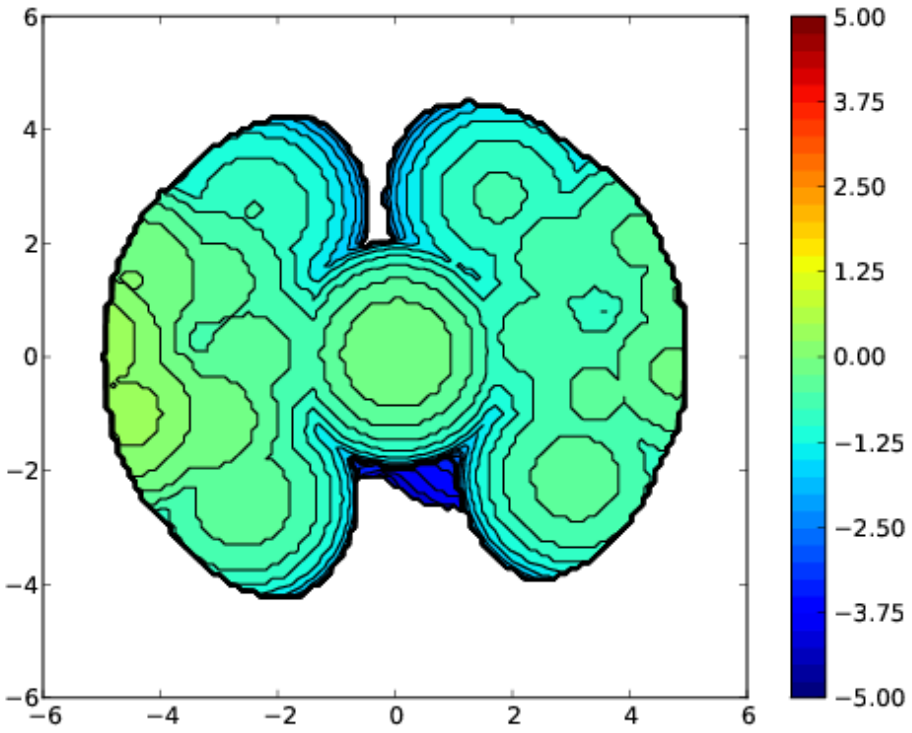
Quadrant	V f	V b	V t	%V f	%V b
SW	29.2	15.7	44.9	65.0	35.0
NW	29.9	15.0	44.9	66.6	33.4
NE	29.2	15.6	44.9	65.2	34.8
SE	31.4	13.4	44.9	70.0	30.0



At 5.0 Å:

%V Free	%V Buried	% V Tot/V Ex
64.4	35.6	99.9

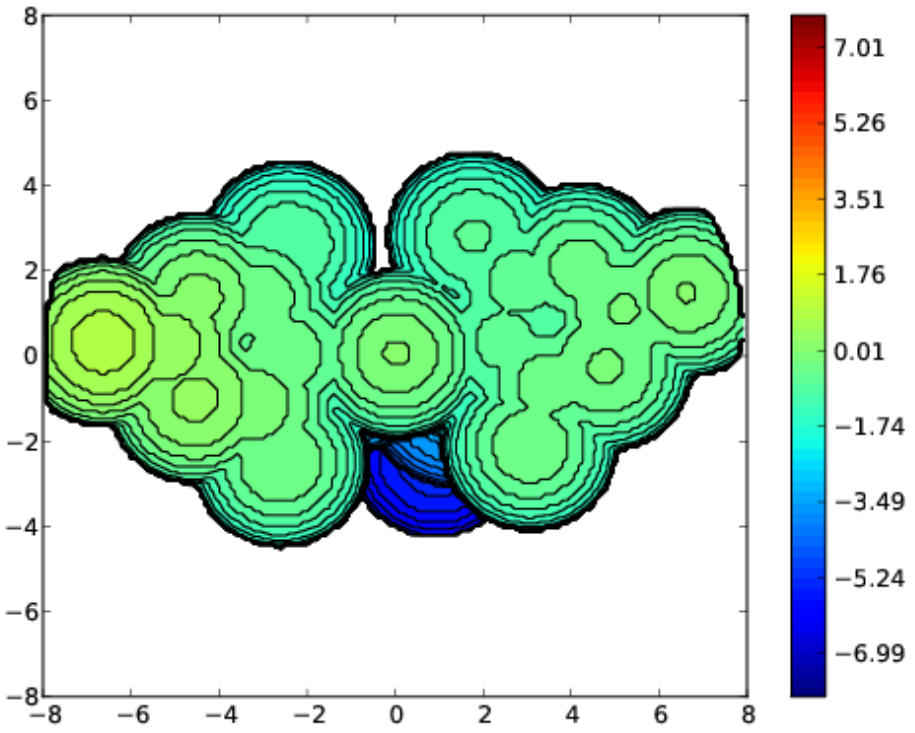
Quadrant	V f	V b	V t	%V f	%V b
SW	82.2	48.6	130.8	62.9	37.1
NW	83.9	46.9	130.8	64.2	35.8
NE	81.4	49.5	130.8	62.2	37.8
SE	89.5	41.4	130.8	68.4	31.6



At 8.0 Å:

%V Free	%V Buried	% V Tot/V Ex
81.3	**18.7**	100.0

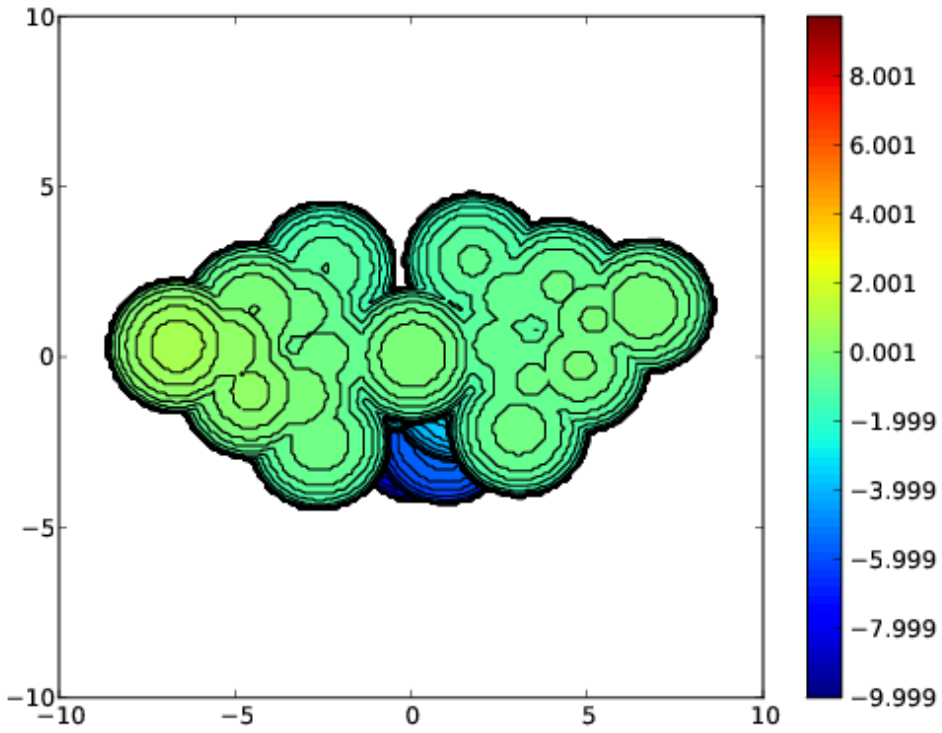
Quadrant	V f	V b	V t	%V f	%V b
SW	443.1	93.0	536.1	82.7	**17.3**
NW	439.9	94.2	534.1	82.4	**17.6**
NE	416.9	115.3	532.2	78.3	**21.7**
SE	437.3	96.8	534.1	81.9	**18.1**



At 10.0 Å:

%V Free	%V Buried	% V Tot/V Ex
89.0	**11.0**	100.0

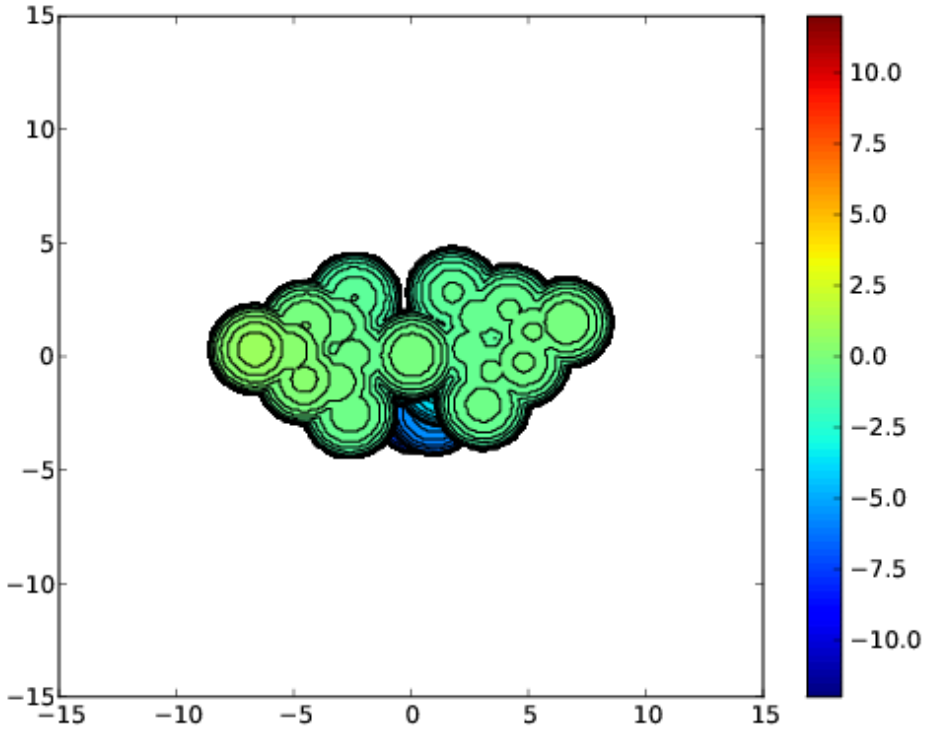
Quadrant	V f	V b	V t	%V f	%V b
SW	941.0	106.1	1047.0	89.9	**10.1**
NW	946.5	100.3	1046.8	90.4	**9.6**
NE	913.2	133.4	1046.5	87.3	**12.7**
SE	924.6	122.2	1046.8	88.3	**11.7**



At 12.0 Å:

%V Free	%V Buried	% V Tot/V Ex
92.9	7.1	100.0

Quadrant	V f	V b	V t	%V f	%V b
SW	1691.2	118.0	1809.1	93.5	6.5
NW	1706.5	102.6	1809.1	94.3	5.7
NE	1666.8	142.3	1809.1	92.1	7.9
SE	1659.3	149.8	1809.1	91.7	8.3



At 15.0 Å:

%V Free	%V Buried	% V Tot/V Ex
96.3	3.7	100.0

Quadrant	V f	V b	V t	%V f	%V b
SW	3414.6	119.7	3534.3	96.6	3.4
NW	3431.0	102.6	3533.6	97.1	2.9
NE	3388.6	144.3	3532.9	95.9	4.1
SE	3376.7	156.8	3533.6	95.6	4.4

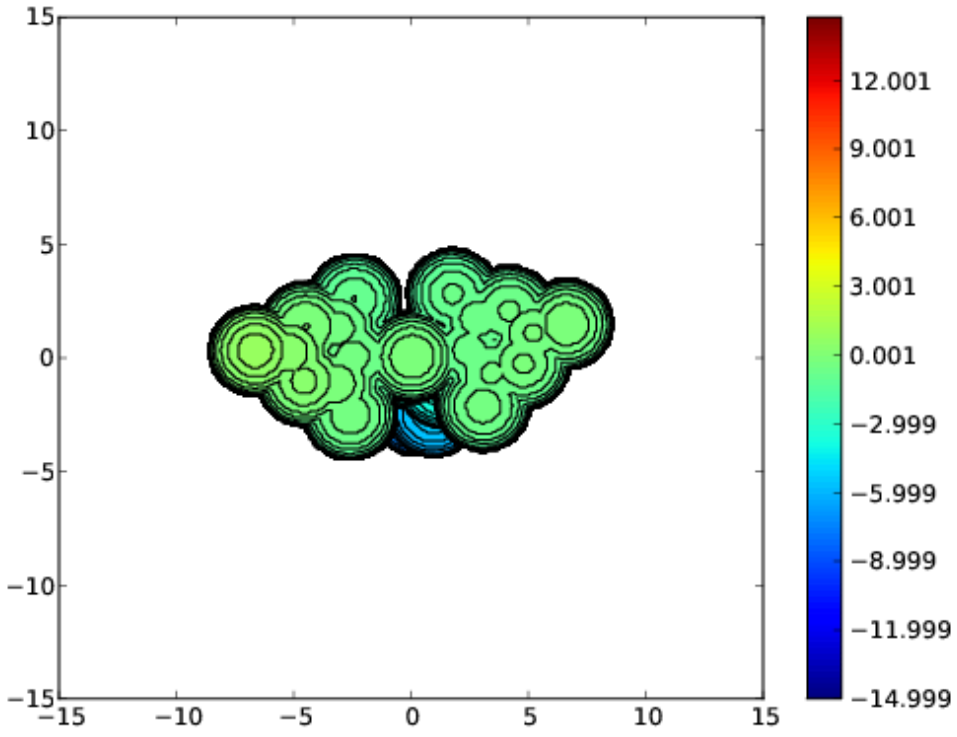
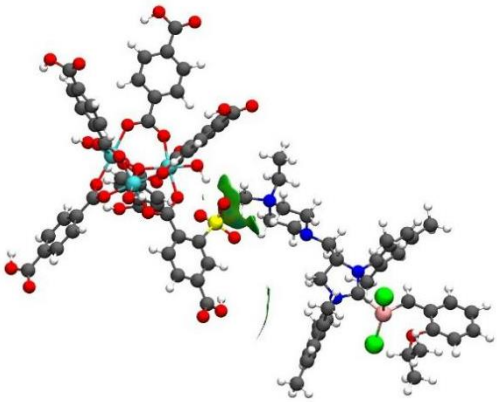
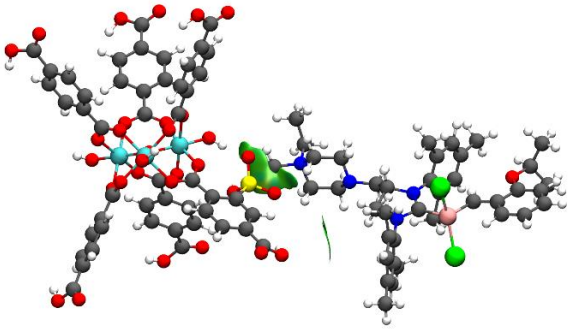
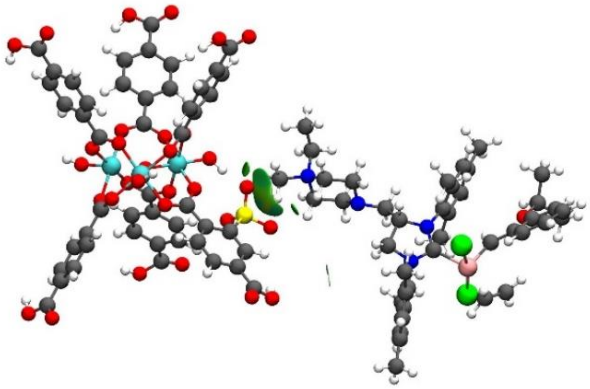
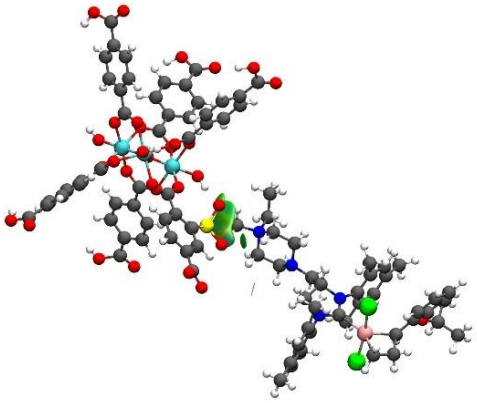
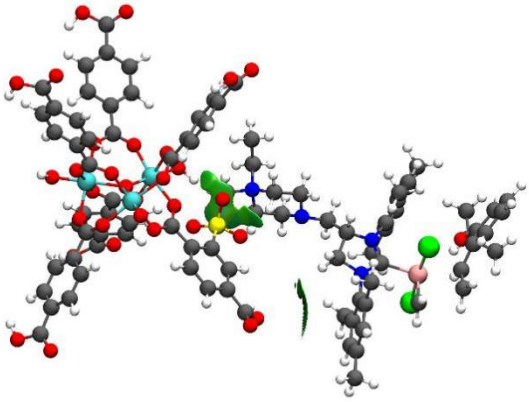
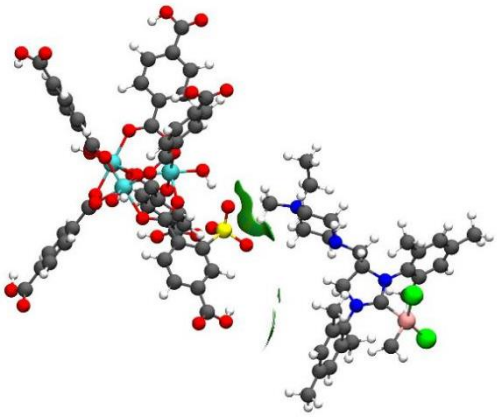


Table S1. NCI plots of the truncated MOF in combination with the Precat. Previously optimised geometries have been evaluated using the promolecular approach suitable for large structures.

Precat	**Act**
	
Cl1	**MCy**
	
Cl2	**I14e**
	

Computational Coordinates

Table S1. Coordinates data set, absolute energies (a.u.) for all DFT optimized neutral complexes.

Precat				TS_Open			
75				75			
precat SCF Done: -2403.24318273 A.U.				ts_open SCF Done: -2403.20586043 A.U.			
Ru	0.151733	0.458008	-0.007440	Ru	0.217673	0.504668	-0.183830
C	0.254906	-1.504528	-0.015556	C	0.813487	-1.327998	0.035166
N	1.464220	-2.178459	-0.020183	N	2.143026	-1.697928	-0.051090
N	-0.722276	-2.473184	-0.049902	N	0.088464	-2.492060	0.171349
C	-0.183916	-3.845632	0.034754	C	0.949950	-3.684622	0.301826
C	1.314556	-3.632101	-0.215360	C	2.312892	-3.158994	-0.162390
H	-0.663588	-4.502865	-0.719736	H	0.564896	-4.514084	-0.325535
H	-0.389749	-4.281543	1.039635	H	0.966888	-4.039744	1.358525
H	1.959489	-4.195124	0.490599	H	3.155082	-3.505980	0.470342
H	1.614181	-3.917960	-1.249498	H	2.536120	-3.443030	-1.216111
C	-2.146321	-2.309062	-0.013834	C	-1.325008	-2.661854	0.348717
C	2.785802	-1.605148	-0.003748	C	3.308318	-0.850097	-0.107781
C	3.465329	-1.337784	-1.223055	C	3.875936	-0.491678	-1.359917
C	4.757001	-0.774507	-1.156338	C	5.028345	0.321837	-1.356759
C	5.404507	-0.522148	0.066777	C	5.649890	0.741672	-0.166290
C	4.742655	-0.896593	1.253935	C	5.112146	0.288612	1.055087
C	3.450029	-1.453845	1.247602	C	3.956838	-0.512261	1.112561
C	2.898576	-1.728115	-2.567963	C	3.339896	-1.019956	-2.669985
H	5.277978	-0.543200	-2.100964	H	5.460573	0.621685	-2.326400
C	6.770959	0.124489	0.111650	C	6.856491	1.652822	-0.194128
H	5.254046	-0.765486	2.222597	H	5.610008	0.564286	2.000004
C	2.815337	-1.913040	2.537728	C	3.440718	-1.007785	2.442372
H	1.794071	-1.713326	-2.578825	H	2.233328	-1.041883	-2.694923
H	3.247801	-2.747973	-2.847933	H	3.716138	-2.050585	-2.859598
H	3.244076	-1.036165	-3.360958	H	3.680641	-0.392064	-3.516726
H	7.309577	0.014753	-0.851158	H	7.427775	1.549868	-1.138897
H	7.403295	-0.309419	0.913591	H	7.544320	1.448415	0.651748
H	6.688399	1.214110	0.320490	H	6.548397	2.718674	-0.112199
H	3.548366	-1.882217	3.367754	H	4.175369	-0.810406	3.247643
H	2.432875	-2.952829	2.459202	H	3.234163	-2.098815	2.428345
H	1.954971	-1.263132	2.805832	H	2.493423	-0.490577	2.703770
C	-2.858770	-2.257139	-1.239323	C	-2.132605	-2.942133	-0.784290
C	-2.814364	-2.252852	1.236375	C	-1.871419	-2.632482	1.657531
C	-4.262606	-2.146306	-1.187749	C	-3.505847	-3.179246	-0.577055
C	-4.219756	-2.143555	1.231639	C	-3.252338	-2.874989	1.808613
C	-4.963496	-2.094254	0.034755	C	-4.087599	-3.148774	0.707575
C	-6.474304	-2.017183	0.061021	C	-5.570945	-3.382988	0.887999
H	-4.824424	-2.094349	-2.135704	H	-4.141348	-3.398208	-1.452027
C	-2.041103	-2.251116	2.534604	C	-1.008727	-2.300534	2.854043
H	-4.748316	-2.087708	2.198373	H	-3.686993	-2.845845	2.821970
C	-2.125238	-2.269894	-2.559887	C	-1.541673	-2.961685	-2.173802
H	-1.428316	-1.407237	-2.639859	H	-1.126817	-1.966531	-2.448275
H	-2.834613	-2.225679	-3.409316	H	-2.303885	-3.244269	-2.926207
H	-1.510155	-3.187415	-2.681828	H	-0.702453	-3.685249	-2.255806
H	-1.445744	-3.180371	2.665593	H	-0.501983	-1.319939	2.725857
H	-2.724307	-2.169840	3.402422	H	-0.208701	-3.055148	3.014178
H	-1.323660	-1.402967	2.575521	H	-1.614285	-2.258478	3.780235
H	-6.843561	-1.512951	0.976987	H	-5.835713	-3.537124	1.952941
H	-6.925264	-3.034239	0.044673	H	-5.915976	-4.269481	0.315860
H	-6.872836	-1.472296	-0.818860	H	-6.158841	-2.513771	0.520399
C	-1.667430	0.782448	0.014408	C	-1.561035	0.420585	0.206019
Cl	0.598285	0.673879	-2.315455	Cl	0.167580	0.408181	-2.529104
Cl	0.650646	0.717999	2.287413	Cl	1.152061	1.436872	1.754750
O	0.087510	2.761148	-0.017944	O	-1.302597	3.008355	0.481858
C	1.305614	3.585856	-0.049285	C	-1.086777	4.231404	1.235462
C	1.414925	4.378743	-1.351629	C	-0.798091	5.429296	0.323528
H	2.078952	2.791073	-0.072042	H	-0.147318	3.971294	1.767904
C	1.484690	4.375099	1.247419	C	-2.175730	4.470456	2.285080
H	0.773252	5.218242	1.349975	H	-3.154179	4.743553	1.840638
H	2.510848	4.797155	1.270087	H	-1.866741	5.300703	2.953334
H	1.367206	3.698229	2.116714	H	-2.316332	3.564915	2.908875
H	1.251468	3.703556	-2.214801	H	-0.034835	5.160418	-0.434028
H	2.438594	4.800576	-1.427782	H	-0.396413	6.267471	0.930236
H	0.699489	5.222580	-1.414798	H	-1.698359	5.800442	-0.206466

C	-1.200442	3.218317	0.009266
C	-2.152519	2.151803	0.024327
C	-1.621242	4.558719	0.022465
C	-3.000721	4.842574	0.049817
C	-3.958169	3.811132	0.063995
C	-3.532661	2.476086	0.051176
H	-3.325683	5.895208	0.060285
H	-0.898320	5.383528	0.012163
H	-4.263385	1.651288	0.062407
H	-5.032024	4.052482	0.085424
H	-2.447742	-0.001196	0.022009

C	-2.438579	2.690545	-0.211031
C	-2.430687	1.317093	-0.585665
C	-3.444597	3.556687	-0.680788
C	-4.434004	3.048476	-1.544811
C	-4.426902	1.700118	-1.941573
C	-3.445801	0.830102	-1.435484
H	-5.214216	3.729312	-1.921439
H	-3.454473	4.618813	-0.403573
H	-3.463929	-0.241963	-1.685847
H	-5.200918	1.319460	-2.625985
H	-2.052822	-0.334128	0.854102

Act

75

act SCF Done: -2403.22255201 A.U.

Ru	0.627109	-0.718288	0.465266
C	1.196552	1.067988	0.019576
N	2.532158	1.375315	-0.173760
N	0.507331	2.261842	-0.008875
C	1.379035	3.410058	-0.331032
C	2.786888	2.826047	-0.151334
H	1.171303	4.260055	0.350923
H	1.190874	3.761513	-1.372407
H	3.487179	3.114951	-0.961892
H	3.243223	3.127667	0.819015
C	-0.909095	2.495595	0.014208
C	3.625094	0.454025	-0.350208
C	4.464025	0.115198	0.744794
C	5.534422	-0.772718	0.508884
C	5.811115	-1.295085	-0.768152
C	5.001939	-0.877716	-1.844237
C	3.916421	-0.001417	-1.665828
C	4.276107	0.719728	2.116326
H	6.178473	-1.055315	1.358724
C	6.934890	-2.284066	-0.981344
H	5.222836	-1.244410	-2.860778
C	3.093018	0.446407	-2.849680
H	3.211124	0.731507	2.423783
H	4.656241	1.765560	2.146753
H	4.842090	0.148385	2.878254
H	7.705500	-2.208620	-0.187836
H	7.431340	-2.135892	-1.962411
H	6.549577	-3.327530	-0.967776
H	3.578275	0.152928	-3.801196
H	2.949693	1.547507	-2.862293
H	2.086783	-0.022370	-2.819726
C	-1.528023	2.880621	1.231713
C	-1.641633	2.427813	-1.198483
C	-2.900845	3.194721	1.206688
C	-3.011855	2.757609	-1.168566
C	-3.659937	3.148408	0.019452
C	-5.124781	3.526910	0.026651
H	-3.391539	3.488078	2.150206
C	-0.988483	1.957642	-2.478137
H	-3.589006	2.705892	-2.107353
C	-0.743336	2.935607	2.520764
H	-0.298688	1.947066	2.765830
H	-1.389439	3.248556	3.364151
H	0.100023	3.656964	2.458701
H	-0.637094	0.907345	-2.382975
H	-0.098907	2.565960	-2.746842
H	-1.696879	2.007062	-3.327961
H	-5.622921	3.258683	-0.926336
H	-5.255997	4.621329	0.173859
H	-5.670611	3.025923	0.853444
C	-1.212821	-0.617475	0.352105
Cl	1.011697	-0.461072	2.763305
Cl	1.073855	-1.976926	-1.443404
O	-3.572466	-1.135935	-0.918593
C	-4.729521	-1.211794	-1.789219
C	-4.743984	-2.481982	-2.648773
H	-4.526620	-0.358681	-2.471243

TS_Ci1

81

ts_ci1 SCF Done: -2481.74738224 A.U.

Ru	-0.578506	-0.558024	-0.365879
C	-1.072999	1.280672	-0.041270
N	-2.394236	1.648533	0.151532
N	-0.344410	2.449143	-0.100110
C	-1.170386	3.646381	0.157067
C	-2.599394	3.102817	0.032910
H	-0.941912	4.442531	-0.580669
H	-0.955845	4.055806	1.171569
H	-3.278407	3.471112	0.829243
H	-3.058074	3.353545	-0.950833
C	1.078152	2.633756	-0.167100
C	-3.523433	0.784367	0.385268
C	-4.365608	0.392880	-0.690322
C	-5.468750	-0.437736	-0.400636
C	-5.780172	-0.845712	0.909758
C	-4.972921	-0.366107	1.960868
C	-3.853575	0.454268	1.729639
C	-4.159184	0.898839	-2.098542
H	-6.114603	-0.761100	-1.234443
C	-6.942863	-1.772503	1.185136
H	-5.224424	-0.634178	3.000873
C	-3.041981	0.976936	2.890549
H	-3.092714	0.882031	-2.398793
H	-4.532783	1.942522	-2.200654
H	-4.724107	0.281902	-2.824953
H	-7.698821	-1.735770	0.374997
H	-7.447012	-1.524442	2.141781
H	-6.597577	-2.826919	1.265520
H	-3.578968	0.822439	3.847088
H	-2.822108	2.060395	2.789835
H	-2.069791	0.443205	2.949807
C	1.681831	2.906353	-1.421734
C	1.833976	2.633357	1.033170
C	3.065447	3.169251	-1.447835
C	3.213956	2.909003	0.951236
C	3.849708	3.180038	-0.276345
C	5.335988	3.453774	-0.346675
H	3.543928	3.376014	-2.420137
C	1.190626	2.292917	2.358273
H	3.808957	2.909102	1.880118
C	0.868540	2.902644	-2.693784
H	0.359815	1.926228	-2.843530
H	1.509386	3.104301	-3.574299
H	0.071945	3.678034	-2.675068
H	0.761932	1.267255	2.344370
H	0.356936	2.982427	2.610765
H	1.927889	2.346781	3.182886
H	5.762099	3.667739	0.653950
H	5.560275	4.317473	-1.006788
H	5.884710	2.581132	-0.764092
C	1.263300	-0.478554	-0.291435
Cl	-0.971026	-0.409153	-2.682484
Cl	-0.969051	-1.507828	1.745710
O	3.520125	-1.060702	1.111009
C	4.524261	-1.263083	2.137919
C	4.356266	-2.596543	2.875258
H	4.251050	-0.457067	2.851900

C	-6.046560	-0.902084	-1.065780
H	-6.388243	-1.721757	-0.403922
H	-6.844225	-0.722624	-1.816282
H	-5.940224	0.015484	-0.453020
H	-3.751957	-2.639461	-3.117579
H	-5.492992	-2.366973	-3.459492
H	-5.004114	-3.394936	-2.078131
C	-3.302677	-1.981430	0.111325
C	-2.054897	-1.728412	0.789944
C	-4.117030	-3.054913	0.531083
C	-3.716082	-3.879148	1.597412
C	-2.503220	-3.649530	2.268458
C	-1.688311	-2.585616	1.862928
H	-4.371010	-4.710888	1.903404
H	-5.068945	-3.263477	0.027863
H	-0.755302	-2.365473	2.406515
H	-2.198866	-4.289518	3.110608
H	-1.733317	0.201606	-0.176656

C	5.949736	-0.966730	1.653336
H	6.365978	-1.757924	0.999258
H	6.622815	-0.870513	2.530612
H	5.975175	-0.008650	1.096514
H	3.300116	-2.735419	3.181612
H	4.982330	-2.590519	3.791525
H	4.657901	-3.471937	2.267393
C	3.323185	-1.863276	0.030982
C	2.120228	-1.585464	-0.715483
C	4.176006	-2.906676	-0.386702
C	3.856419	-3.675083	-1.520681
C	2.688225	-3.419358	-2.257621
C	1.830474	-2.389263	-1.849598
H	4.540662	-4.482887	-1.826932
H	5.096952	-3.129928	0.165828
H	0.923052	-2.156560	-2.428302
H	2.449072	-4.016037	-3.151295
C	-2.065625	-3.564043	-1.130294
C	-0.991201	-4.247533	-0.696548
H	1.788126	0.347249	0.223308
H	-0.671006	-4.196447	0.357237
H	-0.382615	-4.865743	-1.377695
H	-2.670838	-2.952097	-0.440568
H	-2.383807	-3.584975	-2.185737

TS_Con

81

ts_con_2 SCF Done: -2481.74092917 A.U.

C	0.686060	-1.308393	0.002036
C	0.588520	-3.680114	0.106329
H	0.090828	-4.399318	-0.574956
H	0.595393	-4.128541	1.125602
C	1.983377	-3.267853	-0.369432
H	2.801310	-3.712261	0.233091
H	2.164475	-3.529630	-1.436436
C	-2.174424	-2.646162	1.506884
C	-3.559205	-2.895435	1.569989
H	-4.029420	-3.000617	2.562342
C	-4.352242	-3.031733	0.411413
C	-3.720543	-2.910513	-0.841297
H	-4.317002	-3.030151	-1.761271
C	-2.338729	-2.650195	-0.964873
C	-1.578270	-2.499040	0.223604
C	-1.358616	-2.534178	2.772855
H	-1.998926	-2.666526	3.666840
H	-0.847453	-1.548015	2.848037
H	-0.561103	-3.307218	2.818519
C	-5.838148	-3.293648	0.519743
H	-6.276367	-3.580922	-0.456787
H	-6.379634	-2.390079	0.875922
H	-6.056444	-4.104081	1.246334
C	-1.695732	-2.544021	-2.325331
H	-2.438532	-2.714840	-3.128750
H	-0.882813	-3.291512	-2.455084
H	-1.232716	-1.543318	-2.476737
C	3.218813	-1.106433	-0.216591
C	3.927517	-0.955035	1.008095
C	5.201268	-0.354207	0.970383
H	5.750631	-0.224684	1.918112
C	5.790777	0.078423	-0.235157
C	5.084029	-0.141188	-1.432975
H	5.541769	0.154901	-2.391868
C	3.810934	-0.749456	-1.457330
C	3.335725	-1.410844	2.318587
H	4.077836	-1.329708	3.136808
H	2.994118	-2.467051	2.273147
H	2.444910	-0.798481	2.586893
C	7.136991	0.766867	-0.236601
H	7.650853	0.663158	-1.213461
H	7.804527	0.362446	0.551644
H	7.024719	1.855876	-0.039065
C	3.133371	-1.036504	-2.776015

Ci1

81

ci1 SCF Done: -2481.75876594 A.U.

Ru	0.747112	-0.865237	0.228104
C	1.188578	1.111130	0.049888
N	2.502051	1.507078	0.007801
N	0.427539	2.242758	0.121644
C	1.233745	3.483143	0.046082
C	2.669220	2.961872	0.206820
H	0.934767	4.190366	0.846481
H	1.065404	3.990175	-0.931326
H	3.374069	3.380702	-0.540631
H	3.081736	3.168117	1.219489
C	-1.002295	2.375506	0.069276
C	3.658230	0.667494	-0.194946
C	4.433360	0.229669	0.914421
C	5.555561	-0.586078	0.658241
C	5.953907	-0.930626	-0.646897
C	5.223200	-0.391055	-1.724352
C	4.089907	0.420834	-1.529655
C	4.137400	0.674839	2.326212
H	6.146913	-0.947317	1.516521
C	7.132299	-1.846606	-0.889448
H	5.550135	-0.598392	-2.757196
C	3.379931	1.026531	-2.715340
H	3.056553	0.606311	2.565868
H	4.464562	1.727284	2.482780
H	4.689140	0.053287	3.058758
H	7.831639	-1.853841	-0.029147
H	7.700319	-1.552942	-1.796116
H	6.793159	-2.894465	-1.046274
H	3.984835	0.908649	-3.635850
H	3.182708	2.109744	-2.571628
H	2.401210	0.523621	-2.874853
C	-1.721638	2.579913	1.275779
C	-1.644379	2.421217	-1.194897
C	-3.106129	2.821038	1.187779
C	-3.031713	2.670061	-1.224775
C	-3.780242	2.875589	-0.049284
C	-5.269348	3.137534	-0.101021
H	-3.674078	2.975773	2.120724
C	-0.873873	2.177784	-2.471979
H	-3.539530	2.711457	-2.203275
C	-1.022990	2.540774	2.613453
H	-0.441024	1.602048	2.739659
H	-1.752736	2.619938	3.442858
H	-0.303066	3.381629	2.724536

H	3.697951	-0.583683	-3.614653
H	2.093046	-0.645387	-2.803890
H	3.080894	-2.130195	-2.972184
C	-1.504054	0.487568	0.365528
H	-1.891980	-0.094059	1.227338
C	-2.501855	1.317023	-0.323448
C	-3.735156	0.755547	-0.746870
H	-3.937266	-0.303327	-0.524740
C	-4.660979	1.511924	-1.479008
H	-5.597285	1.045280	-1.823646
C	-4.389575	2.859820	-1.776946
H	-5.108015	3.455948	-2.361805
C	-3.204314	3.453348	-1.312587
C	-2.271236	2.698915	-0.580119
N	-0.146917	-2.395106	0.118862
N	1.957240	-1.801326	-0.197028
Cl	0.420400	0.651491	2.482731
Cl	0.021300	0.639189	-2.395484
Ru	0.313038	0.629012	0.001772
H	-2.981385	4.512423	-1.511275
O	-1.130718	3.310832	-0.096305
C	-1.169119	3.864729	1.276359
C	1.886420	2.326484	-0.707853
C	2.307735	2.109346	0.578046
H	1.124305	3.084998	-0.950840
H	2.394419	1.859561	-1.564827
H	3.155102	1.445708	0.802897
H	1.897834	2.671675	1.429767
C	-0.108724	4.961068	1.314551
H	0.875796	4.584128	0.976108
H	0.009493	5.339753	2.350498
H	-0.397346	5.810375	0.660398
C	-2.545374	4.382364	1.691565
H	-0.874756	3.030070	1.954487
H	-2.887846	5.217712	1.045486
H	-2.477309	4.761191	2.732323
H	-3.317172	3.587835	1.674903

TS_MCy

81

ts_mcy SCF Done: -2481.75565653 A.U.

Ru	0.689004	-0.806804	0.259894
C	1.354959	1.037650	-0.301871
N	2.673566	1.339157	-0.489237
N	0.620946	2.143698	-0.600341
C	1.451796	3.272284	-1.079044
C	2.887332	2.745033	-0.899530
H	1.246264	4.184938	-0.481131
H	1.208147	3.504986	-2.138965
H	3.484099	2.790286	-1.834381
H	3.452720	3.293579	-0.114384
C	-0.805607	2.310826	-0.522327
C	3.807450	0.469482	-0.281219
C	4.430018	0.425856	0.996911
C	5.548126	-0.417439	1.161710
C	6.080719	-1.175081	0.101274
C	5.489680	-1.039264	-1.170354
C	4.369617	-0.214854	-1.395138
C	3.946828	1.271545	2.149162
H	6.027205	-0.464975	2.154198
C	7.252512	-2.105922	0.318303
H	5.920778	-1.582965	-2.027845
C	3.816458	-0.052593	-2.789128
H	2.948204	0.932276	2.503405
H	3.847236	2.340447	1.864068
H	4.654636	1.215103	2.999274
H	6.902041	-3.136121	0.549961
H	7.885875	-1.778797	1.167751
H	7.892865	-2.177157	-0.584586
H	4.428697	-0.614229	-3.521578
H	3.808201	1.012282	-3.107815
H	2.770736	-0.426761	-2.844077

MCy

81

mcy SCF Done: -2481.76698777 A.U.

Ru	0.612952	-0.761675	-0.040240
C	1.386553	1.099518	-0.097620
N	2.708579	1.412666	-0.163184
N	0.658780	2.246598	-0.093933
C	1.517394	3.453266	-0.084152
C	2.925429	2.871654	-0.307601
H	1.418428	3.981724	0.889878
H	1.205425	4.157115	-0.883099
H	3.324622	3.097468	-1.320794
H	3.667617	3.228746	0.435721
C	-0.770136	2.379953	0.055961
C	3.838391	0.512800	-0.156574
C	4.484954	0.240819	1.079261
C	5.606994	-0.611454	1.067393
C	6.109493	-1.173681	-0.122080
C	5.478969	-0.830515	-1.333860
C	4.356531	0.020887	-1.384908
C	4.002031	0.839236	2.377872
H	6.107728	-0.834035	2.024689
C	7.287734	-2.121718	-0.097549
H	5.880394	-1.225243	-2.282519
C	3.756383	0.403841	-2.715287
H	3.024505	0.395620	2.669394
H	3.854757	1.937672	2.304755
H	4.728507	0.649728	3.192181
H	7.979734	-1.894108	0.738702
H	7.863861	-2.085290	-1.044402
H	6.948449	-3.172623	0.037817
H	4.333056	-0.044299	-3.548047
H	3.759853	1.505361	-2.865632
H	2.698533	0.068263	-2.799540

C	-1.364823	2.841080	0.669639	C	-1.334324	2.415889	1.361106
C	-1.601913	2.055889	-1.667963	C	-1.560684	2.609770	-1.100382
C	-2.749957	3.089954	0.698343	C	-2.722314	2.624944	1.473442
C	-2.984758	2.320114	-1.581095	C	-2.942977	2.823754	-0.924472
C	-3.579103	2.833440	-0.412415	C	-3.545401	2.826619	0.347777
C	-5.068092	3.087879	-0.335998	C	-5.033981	3.036728	0.513153
H	-3.193982	3.499812	1.621012	H	-3.170238	2.643961	2.481024
C	-0.997180	1.525882	-2.945827	C	-0.952577	2.626930	-2.480859
H	-3.613775	2.127869	-2.466783	H	-3.564434	3.004090	-1.817739
C	-0.502491	3.124950	1.876911	C	-0.488454	2.255713	2.601376
H	-0.017212	2.197630	2.254139	H	-0.054455	1.233743	2.676617
H	-1.103260	3.562926	2.697987	H	-1.091800	2.440776	3.511508
H	0.315620	3.840665	1.644161	H	0.365131	2.967009	2.616183
H	-0.230455	2.218275	-3.356729	H	-0.129008	3.368602	-2.563816
H	-1.773966	1.395042	-3.724684	H	-1.712858	2.883836	-3.244303
H	-0.490007	0.547616	-2.787172	H	-0.518882	1.632788	-2.730462
H	-5.572449	2.300859	0.266220	H	-5.255011	3.781230	1.306605
H	-5.536572	3.091544	-1.340703	H	-5.535874	2.090867	0.812193
H	-5.292427	4.059772	0.151140	H	-5.507286	3.386019	-0.426264
C	-1.189563	-1.036042	0.084541	C	-1.171096	-1.728946	-0.185586
Cl	0.900230	-0.287292	2.612870	Cl	1.014993	-0.976059	2.324912
Cl	0.792700	-1.534919	-2.060050	Cl	0.427303	-0.648842	-2.460129
O	-3.604462	-1.924327	-0.794749	O	-3.682523	-1.229584	-1.151093
C	-4.725240	-2.551653	-1.473185	C	-4.831675	-1.520122	-1.990048
C	-5.289434	-3.753662	-0.705870	C	-5.391151	-2.929024	-1.769519
H	-4.214784	-2.950352	-2.375421	H	-4.363382	-1.499172	-2.997480
C	-5.774469	-1.545364	-1.962750	C	-5.885704	-0.405259	-1.965415
H	-6.418152	-1.147729	-1.153735	H	-6.513651	-0.415849	-1.051854
H	-6.435939	-2.041295	-2.702997	H	-6.564954	-0.518570	-2.836049
H	-5.280587	-0.690205	-2.465905	H	-5.394870	0.585576	-2.040169
H	-4.470890	-4.435434	-0.399018	H	-4.579318	-3.682253	-1.822124
H	-5.973455	-4.321894	-1.369678	H	-6.126377	-3.162010	-2.567219
H	-5.859467	-3.468436	0.199921	H	-5.903426	-3.040330	-0.793449
C	-3.646800	-1.291006	0.404769	C	-3.627140	-1.429882	0.196323
C	-2.375068	-0.817960	0.913319	C	-2.318708	-1.653455	0.751576
C	-4.820530	-1.089558	1.165616	C	-4.755653	-1.401673	1.047424
C	-4.758020	-0.456490	2.417332	C	-4.613557	-1.603065	2.429066
C	-3.530707	-0.006583	2.934207	C	-3.341995	-1.824216	2.985750
C	-2.364077	-0.184880	2.183046	C	-2.217312	-1.839844	2.151250
H	-5.687988	-0.320987	2.993561	H	-5.508053	-1.575580	3.072346
H	-5.790586	-1.436256	0.790427	H	-5.752031	-1.210636	0.629282
H	-1.389142	0.146006	2.570800	H	-1.213269	-1.966075	2.584953
H	-3.484678	0.482493	3.919325	H	-3.224385	-1.972337	4.070432
C	1.277149	-2.846915	0.711549	C	1.402802	-2.562348	-0.270457
C	-0.118321	-2.922475	0.909822	C	-0.110410	-2.916226	-0.031543
H	-1.456800	-1.436790	-0.914154	H	-1.513707	-1.653223	-1.231148
H	-0.744144	-3.438566	0.163678	H	-0.389408	-3.590455	-0.866773
H	-0.538498	-2.810205	1.921518	H	-0.236098	-3.389408	0.959094
H	1.725661	-3.277706	-0.198926	H	1.773018	-2.802253	-1.284727
H	1.929423	-2.720677	1.593432	H	2.058453	-2.892957	0.557129

TS_Ci2				Ci2			
81				81			
ts_ci2 SCF Done: -2481.74740294 A.U.				ci2 SCF Done: -2481.75117097 A.U.			
Ru	0.560189	-0.789672	0.062175	Ru	0.271097	-0.103196	0.934492
C	1.345739	1.076579	-0.047282	C	1.339054	1.051165	-0.420273
N	2.670023	1.403375	-0.105605	N	2.597895	0.867690	-0.905126
N	0.622640	2.231076	-0.059121	N	0.823479	2.178464	-0.981962
C	1.472030	3.442301	-0.067498	C	1.731300	2.781154	-1.985373
C	2.889651	2.863292	-0.223282	C	3.022596	1.968219	-1.803486
H	1.339383	4.008217	0.880656	H	1.865345	3.864276	-1.787117
H	1.182341	4.114500	-0.902177	H	1.294325	2.674354	-3.002543
H	3.344445	3.102184	-1.209791	H	3.417860	1.559808	-2.755686
H	3.590023	3.216079	0.562304	H	3.836110	2.553594	-1.321698
C	-0.810465	2.370005	0.019964	C	-0.473910	2.775750	-0.763552
C	3.809945	0.526321	-0.172919	C	3.548507	-0.176370	-0.614399
C	4.526874	0.234392	1.019116	C	4.467582	-0.009866	0.457660
C	5.674144	-0.577643	0.921214	C	5.417306	-1.027875	0.679483
C	6.131550	-1.085953	-0.311231	C	5.498760	-2.171903	-0.137906
C	5.419084	-0.740449	-1.475918	C	4.614243	-2.268355	-1.230455
C	4.266298	0.071379	-1.439751	C	3.644097	-1.283414	-1.501645
C	4.079424	0.768637	2.357604	C	4.461488	1.224526	1.326282

H	6.232088	-0.811998	1.843589	H	6.124839	-0.909638	1.517408
C	7.347042	-1.984116	-0.376543	C	6.500640	-3.267023	0.151769
H	5.776323	-1.102247	-2.454910	H	4.684096	-3.136328	-1.907508
C	3.554079	0.442315	-2.717576	C	2.752479	-1.403907	-2.712738
H	3.075336	0.369655	2.625481	H	3.476598	1.382023	1.819171
H	3.999307	1.877103	2.356859	H	4.676607	2.140323	0.732884
H	4.795156	0.486155	3.154300	H	5.238562	1.153974	2.112346
H	7.811366	-1.973557	-1.383231	H	7.404820	-2.872729	0.658357
H	7.075828	-3.039261	-0.151022	H	6.820584	-3.785750	-0.774709
H	8.117749	-1.684611	0.363103	H	6.061987	-4.039011	0.822163
H	4.100484	0.053054	-3.598960	H	2.965056	-2.339076	-3.266983
H	3.470217	1.543986	-2.838173	H	2.904322	-0.559077	-3.420001
H	2.516266	0.038407	-2.742028	H	1.680503	-1.403309	-2.417716
C	-1.434858	2.471606	1.294558	C	-0.583334	3.856220	0.158629
C	-1.547024	2.554000	-1.180673	C	-1.567513	2.400604	-1.590651
C	-2.826204	2.686234	1.332827	C	-1.839277	4.475654	0.307433
C	-2.935615	2.777989	-1.078534	C	-2.798399	3.063505	-1.399868
C	-3.596647	2.835722	0.162787	C	-2.963200	4.088054	-0.449727
C	-5.089830	3.059619	0.249982	C	-4.302250	4.761271	-0.246166
H	-3.318942	2.756545	2.316977	H	-1.931684	5.306303	1.027277
C	-0.879248	2.517820	-2.533154	C	-1.437785	1.353327	-2.668693
H	-3.512918	2.927262	-2.006546	H	-3.651800	2.771061	-2.033555
C	-0.646569	2.381342	2.578195	C	0.604290	4.360481	0.940180
H	-0.199940	1.371296	2.716284	H	0.974688	3.581451	1.642481
H	-1.294237	2.597147	3.450298	H	0.335605	5.263603	1.522222
H	0.194833	3.106975	2.598211	H	1.452546	4.630007	0.274837
H	-0.017009	3.215884	-2.592782	H	-0.619668	1.595407	-3.380689
H	-1.593235	2.796883	-3.332786	H	-2.375722	1.276321	-3.252079
H	-0.487553	1.498367	-2.748468	H	-1.206758	0.351322	-2.243328
H	-5.339111	3.867370	0.969972	H	-4.799471	4.388547	0.676308
H	-5.607439	2.142480	0.606072	H	-4.990649	4.570229	-1.093646
H	-5.523921	3.330727	-0.733056	H	-4.194131	5.859666	-0.129629
C	-1.151930	-2.321227	-0.021221	C	-1.659097	-1.250011	1.756619
Cl	0.888590	-0.787815	2.467902	Cl	1.176790	1.408294	2.632707
Cl	0.239582	-0.829965	-2.342011	Cl	-0.307211	-1.492972	-0.988752
O	-3.488128	-1.540932	-1.182473	O	-2.887745	-3.449016	0.690235
C	-4.640927	-1.665549	-2.055493	C	-2.999005	-4.659407	-0.105688
C	-5.485079	-2.907919	-1.751725	C	-4.264012	-5.461658	0.228873
H	-4.139562	-1.830484	-3.032923	H	-2.133312	-5.241336	0.278173
C	-5.443192	-0.363953	-2.180687	C	-2.762715	-4.421761	-1.599724
H	-6.102847	-0.168756	-1.311566	H	-3.615777	-3.919340	-2.097283
H	-6.088676	-0.415098	-3.082248	H	-2.604754	-5.397810	-2.103710
H	-4.755533	0.497188	-2.296467	H	-1.859221	-3.795858	-1.744564
H	-4.844260	-3.811213	-1.701243	H	-4.393019	-5.539229	1.327399
H	-6.224766	-3.058073	-2.565150	H	-4.170013	-6.489920	-0.178653
H	-6.043421	-2.826404	-0.798078	H	-5.186096	-5.017946	-0.197647
C	-3.524114	-1.559663	0.177733	C	-3.503399	-2.268596	0.403038
C	-2.291598	-1.909739	0.830258	C	-2.890890	-1.097326	0.958699
C	-4.663488	-1.253207	0.956662	C	-4.711842	-2.148380	-0.319027
C	-4.601000	-1.292705	2.358239	C	-5.314451	-0.892951	-0.497883
C	-3.402013	-1.633235	3.008254	C	-4.727690	0.261589	0.047262
C	-2.268091	-1.936790	2.245076	C	-3.530802	0.147663	0.767932
H	-5.502380	-1.049017	2.943649	H	-6.258792	-0.824656	-1.061622
H	-5.604132	-0.973858	0.466222	H	-5.198879	-3.042715	-0.727674
H	-1.320041	-2.172438	2.750062	H	-3.066954	1.056495	1.183670
H	-3.348755	-1.659072	4.107483	H	-5.200528	1.246341	-0.085623
C	1.956531	-1.968620	-0.120442	C	1.571071	-1.295638	1.356529
C	-0.022130	-3.067663	0.385643	C	-1.147889	-0.307923	2.657070
H	-1.390780	-2.339321	-1.095546	H	-1.295413	-2.286340	1.818465
H	0.422914	-3.755617	-0.351135	H	-0.498377	-0.620956	3.487484
H	0.166235	-3.294627	1.446906	H	-1.638658	0.669287	2.803482
H	2.245438	-2.382077	-1.113154	H	1.679528	-2.247090	0.790414
H	2.558646	-2.302353	0.754926	H	2.261224	-1.117946	2.210736

TS_I14e				I14e			
81				55			
ts_I14e SCF Done: -2481.74389163 A.U.				I14e SCF Done: -1979.31478192 A.U.			
Ru	-0.409997	-0.120105	-0.826076	Ru	0.091304	-0.062519	-1.461499
C	-1.489486	0.951817	0.454007	C	-0.085405	0.063361	0.459131
N	-2.756637	0.742310	0.920731	N	-1.210029	0.152327	1.247084
N	-1.004488	2.087419	1.041473	N	1.004148	0.099519	1.307570
C	-1.934925	2.650249	2.042466	C	0.625830	0.366802	2.706547

C	-3.212692	1.821635	1.823328
H	-2.085961	3.735638	1.867684
H	-1.516697	2.528259	3.066464
H	-3.619821	1.396193	2.763769
H	-4.025320	2.407302	1.338699
C	0.281539	2.708138	0.831791
C	-3.674872	-0.308603	0.577903
C	-4.571666	-0.127388	-0.511136
C	-5.511950	-1.144808	-0.770603
C	-5.596775	-2.307758	0.020155
C	-4.717150	-2.433940	1.114705
C	-3.757143	-1.450528	1.422272
C	-4.522965	1.109772	-1.374251
H	-6.205955	-1.014822	-1.618023
C	-6.591922	-3.399106	-0.305020
H	-4.782710	-3.326141	1.759963
C	-2.836631	-1.615094	2.605354
H	-3.541090	1.212965	-1.890222
H	-4.665339	2.035830	-0.776275
H	-5.320273	1.084821	-2.142510
H	-6.136782	-4.165338	-0.971030
H	-7.482941	-2.999450	-0.830168
H	-6.934817	-3.926428	0.608390
H	-3.091926	-2.525304	3.182681
H	-2.894331	-0.748898	3.299206
H	-1.775673	-1.690354	2.274616
C	0.375568	3.789576	-0.091256
C	1.381417	2.346081	1.656163
C	1.619327	4.433063	-0.234215
C	2.602912	3.027113	1.465783
C	2.748377	4.061894	0.524165
C	4.067991	4.778035	0.339420
H	1.699047	5.266823	-0.952159
C	1.265688	1.292918	2.730256
H	3.463492	2.743287	2.093732
C	-0.816283	4.258709	-0.887569
H	-1.124287	3.481442	-1.621991
H	-0.579178	5.190380	-1.437609
H	-1.695012	4.462605	-0.239417
H	0.429168	1.508371	3.428999
H	2.196005	1.242322	3.328951
H	1.072821	0.285501	2.297579
H	4.825370	4.439361	1.074034
H	3.951874	5.877103	0.451552
H	4.481140	4.604924	-0.677914
C	1.893721	-1.394586	-1.867651
Cl	-1.129813	1.293146	-2.658440
Cl	0.357315	-1.573976	0.958961
O	3.385273	-3.284189	-0.576208
C	3.618151	-4.339214	0.398446
C	4.944596	-5.070087	0.153360
H	2.801067	-5.045990	0.138241
C	3.389206	-3.885797	1.842268
H	4.203645	-3.239798	2.225934
H	3.329088	-4.778493	2.498819
H	2.434684	-3.326794	1.917992
H	5.060966	-5.311082	-0.922589
H	4.952365	-6.023824	0.721181
H	5.829172	-4.484474	0.475701
C	3.876341	-2.019514	-0.480724
C	3.127875	-1.008165	-1.167411
C	5.082966	-1.672055	0.169165
C	5.545862	-0.347393	0.148146
C	4.819835	0.653801	-0.521635
C	3.625767	0.315128	-1.170513
H	6.491006	-0.100571	0.658190
H	5.677352	-2.443158	0.675443
H	3.042584	1.101904	-1.674812
H	5.180474	1.693281	-0.533330
C	-1.709974	-1.324532	-1.222454
C	1.246546	-0.673320	-2.840233

C	-0.894398	0.148635	2.690274
H	0.900553	1.408336	2.989011
H	1.156735	-0.321210	3.396604
H	-1.191130	-0.823316	3.146978
H	-1.454820	0.949584	3.215332
C	2.398042	0.049647	0.944403
C	-2.588736	0.077811	0.856269
C	-3.303592	1.284697	0.649826
C	-4.670981	1.199774	0.318281
C	-5.333144	-0.038373	0.193669
C	-4.586371	-1.216711	0.401806
C	-3.217858	-1.188503	0.735406
C	-2.602601	2.621136	0.727464
H	-5.233467	2.132883	0.146384
C	-6.808631	-0.105436	-0.132078
H	-5.082806	-2.196169	0.296233
C	-2.437691	-2.470656	0.907736
H	-1.784871	2.685370	-0.022341
H	-2.137089	2.790590	1.721966
H	-3.309574	3.452927	0.541430
H	-7.166284	0.829243	-0.608449
H	-7.413458	-0.259132	0.788870
H	-7.038599	-0.950141	-0.813392
H	-3.098408	-3.353123	0.802844
H	-1.952272	-2.533692	1.905141
H	-1.627392	-2.553219	0.151105
C	3.120530	1.255079	0.732362
C	3.059512	-1.210398	0.942606
C	4.484536	1.161005	0.391575
C	4.425307	-1.243479	0.601594
C	5.151275	-0.075123	0.296524
C	6.601873	-0.147679	-0.123739
H	5.044853	2.092394	0.203357
C	2.344652	-2.483669	1.326777
H	4.940239	-2.218744	0.585772
C	2.499833	2.616667	0.945660
H	1.411997	2.619703	0.750311
H	2.956878	3.370084	0.274843
H	2.673529	2.960083	1.990708
H	1.746326	-2.358332	2.253639
H	3.070177	-3.303149	1.497278
H	1.644521	-2.802627	0.525668
H	7.110112	-1.034501	0.306320
H	7.164522	0.757849	0.181881
H	6.687974	-0.226723	-1.230037
Cl	0.864954	2.078650	-1.926201
Cl	0.558716	-2.337906	-1.652329
C	-1.607842	0.029259	-2.075066
H	-1.679703	-0.040820	-3.192039
H	-2.561940	0.158018	-1.529198

H	1.539551	-2.411793	-1.640610
H	0.419701	-1.118797	-3.411661
H	1.598924	0.309430	-3.189224
H	-1.805588	-2.282508	-0.663254
H	-2.393276	-1.175825	-2.089179

Table S3. Coordinates data set, absolute energies (a.u.) for DFT all the optimized ammonium tagged complexes (AquaMet™).

Precat				TS_Open			
103				103			
PENJOLL-precat SCF Done: -3287.58987447 A.U.				PENJOLL-TSopenFFall SCF Done: -3287.55982492 A.U.			
Ru	-2.211045	0.191413	-0.104445	Ru	-2.095474	0.500935	-0.401998
C	-0.249587	0.134430	-0.218149	C	-0.174935	0.236599	-0.373055
N	0.508955	1.281724	-0.279198	N	0.709572	1.287424	-0.458265
N	0.636532	-0.925386	-0.337063	N	0.586913	-0.922335	-0.320113
C	2.053832	-0.477633	-0.264688	C	2.029721	-0.612464	-0.124214
C	1.929351	1.019671	-0.563035	C	2.105729	0.840829	-0.598600
H	2.611141	1.630666	0.070325	H	2.267265	-0.650693	0.967101
H	2.143791	1.235276	-1.638780	H	2.810738	1.450105	0.010814
C	0.346830	-2.313902	-0.110387	H	2.412412	0.900239	-1.672497
C	0.052658	2.646009	-0.170383	C	0.122915	-2.261062	-0.092944
C	-0.319621	3.369422	-1.335344	C	0.409397	2.696675	-0.507757
C	-0.757454	4.702083	-1.179375	C	0.185634	3.334050	-1.755912
C	-0.781925	5.339919	0.074265	C	-0.098901	4.716357	-1.754850
C	-0.307680	4.622576	1.190638	C	-0.112983	5.475727	-0.571513
C	0.131639	3.288356	1.097836	C	0.208452	4.825164	0.637241
C	-0.159847	2.795417	-2.724328	C	0.487421	3.447935	0.698852
H	-1.066802	5.262304	-2.078271	C	0.356506	2.614325	-3.074262
C	-1.292495	6.756305	0.223762	H	-0.296704	5.213474	-2.719749
H	-0.267258	5.119249	2.174748	C	-0.460432	6.947864	-0.587673
C	0.733123	2.600427	2.297988	H	0.250376	5.410396	1.571290
H	-0.528547	1.753533	-2.798320	C	0.926436	2.816559	1.996948
H	0.910893	2.810678	-3.029117	H	0.090106	1.543357	-3.013616
H	-0.716297	3.401400	-3.466763	H	1.412393	2.696968	-3.418623
H	-1.327125	7.285364	-0.750106	H	-0.279120	3.067880	-3.860362
H	-0.657763	7.348373	0.915593	H	-0.371923	7.380236	-1.604802
H	-2.322568	6.767738	0.644003	H	0.195120	7.529426	0.093521
H	0.540506	3.185744	3.218771	H	-1.506617	7.113940	-0.247809
H	1.838374	2.498931	2.188349	H	0.714831	3.491108	2.849922
H	0.301579	1.591192	2.441773	H	2.023928	2.616867	1.989342
C	0.077986	-3.156239	-1.222200	H	0.399537	1.860626	2.181844
C	0.362917	-2.829512	1.214643	C	-0.148565	-3.096798	-1.210178
C	-0.139395	-4.528605	-0.982557	C	-0.017295	-2.743807	1.235626
C	0.147363	-4.211528	1.395724	C	-0.538043	-4.428750	-0.967816
C	-0.095680	-5.081001	0.313527	C	-0.404147	-4.087974	1.420657
C	-0.287256	-6.565800	0.533498	C	-0.666608	-4.948103	0.337005
H	-0.357257	-5.185521	-1.841777	C	-1.111376	-6.377074	0.558295
C	0.510631	-1.919121	2.412509	H	-0.751899	-5.081018	-1.831646
H	0.151633	-4.614926	2.422707	C	0.157344	-1.827876	2.426093
C	-0.023528	-2.597774	-2.621906	H	-0.521692	-4.466246	2.450286
H	-0.772038	-1.777708	-2.675318	C	-0.067508	-2.564868	-2.621276
H	-0.315152	-3.388437	-3.341022	H	-0.786908	-1.731438	-2.776686
H	0.940239	-2.167055	-2.967162	H	-0.288209	-3.361446	-3.358804
H	1.463889	-1.349638	2.406814	H	0.936941	-2.153405	-2.853473
H	0.471881	-2.498007	3.355947	H	-0.489789	-0.929713	2.330004
H	-0.306291	-1.165057	2.436384	H	1.199819	-1.459017	2.535319
H	-0.669471	-6.783970	1.551320	H	-0.111799	-2.346835	3.366643
H	0.674561	-7.114403	0.421886	H	-2.195070	-6.495708	0.339262
H	-0.994436	-7.001345	-0.201715	H	-0.947678	-6.700757	1.605560
C	-2.677594	-1.563635	0.235568	H	-0.570661	-7.081037	-0.108454
Cl	-2.500632	0.293215	-2.451600	C	-2.789967	-1.151729	-0.028632
Cl	-2.313410	1.066997	2.079832	Cl	-2.355897	0.560803	-2.725239
O	-4.517033	0.323130	-0.033151	Cl	-2.313925	1.704964	1.574403
C	-5.238458	1.596286	-0.171492	O	-4.908789	-0.212620	1.620470
C	-6.094989	1.620388	-1.438026	C	-5.707299	0.796129	2.294638
H	-4.383637	2.286720	-0.323162	C	-6.274817	1.844393	1.334081
C	-5.937478	1.993957	1.128628	H	-4.926523	1.297349	2.903885
H	-6.829444	1.376186	1.354483	C	-6.732185	0.183257	3.258489

H	-6.271198	3.049194	1.046364	H	-7.612550	-0.252551	2.743903
H	-5.224163	1.918836	1.973036	H	-7.105605	0.968361	3.948792
H	-5.491432	1.288053	-2.305644	H	-6.258730	-0.611295	3.869977
H	-6.429835	2.661919	-1.624406	H	-5.463813	2.253212	0.698871
H	-7.000226	0.984986	-1.366497	H	-6.705216	2.683005	1.919722
C	-5.069617	-0.900913	0.218410	H	-7.073118	1.446381	0.676228
C	-4.080311	-1.923788	0.361429	C	-5.294389	-0.902839	0.516116
C	-6.437305	-1.201534	0.333737	C	-4.229502	-1.422249	-0.284584
C	-6.828063	-2.529441	0.595112	C	-6.633327	-1.199659	0.166151
C	-5.874499	-3.554169	0.740690	C	-6.918925	-2.002162	-0.949610
C	-4.511594	-3.248731	0.623474	C	-5.879716	-2.540771	-1.727855
H	-7.901794	-2.759214	0.685457	C	-4.550789	-2.254355	-1.385705
H	-7.200599	-0.421630	0.224025	H	-7.969976	-2.217301	-1.201487
H	-3.746775	-4.034511	0.734114	H	-7.457768	-0.820905	0.783918
H	-6.197473	-4.586566	0.945562	H	-3.725167	-2.657042	-1.993728
H	-1.957766	-2.392155	0.372200	H	-6.102485	-3.176528	-2.598770
C	3.027196	-1.231894	-1.194063	H	-2.169490	-2.024110	0.259724
H	2.430661	-0.611888	0.778622	C	3.010174	-1.565916	-0.836125
N	4.405370	-0.885060	-0.881193	H	2.719448	-2.626583	-0.644208
H	2.811799	-0.975963	-2.254542	H	2.947872	-1.416543	-1.935628
H	2.863893	-2.330485	-1.096813	C	4.874466	-1.972703	0.777711
C	5.225277	-0.115022	-1.781283	C	5.399275	-0.875874	-1.311593
C	5.149634	-1.671671	0.071703	C	5.856002	-1.072116	1.529096
C	6.057599	-0.771467	0.908163	H	5.323029	-2.981191	0.540943
H	5.730633	-2.511074	-0.409922	H	4.042073	-2.173417	1.484301
H	4.450601	-2.157446	0.783601	C	6.373032	0.067636	-0.603208
C	6.156841	0.809885	-0.991433	H	5.944699	-1.737107	-1.797222
H	4.586884	0.548798	-2.400211	H	4.946631	-0.292846	-2.139793
H	5.803336	-0.754231	-2.511201	H	6.325620	-1.587294	2.391756
N	7.008946	0.055584	0.039251	H	5.328150	-0.131942	1.845572
H	5.438010	0.003651	1.435484	H	7.200163	0.399451	-1.260326
H	6.676983	-1.339957	1.628793	H	5.811438	0.948041	-0.190855
H	5.546340	1.516842	-0.369798	N	4.370083	-1.296078	-0.392843
H	6.864594	1.354998	-1.648983	N	7.000913	-0.571352	0.638250
C	7.652917	1.092878	0.927466	C	7.713241	0.520569	1.400795
H	8.325395	1.717607	0.308737	H	8.156680	0.079545	2.314035
H	8.226584	0.582777	1.722377	H	8.503519	0.952730	0.760514
H	6.817560	1.697625	1.365676	H	6.937720	1.288966	1.651498
C	8.059783	-0.780574	-0.676904	C	7.945860	-1.720657	0.318552
C	8.947527	-1.649300	0.207256	H	8.323400	-2.067219	1.302432
H	8.667927	-0.051590	-1.250853	H	7.326151	-2.537737	-0.098421
H	7.520554	-1.406784	-1.413538	C	9.101201	-1.401196	-0.623082
H	9.511724	-1.066056	0.961823	H	9.755015	-0.588832	-0.248224
H	9.694026	-2.148665	-0.443298	H	9.730362	-2.310044	-0.712548
H	8.382776	-2.448353	0.726558	H	8.761458	-1.140112	-1.644623
Cl	4.536856	2.115094	1.619830	Cl	4.727693	2.051531	1.533478

Act				TS_Ci1			
103				109			
PENJOLL-Act SCF Done: -3287.57212486 A.U.				PENJOLL-TS1FFllqst3 SCF Done: -3366.09107456 A.U.			
Ru	1.936656	1.362824	0.484197	Ru	1.593471	1.114867	0.408198
C	0.082674	0.812713	0.413269	C	0.013667	0.309301	-0.366062
N	-0.932690	1.720496	0.213937	N	-1.076116	1.066967	-0.711070
N	-0.511405	-0.411331	0.670537	N	-0.361763	-1.023144	-0.463570
C	-1.995519	-0.367524	0.511344	C	-1.804260	-1.178020	-0.788858
C	-2.271316	1.139560	0.389910	C	-2.254475	0.267076	-1.088753
H	-2.288224	-0.855602	-0.447782	H	-1.894159	-1.822102	-1.692369
H	-2.917682	1.356801	-0.487224	H	-2.491565	0.423231	-2.165182
H	-2.746369	1.558418	1.310550	H	-3.163622	0.568984	-0.521016
C	0.105182	-1.711204	0.627129	C	0.494159	-2.171759	-0.598996
C	-0.817670	3.114998	-0.132257	C	-1.137088	2.506927	-0.794937
C	-0.825291	4.101219	0.890111	C	-1.693464	3.256810	0.275807
C	-0.757154	5.456647	0.506240	C	-1.728866	4.661671	0.148820
C	-0.719570	5.850391	-0.844410	C	-1.291654	5.324279	-1.012181
C	-0.784991	4.845806	-1.830088	C	-0.843046	4.538619	-2.092889
C	-0.844655	3.476725	-1.507557	C	-0.769326	3.136146	-2.016862
C	-0.953160	3.737023	2.351438	C	-2.344669	2.597967	1.465868
H	-0.746676	6.227264	1.295661	H	-2.144571	5.251127	0.983297
C	-0.598572	7.308041	-1.230060	C	-1.308133	6.833870	-1.104264
H	-0.789450	5.133659	-2.894955	H	-0.547958	5.031487	-3.034568
C	-0.938925	2.438018	-2.597737	C	-0.335004	2.336942	-3.222787
H	-0.157999	3.035221	2.679076	H	-1.803633	1.687807	1.788723

H	-1.931051	3.250980	2.564149
H	-0.892328	4.642693	2.986745
H	-0.958282	7.978754	-0.423446
H	-1.171022	7.536984	-2.152622
H	0.461816	7.577178	-1.432355
H	-1.007763	2.923672	-3.591121
H	-1.818933	1.766424	-2.488067
H	-0.031573	1.799586	-2.597964
C	0.525095	-2.335217	1.834127
C	0.215239	-2.381259	-0.623490
C	1.020869	-3.652846	1.765820
C	0.712850	-3.702171	-0.628076
C	1.109194	-4.361275	0.550888
C	1.613051	-5.788068	0.524982
H	1.350975	-4.138673	2.699885
C	-0.113172	-1.690634	-1.927190
H	0.803205	-4.224772	-1.595598
C	0.491077	-1.610235	3.158085
H	1.190337	-0.746818	3.161502
H	0.769634	-2.290356	3.987186
H	-0.509780	-1.187152	3.379988
H	0.436338	-0.729090	-2.010068
H	-1.193093	-1.448073	-2.052085
H	0.181687	-2.324285	-2.786737
H	1.796938	-6.140213	-0.509847
H	0.878508	-6.483828	0.987170
H	2.557756	-5.896806	1.098195
C	2.833654	-0.238362	0.294405
Cl	1.966540	1.757725	2.796195
Cl	2.385084	2.303537	-1.593941
O	4.277394	-2.005350	-1.201598
C	4.791470	-2.921148	-2.199651
C	5.620738	-2.215000	-3.279354
H	3.845305	-3.252911	-2.677903
C	5.445516	-4.169902	-1.592887
H	6.449346	-3.978678	-1.165337
H	5.559386	-4.944128	-2.380019
H	4.802178	-4.587373	-0.792547
H	5.077106	-1.327259	-3.659990
H	5.784787	-2.909092	-4.129614
H	6.613810	-1.882645	-2.918390
C	5.030730	-1.260079	-0.349199
C	4.284928	-0.320446	0.451583
C	6.433126	-1.334417	-0.210181
C	7.104343	-0.498226	0.699691
C	6.394154	0.421446	1.489491
C	5.001832	0.503805	1.359772
H	8.200106	-0.576338	0.787481
H	7.015717	-2.042457	-0.812158
H	4.424717	1.193794	1.996746
H	6.921390	1.066216	2.209212
H	2.340401	-1.142612	-0.105863
C	-2.742982	-1.083695	1.665406
H	-2.187445	-2.013705	1.910558
H	-2.707962	-0.450007	2.582416
C	-4.460128	-2.742200	0.822089
C	-5.211722	-0.516219	1.435935
C	-5.157475	-2.621268	-0.540687
H	-5.082807	-3.355602	1.529284
H	-3.536547	-3.331626	0.649409
C	-5.893074	-0.345952	0.071227
H	-5.971439	-0.800701	2.214785
H	-4.835005	0.482014	1.737429
H	-5.525850	-3.600819	-0.909662
H	-4.477119	-2.143740	-1.292082
H	-6.771390	0.327546	0.116160
H	-5.165118	0.018305	-0.697834
N	-4.121440	-1.461033	1.393832
N	-6.374405	-1.684103	-0.496660
C	-6.819129	-1.450601	-1.919964
H	-7.150375	-2.416746	-2.346704
H	-3.393382	2.325768	1.198685
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H	-2.066792	7.277753	-0.428222
H	-1.521272	7.178402	-2.137100
H	-0.321689	7.260980	-0.816911
H	-0.300334	2.979814	-4.124430
H	-1.027485	1.495316	-3.433054
H	0.679546	1.915031	-3.066336
C	0.787250	-3.010198	0.509249
C	1.004338	-2.472047	-1.893403
C	1.557054	-4.170688	0.278397
C	1.760938	-3.645736	-2.067670
C	2.038441	-4.519258	-0.996770
C	2.818673	-5.797355	-1.212181
H	1.795524	-4.819506	1.138534
C	0.792561	-1.520389	-3.048034
H	2.154932	-3.877288	-3.071889
C	0.337812	-2.690520	1.916975
H	0.205414	-1.602555	2.079170
H	1.086946	-3.053724	2.649001
H	-0.620832	-3.197322	2.163583
H	1.255324	-0.533334	-2.833253
H	-0.282729	-1.327714	-3.249183
H	1.243566	-1.917311	-3.978444
H	2.135682	-6.660385	-1.376552
H	3.447137	-6.046421	-0.332667
H	3.478312	-5.731488	-2.101079
C	2.774602	-0.303442	0.398833
Cl	0.628017	0.992773	2.556190
Cl	2.536671	2.299300	-1.389962
O	5.044219	-1.415364	-0.632327
C	6.128243	-1.807200	-1.512289
C	7.101652	-0.658163	-1.797262
H	5.568725	-2.005565	-2.451288
C	6.791683	-3.128863	-1.100425
H	7.468466	-3.029656	-0.228874
H	7.394300	-3.517349	-1.947769
H	6.019708	-3.885384	-0.854579
H	6.543998	0.252498	-2.094288
H	7.770138	-0.942590	-2.636142
H	7.739761	-0.404615	-0.927955
C	5.193022	-0.921610	0.626586
C	4.007985	-0.318745	1.185417
C	6.379658	-0.961348	1.388806
C	6.411098	-0.417884	2.685844
C	5.264930	0.169584	3.246961
C	4.082397	0.221160	2.496792
H	7.350593	-0.463083	3.260290
H	7.288831	-1.418514	0.979352
H	3.165271	0.657654	2.923112
H	5.290714	0.582711	4.267160
C	2.524108	4.007914	1.890664
C	3.828517	3.715828	1.735545
H	2.683489	-1.121734	-0.340414
H	4.287352	3.670968	0.734141
H	4.479886	3.492201	2.597087
H	1.880700	4.235456	1.024432
H	2.045995	4.032888	2.883588
C	-2.567469	-1.844774	0.387871
H	-2.256477	-2.921115	0.456712
H	-2.231917	-1.349852	1.322042
C	-4.708190	-2.272239	-0.811246
C	-4.748774	-1.801236	1.542089
C	-6.063961	-1.591032	-0.998265
H	-4.801038	-3.393877	-0.717164
H	-4.149198	-2.096162	-1.753873
C	-6.097133	-1.099399	1.418282
H	-4.858929	-2.874271	1.876741
H	-4.197958	-1.280651	2.353433
H	-6.654557	-2.051093	-1.816150
H	-5.903129	-0.491923	-1.168268

H -7.650936 -0.722864 -1.925186 H -5.934522 -1.044369 -2.472167 C -7.491016 -2.323499 0.318098 H -7.737487 -3.262702 -0.218180 H -7.053546 -2.611581 1.292795 C -8.740037 -1.474769 0.528373 H -9.217996 -1.164415 -0.421670 H -9.481059 -2.087899 1.080486 H -8.546453 -0.571401 1.139586 Cl -3.716423 -0.343550 -2.534280	H -6.706084 -1.182709 2.338569 H -5.926854 -0.022359 1.138698 N -4.006614 -1.670819 0.303502 N -6.936042 -1.643526 0.260802 C -8.086816 -0.688762 0.047048 H -8.688986 -1.047341 -0.809894 H -8.704027 -0.655727 0.963114 H -7.627688 0.313264 -0.159004 C -7.433670 -3.063588 0.485427 H -8.018807 -3.314591 -0.423198 H -6.539903 -3.717205 0.489353 C -8.263125 -3.293829 1.743987 H -9.174125 -2.664271 1.782697 H -8.597059 -4.351319 1.745552 H -7.682909 -3.134826 2.674249 Cl -5.709361 1.645946 -0.353548
TS_Conc	Ci1
109 PENJOLL-TSconc SCF Done: -3366.08812308 A.U. C 0.181844 0.249948 0.183002 C -1.981981 -0.689529 -0.044232 H -2.244434 -0.629092 -1.127142 C -2.108962 0.703385 0.571237 H -2.863787 1.334130 0.048931 H -2.372818 0.652827 1.656974 C -0.090201 -3.030616 -1.170534 C 0.263994 -4.395044 -1.143603 H 0.226139 -4.965807 -2.087107 C 0.659772 -5.045843 0.041334 C 0.693528 -4.288064 1.228439 H 0.982264 -4.779132 2.173256 C 0.355328 -2.918550 1.262015 C -0.028994 -2.290462 0.044281 C -0.519064 -2.388864 -2.468812 H -0.252684 -3.031871 -3.330886 H -0.037424 -1.396208 -2.607473 H -1.620330 -2.232920 -2.509453 C 1.060668 -6.504557 0.032897 H 0.902748 -6.979141 1.022725 H 2.138619 -6.621695 -0.216776 H 0.490582 -7.082544 -0.723024 C 0.398954 -2.163292 2.566107 H 0.528587 -2.856733 3.420141 H -0.527337 -1.574198 2.732309 H 1.234427 -1.426101 2.583032 C -0.547194 2.658175 0.548424 C -0.759570 3.486182 -0.589160 C -0.638845 4.880670 -0.420270 H -0.790228 5.528633 -1.300001 C -0.357652 5.467196 0.829245 C -0.229322 4.618106 1.945189 H -0.055486 5.057553 2.942053 C -0.338573 3.216068 1.838871 C -1.155992 2.912418 -1.927054 H -1.081861 3.685457 -2.717787 H -2.217830 2.570154 -1.903340 H -0.515664 2.054010 -2.220702 C -0.199742 6.965302 0.964534 H -0.902305 7.511506 0.301918 H 0.827605 7.284771 0.681080 H -0.372539 7.303799 2.006208 C -0.259413 2.357590 3.078293 H -0.208711 2.988533 3.987539 H 0.639197 1.701876 3.058051 H -1.146990 1.696755 3.177479 C 2.686924 -1.063082 -0.378598 H 2.219986 -1.706978 -1.153828 C 3.937200 -1.579024 0.195816 C 4.018258 -2.897995 0.712525 H 3.123127 -3.537126 0.667708 C 5.195638 -3.370809 1.309839	109 PENJOLL-CI1 SCF Done: -3366.10527741 A.U. Ru 1.874612 1.534905 0.238952 C 0.023227 0.693813 0.262365 N -1.073239 1.507479 0.211509 N -0.432213 -0.597323 0.383732 C -1.913274 -0.677383 0.212502 C -2.337284 0.779382 0.429676 H -2.139485 -0.971571 -0.840769 H -3.140838 1.096840 -0.271937 H -2.688559 0.947101 1.476891 C 0.339396 -1.809724 0.320524 C -1.079220 2.936218 -0.000251 C -1.041501 3.822597 1.111053 C -1.037878 5.209921 0.852910 C -1.128956 5.729971 -0.451308 C -1.279623 4.820063 -1.516731 C -1.282737 3.425561 -1.322740 C -1.110515 3.327813 2.536462 H -0.987563 5.903041 1.709812 C -1.081366 7.220224 -0.706329 H -1.413992 5.204976 -2.541566 C -1.573724 2.499728 -2.477043 H -0.367110 2.531792 2.745283 H -2.123674 2.925485 2.760697 H -0.925174 4.157316 3.247286 H -1.297862 7.801388 0.212763 H -1.808943 7.524275 -1.487316 H -0.075357 7.531370 -1.065138 H -1.542291 3.054141 -3.435626 H -2.590138 2.051241 -2.381618 H -0.827485 1.683751 -2.535651 C 0.781078 -2.418552 1.526926 C 0.565871 -2.426348 -0.939572 C 1.427092 -3.667662 1.444181 C 1.210760 -3.680801 -0.961190 C 1.641019 -4.323453 0.215155 C 2.333310 -5.668183 0.171701 H 1.771406 -4.143503 2.378031 C 0.188433 -1.740722 -2.233102 H 1.386064 -4.165452 -1.936795 C 0.578457 -1.750742 2.864966 H 1.028680 -0.733889 2.882914 H 1.030810 -2.352424 3.677689 H -0.498750 -1.619066 3.102078 H 0.641784 -0.725797 -2.303114 H -0.908806 -1.601592 -2.340008 H 0.532525 -2.330683 -3.105204 H 2.305233 -6.112818 -0.843409 H 1.862851 -6.390486 0.872234 H 3.399760 -5.581362 0.473006 C 2.867427 -0.041006 0.064354 Cl 1.871940 1.646681 2.661549 Cl 1.765189 1.837921 -2.148810

H	5.225067	-4.388528	1.730489	O	4.435210	-1.695419	-1.417125
C	6.331999	-2.544095	1.376971	C	5.172260	-2.321142	-2.499088
H	7.255511	-2.904960	1.857223	C	6.450436	-1.557799	-2.862771
C	6.291988	-1.255447	0.819754	H	4.456923	-2.183684	-3.337574
C	5.113498	-0.776950	0.220309	C	5.355886	-3.832950	-2.311227
N	-0.513836	-0.939830	0.077828	H	6.135295	-4.094224	-1.568380
N	-0.741525	1.234830	0.415648	H	5.652605	-4.288690	-3.278840
Cl	1.610287	0.531138	-2.510798	H	4.402153	-4.298749	-1.992029
Cl	2.651196	0.600881	2.276392	H	6.229994	-0.479776	-2.995735
Ru	2.097842	0.674343	-0.079153	H	6.848340	-1.946612	-3.822929
H	7.172426	-0.595830	0.847947	H	7.248552	-1.658289	-2.101272
O	5.090950	0.479908	-0.349247	C	4.910394	-1.450889	-0.168804
C	5.515255	0.639362	-1.758202	C	4.113976	-0.543389	0.626240
C	3.034163	2.848777	0.303245	C	6.095590	-1.996611	0.371724
C	2.640679	2.898271	-1.012211	C	6.506757	-1.655085	1.671270
H	4.054213	2.555734	0.596135	C	5.750527	-0.765137	2.454462
H	2.389020	3.242275	1.104486	C	4.577693	-0.211593	1.927471
H	1.675664	3.329931	-1.310440	H	7.437452	-2.092175	2.068537
H	3.325438	2.642955	-1.834013	H	6.707877	-2.690700	-0.217133
C	6.216888	1.992886	-1.840058	H	3.960079	0.481554	2.520893
H	5.585758	2.798048	-1.415380	H	6.077533	-0.500878	3.472055
H	6.434094	2.249396	-2.897588	C	3.041026	3.479251	0.422675
H	7.174854	1.974041	-1.279084	C	4.034943	2.599103	0.037107
C	6.386754	-0.499586	-2.284706	H	2.474301	-0.697314	-0.737182
H	4.573503	0.663357	-2.354865	H	4.264657	2.430776	-1.026330
H	7.354948	-0.571421	-1.747219	H	4.726909	2.174173	0.779092
H	6.603664	-0.304580	-3.355357	H	2.483493	4.060143	-0.334979
H	5.876999	-1.480960	-2.218046	H	2.942607	3.799611	1.472287
C	-2.893351	-1.753237	0.599356	C	-2.627408	-1.689818	1.130043
N	-4.287570	-1.451153	0.304804	H	-2.094342	-2.669569	1.103106
H	-2.740191	-1.767020	1.700150	H	-2.584737	-1.336865	2.182863
H	-2.613390	-2.769263	0.236298	C	-4.372650	-2.824738	-0.260098
C	-5.228192	-1.124684	1.348507	C	-5.106123	-1.458043	1.596236
C	-4.899510	-2.019800	-0.871293	C	-5.531832	-2.323057	-1.121688
C	-6.262764	-0.127502	0.824032	H	-4.589929	-3.835770	0.192210
H	-4.701440	-0.617848	2.183042	H	-3.521672	-2.984725	-0.954909
H	-5.726465	-2.032006	1.799861	C	-6.271285	-0.911090	0.768213
C	-5.941932	-1.058840	-1.444098	H	-5.444266	-2.293407	2.277033
H	-5.329215	-3.047321	-0.687929	H	-4.784333	-0.632174	2.263656
H	-4.135968	-2.150670	-1.666447	H	-5.883977	-3.088657	-1.842846
N	-7.002455	-0.651309	-0.410737	H	-5.225003	-1.375164	-1.641487
H	-6.488376	-1.492621	-2.306173	H	-7.146246	-0.641537	1.391015
H	-5.444276	-0.089195	-1.716801	H	-5.923294	-0.032263	0.162491
H	-7.026620	0.131087	1.582711	N	-4.018733	-1.834110	0.727603
H	-5.744155	0.794363	0.448645	N	-6.752595	-1.908578	-0.288788
C	-7.916156	-1.831504	-0.113510	C	-7.693505	-1.173985	-1.213917
C	-8.995963	-1.595972	0.936817	H	-8.042625	-1.878644	-1.992983
H	-7.263324	-2.674023	0.185470	H	-8.550348	-0.790547	-0.630743
H	-8.368812	-2.101094	-1.089790	H	-7.105483	-0.329541	-1.656950
H	-8.579032	-1.405555	1.945319	C	-7.416877	-3.142313	0.303218
H	-9.611505	-2.515653	1.007692	H	-7.691206	-3.771631	-0.568182
H	-9.679763	-0.765300	0.672692	H	-6.633333	-3.686575	0.864398
C	-7.780518	0.499938	-1.002700	C	-8.629476	-2.893692	1.193327
H	-7.030925	1.293090	-1.255690	H	-9.451806	-2.369391	0.667824
H	-8.505765	0.870279	-0.255741	H	-9.024553	-3.878499	1.515720
H	-8.308445	0.138345	-1.905849	H	-8.378609	-2.328175	2.112529
Cl	-4.839008	2.073677	-1.263929	Cl	-5.126846	0.900851	-1.808296

TS_MCy				MCy			
109				109			
PENJOLL-TSMCy SCF Done: -3366.10238633 A.U.				PENJOLL-MCy SCF Done: -3366.11455475 A.U.			
Ru	1.771061	1.627781	0.003773	Ru	1.779185	1.462610	0.123671
C	-0.074028	0.820485	0.327050	C	-0.112862	0.801682	0.335753
N	-1.231683	1.533035	0.263924	N	-1.240458	1.549370	0.257586
N	-0.398719	-0.505821	0.446508	N	-0.460066	-0.513395	0.475683
C	-1.850426	-0.721938	0.182031	C	-1.918170	-0.695475	0.219017
C	-2.424389	0.676035	0.437154	C	-2.453001	0.722804	0.458751
C	-2.506729	-1.847039	1.000884	C	-2.596339	-1.793684	1.057243
H	-1.979213	-0.969779	-0.898791	H	-2.056979	-0.956036	-0.857518
H	-3.250458	0.938512	-0.260882	H	-3.279060	0.996620	-0.235454
H	-2.809770	0.776577	1.482190	H	-2.819785	0.850334	1.506787
C	0.512930	-1.605391	0.598040	C	0.454077	-1.621466	0.603622

C	-1.357288	2.967587	0.167414
C	-1.269426	3.753193	1.347587
C	-1.396049	5.153444	1.224364
C	-1.645763	5.774902	-0.012000
C	-1.817383	4.953134	-1.144951
C	-1.704518	3.551116	-1.085239
C	-1.088327	3.131341	2.711581
H	-1.314281	5.771516	2.134443
C	-1.762832	7.278667	-0.130416
H	-2.066713	5.414950	-2.115319
C	-2.016198	2.710789	-2.297706
H	-0.042510	2.783779	2.861328
H	-1.748954	2.250329	2.851691
H	-1.325208	3.864253	3.508127
H	-1.606509	7.781778	0.844602
H	-2.762097	7.578827	-0.513002
H	-1.014305	7.684252	-0.844911
H	-2.063862	3.343582	-3.206095
H	-3.006499	2.209516	-2.189856
H	-1.241146	1.935212	-2.460894
C	0.985475	-1.922774	1.901333
C	0.867929	-2.397434	-0.525932
C	1.816134	-3.049546	2.053190
C	1.702400	-3.515061	-0.313242
C	2.188061	-3.859949	0.961966
C	3.109738	-5.043063	1.157469
H	2.183535	-3.301102	3.062298
C	0.383155	-2.064848	-1.917819
H	1.980044	-4.135671	-1.182423
C	0.624804	-1.073826	3.096135
H	1.114096	-0.074486	3.039160
H	0.940917	-1.561795	4.039140
H	-0.466467	-0.879716	3.153605
H	-0.693757	-2.310099	-2.055031
H	0.943677	-2.646244	-2.676378
H	0.507739	-0.983513	-2.148156
H	2.874169	-5.594697	2.091199
H	4.167721	-4.708778	1.237016
H	3.048922	-5.756456	0.310731
C	3.131613	0.354749	-0.384204
Cl	2.199441	2.150337	2.330804
Cl	1.255762	1.504693	-2.368048
O	4.781805	-1.366128	-1.704520
C	5.599568	-2.077187	-2.668280
C	7.043209	-1.561668	-2.719200
H	5.108866	-1.767389	-3.615306
C	5.455683	-3.602023	-2.573794
H	6.009970	-4.048067	-1.725153
H	5.841697	-4.063604	-3.506151
H	4.386974	-3.876962	-2.471995
H	7.052542	-0.455791	-2.795854
H	7.548113	-1.968954	-3.619542
H	7.644157	-1.851046	-1.834914
C	4.975415	-1.327618	-0.361202
C	4.109951	-0.428758	0.374830
C	5.944478	-2.087143	0.333761
C	6.078978	-1.970276	1.726740
C	5.250721	-1.100594	2.456269
C	4.281394	-0.350949	1.780773
H	6.847863	-2.570557	2.240463
H	6.608727	-2.771263	-0.207796
H	3.626532	0.345197	2.327709
H	5.359886	-1.007139	3.547752
C	2.828279	3.441330	-0.511116
C	3.892283	2.507685	-0.509018
H	3.167419	0.118899	-1.466851
H	4.319549	2.181021	-1.471006
H	4.532768	2.406714	0.381110
H	2.419974	3.802602	-1.469645
H	2.690005	4.081863	0.377201
N	-3.876034	-2.048657	0.545876

C	-1.334091	2.983033	0.113440
C	-1.218250	3.807656	1.263810
C	-1.322611	5.203321	1.091007
C	-1.570197	5.784940	-0.166645
C	-1.757925	4.926861	-1.268090
C	-1.665734	3.525210	-1.158740
C	-1.030549	3.230198	2.646825
H	-1.225908	5.851785	1.978296
C	-1.638534	7.286947	-0.334774
H	-2.000044	5.357876	-2.254195
C	-1.968807	2.647640	-2.347179
H	-1.181577	4.011310	3.417983
H	-0.012355	2.803362	2.783797
H	-1.753474	2.411880	2.850274
H	-0.680227	7.688162	-0.733033
H	-1.833887	7.799692	0.628814
H	-2.433198	7.582303	-1.050848
H	-2.024774	3.254999	-3.272269
H	-2.951646	2.134477	-2.228093
H	-1.181222	1.879874	-2.488474
C	0.902395	-1.990498	1.903717
C	0.821830	-2.379534	-0.542389
C	1.764440	-3.098425	2.020739
C	1.676784	-3.485350	-0.359371
C	2.169690	-3.856214	0.905621
C	3.127820	-5.014637	1.064670
H	2.123379	-3.380682	3.024709
C	0.328868	-2.031655	-1.926634
H	1.967613	-4.073731	-1.245869
C	0.485642	-1.231725	3.139029
H	1.041374	-0.269662	3.214008
H	0.689675	-1.824407	4.052629
H	-0.591780	-0.969454	3.123761
H	-0.759754	-2.228484	-2.045518
H	0.853189	-2.639563	-2.689884
H	0.501786	-0.958208	-2.163744
H	2.943853	-5.574230	2.005053
H	4.176533	-4.646332	1.104855
H	3.057777	-5.727307	0.217940
C	3.610056	0.771242	-0.428512
Cl	2.165873	1.787490	2.484288
Cl	1.333165	1.383185	-2.259359
O	4.578907	-1.463020	-1.700946
C	5.394936	-1.997134	-2.777146
C	6.799978	-1.389164	-2.819095
H	4.839839	-1.628459	-3.666585
C	5.370618	-3.530752	-2.838854
H	6.015206	-4.008521	-2.073569
H	5.730128	-3.868340	-3.833372
H	4.335285	-3.902520	-2.704606
H	6.746179	-0.281844	-2.808418
H	7.309344	-1.698726	-3.754964
H	7.429273	-1.712789	-1.966154
C	5.005475	-1.308641	-0.412205
C	4.473432	-0.185370	0.309237
C	5.893263	-2.202138	0.229402
C	6.264713	-2.001964	1.568185
C	5.742544	-0.915010	2.290663
C	4.855878	-0.030343	1.663441
H	6.958470	-2.711080	2.048522
H	6.287517	-3.067156	-0.319440
H	4.406786	0.796902	2.234205
H	6.018183	-0.761265	3.345632
C	2.566505	3.252391	-0.178473
C	3.848177	2.340977	-0.247872
H	3.564877	0.508484	-1.499056
H	4.354186	2.619355	-1.194623
H	4.482813	2.514666	0.640066
H	2.300600	3.741193	-1.134074
H	2.553582	3.914441	0.707775
N	-3.963340	-1.987342	0.594765

H -2.520105 -1.570835 2.076889	H -2.615084 -1.493391 2.126410
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C -6.234182 -1.472635 0.720729	C -6.306889 -1.350982 0.724925
H -4.774312 -1.218676 2.247773	H -4.862416 -1.097211 2.266486
H -5.196157 -2.939481 2.001127	H -5.321614 -2.812677 2.053241
C -5.343572 -2.463527 -1.358048	C -5.414681 -2.419950 -1.316267
H -4.180481 -4.009944 -0.279924	H -4.303517 -3.963087 -0.180063
H -3.260898 -2.861211 -1.288706	H -3.343139 -2.865419 -1.207646
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H -7.125355 -1.425902 1.375821	H -7.205841 -1.263497 1.364971
H -6.025000 -0.472612 0.255189	H -6.062968 -0.369103 0.238247
C -7.066621 -3.749255 -0.080398	C -7.190828 -3.623321 -0.029873
C -8.258389 -3.809737 0.868677	C -8.399013 -3.624612 0.900595
H -6.196061 -4.270231 0.362411	H -6.341901 -4.155691 0.440669
H -7.297855 -4.258609 -1.038464	H -7.421618 -4.152268 -0.977347
H -8.027498 -3.395890 1.870105	H -8.176652 -3.179490 1.890446
H -8.529476 -4.875600 1.011003	H -8.695056 -4.678719 1.076653
H -9.155291 -3.295858 0.469948	H -9.278157 -3.106976 0.468138
C -7.648586 -1.634018 -1.277954	C -7.695610 -1.525185 -1.290453
H -7.190362 -0.662678 -1.599517	H -7.213713 -0.567061 -1.614838
H -8.532779 -1.457709 -0.638917	H -8.591209 -1.326178 -0.674513
H -7.921461 -2.262867 -2.147114	H -7.958914 -2.160631 -2.157682
Cl -5.437487 0.853613 -1.555257	Cl -5.393784 0.888794 -1.590270
TS_Ci2	Ci2
109	109
PENJOLL-TS2 SCF Done: -3366.09225128 A.U.	PENJOLL-CI2 SCF Done: -3366.09868040 A.U.
Ru 1.653322 1.419209 0.235439	Ru -1.903775 0.830631 -1.035166
C -0.051437 0.679886 -0.551171	C 0.132365 0.672602 -0.645949
N -1.242116 1.328635 -0.658702	N 1.022692 1.661758 -0.378300
N -0.237122 -0.630573 -0.905892	N 0.807480 -0.512252 -0.718919
C -1.677654 -0.947870 -1.098355	C 2.257634 -0.363748 -0.381311
C -2.312943 0.452213 -1.191043	C 2.411834 1.163240 -0.287982
H -1.794874 -1.512018 -2.048723	H 2.449147 -0.795493 0.627876
H -2.543404 0.743572 -2.240469	H 2.874154 1.456625 0.678685
H -3.260880 0.540332 -0.614640	H 3.007432 1.585786 -1.130517
C 0.770430 -1.617279 -1.212631	C 0.228411 -1.839216 -0.736932
C -1.489215 2.740343 -0.508877	C 0.795132 3.065699 -0.145567
C -2.213124 3.210461 0.619810	C 0.992281 3.996831 -1.202272
C -2.450631 4.595543 0.721128	C 0.817904 5.366713 -0.920695
C -2.024990 5.508904 -0.263305	C 0.492839 5.832853 0.368159
C -1.364612 4.998611 -1.397067	C 0.375923 4.885794 1.403889
C -1.097880 3.622680 -1.553920	C 0.538453 3.502272 1.185040
C -2.772961 2.268251 1.654467	C 1.403717 3.557539 -2.586952
H -3.003820 4.967222 1.600195	H 0.952179 6.092119 -1.741081
C -2.278031 6.991897 -0.103751	C 0.268409 7.305577 0.630166
H -1.060197 5.688413 -2.202412	H 0.163558 5.230175 2.430110
C -0.436844 3.118542 -2.813521	C 0.459599 2.533008 2.336573
H -2.060245 1.448557 1.874882	H 0.743905 2.750225 -2.972006
H -3.738777 1.843208 1.290914	H 2.447940 3.172080 -2.595703
H -2.981462 2.806287 2.600716	H 1.366725 4.408338 -3.295713
H -2.133137 7.537701 -1.057702	H 0.552934 7.585846 1.664957
H -1.585727 7.439109 0.643345	H -0.804193 7.573688 0.504306
H -3.309539 7.192377 0.253854	H 0.846292 7.940427 -0.072160
H -0.380991 3.922234 -3.573984	H 0.319751 3.076790 3.291634
H -1.000934 2.271967 -3.259215	H 1.378538 1.912740 2.433541
H 0.595871 2.748377 -2.623270	H -0.394134 1.831532 2.208203
C 1.309619 -2.465408 -0.211332	C 0.017625 -2.508012 -1.977260
C 1.134892 -1.779839 -2.582312	C 0.006238 -2.508820 0.505537
C 2.184482 -3.499684 -0.616919	C -0.462273 -3.836318 -1.944973
C 1.993941 -2.836514 -2.928115	C -0.457496 -3.839052 0.465215
C 2.517713 -3.722695 -1.962972	C -0.697945 -4.523548 -0.741164
C 3.387104 -4.889862 -2.377336	C -1.159704 -5.964341 -0.735358
H 2.606110 -4.159276 0.160381	H -0.636299 -4.351747 -2.904747
C 0.655224 -0.815093 -3.638966	C 0.214426 -1.842101 1.842358
H 2.269531 -2.966223 -3.988545	H -0.643774 -4.352426 1.423481
C 0.979837 -2.329676 1.258072	C 0.323683 -1.875830 -3.314723
H 0.569520 -1.336309 1.523971	H -0.126668 -0.866322 -3.425115

H 1.892641 -2.479416 1.870147	H -0.047743 -2.517398 -4.138387
H 0.248796 -3.106215 1.575097	H 1.417727 -1.752163 -3.466346
H -0.447151 -0.683771 -3.635788	H 1.242757 -1.452369 2.006163
H 0.954416 -1.153871 -4.650225	H -0.004641 -2.553144 2.663045
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H 3.955095 -5.304822 -1.520660	H -1.591330 -6.262629 -1.712020
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Cl 0.581302 1.096289 2.396218	Cl -1.135891 1.267572 -3.331447
Cl 2.710351 1.647185 -1.927715	Cl -2.294768 0.512056 1.343593
O 5.359204 -0.620389 -0.076525	O -5.948124 0.063063 1.092045
C 6.558842 -1.157349 -0.690413	C -6.426340 0.389039 2.423980
C 7.823073 -0.869494 0.125869	C -7.876291 -0.063707 2.646150
H 6.607110 -0.545803 -1.616543	H -6.435459 1.499750 2.378472
C 6.401842 -2.618714 -1.129394	C -5.451284 -0.014349 3.533090
H 6.497915 -3.340770 -0.293461	H -5.430459 -1.107717 3.711972
H 7.186744 -2.867003 -1.873973	H -5.753511 0.477837 4.480846
H 5.412597 -2.764430 -1.606292	H -4.424985 0.313910 3.272928
H 7.886320 0.207986 0.379347	H -8.506078 0.216168 1.777461
H 8.718041 -1.133601 -0.474667	H -8.289326 0.438728 3.545904
H 7.864512 -1.449929 1.068961	H -7.969924 -1.157324 2.803339
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C 3.669021 -0.008295 3.109138	C -3.994444 -2.340225 -0.850186
H 5.179954 -2.984445 3.887043	H -5.522187 -4.530047 1.296378
H 5.985242 -2.736132 1.553640	H -6.484064 -2.406734 2.148490
H 2.990842 0.741192 3.541738	H -3.284223 -2.334372 -1.692704
H 3.674738 -1.232124 4.902755	H -3.919138 -4.502244 -0.652129
C 1.386552 3.232836 0.350326	C -2.061317 2.621927 -0.797308
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H 4.392358 1.419756 0.023023	H -4.678343 1.043332 -0.522080
H 3.647705 3.525849 0.962679	H -3.858959 1.285672 -2.861338
H 2.941577 2.695353 2.486866	H -3.431598 -0.514984 -2.936300
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C -2.195403 -1.803935 0.088174	C 3.194133 -1.073410 -1.391049
H -1.697342 -2.808830 0.050079	H 2.742983 -2.056152 -1.644818
H -1.857197 -1.311723 1.023295	H 3.230866 -0.493080 -2.342100
C -4.324818 -2.588811 -0.925577	C 4.902165 -2.537708 -0.228557
C -4.225157 -2.180848 1.436231	C 5.575184 -0.310291 -0.919370
C -5.795805 -2.173755 -0.965618	C 5.425873 -2.277529 1.191783
H -4.197177 -3.709155 -0.860181	H 5.644172 -3.145482 -0.815665
H -3.900810 -2.295477 -1.908477	H 4.006437 -3.182888 -0.119727
C -5.686014 -1.745228 1.462188	C 6.078986 0.000608 0.495848
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H -3.705574 -1.582248 2.213654	H 5.174764 0.635841 -1.336046
H -6.365737 -2.723074 -1.742141	H 5.812372 -3.200764 1.670809
H -5.859853 -1.061069 -1.110775	H 4.633036 -1.802668 1.824847
H -6.177495 -1.959965 2.430208	H 6.911613 0.731218 0.500689
H -5.746111 -0.650252 1.208992	H 5.242478 0.361508 1.147675
N -3.644146 -1.884771 0.141143	N 4.548432 -1.323988 -0.924336
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C -6.721875 -3.905765 0.579117	C 7.821230 -1.865179 0.585915
H -7.348176 -4.239109 -0.273879	H 8.063438 -2.745642 1.215903
H -5.730100 -4.383498 0.461123	H 7.525899 -2.250236 -0.408585
C -7.351233 -4.315650 1.905953	C 9.028135 -0.941992 0.457799
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H -7.490165 -5.415823 1.893718	H 9.867445 -1.532638 0.037675
H -6.707375 -4.078953 2.775774	H 8.848252 -0.095443 -0.233890
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TS_I14e	I14e
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Ru	-1.650780	-0.786407	-0.238408	Ru	3.154852	0.752716	-0.029989
C	0.205730	-0.227864	-0.440500	C	1.347074	0.070751	-0.195657
N	0.761054	1.018440	-0.472902	N	0.888154	-1.219899	-0.253813
N	1.237231	-1.148921	-0.434006	N	0.255488	0.904730	-0.386180
C	2.531610	-0.479341	-0.146718	C	-1.031169	0.154056	-0.429687
C	2.232977	0.961794	-0.582590	C	-0.554344	-1.301438	-0.547600
H	2.711828	-0.486247	0.955112	H	-1.566330	0.264031	0.541894
H	2.736698	1.716664	0.062691	H	-1.072849	-1.949783	0.190665
H	2.540390	1.136460	-1.644158	H	-0.703725	-1.714145	-1.574982
C	1.054528	-2.578145	-0.403258	C	0.212530	2.316006	-0.078229
C	0.075936	2.276563	-0.553700	C	1.602090	-2.453416	-0.078724
C	-0.340926	2.762957	-1.822835	C	2.151821	-3.114221	-1.205479
C	-0.940466	4.037473	-1.880391	C	2.791307	-4.354898	-1.000535
C	-1.113007	4.833585	-0.731355	C	2.884500	-4.947264	0.273391
C	-0.665382	4.327205	0.506447	C	2.310735	-4.266143	1.367470
C	-0.059719	3.061950	0.626340	C	1.661850	-3.024082	1.221773
C	-0.158132	1.941121	-3.075788	C	2.079755	-2.504245	-2.585448
H	-1.271646	4.422020	-2.859924	H	3.229342	-4.872982	-1.870471
C	-1.748557	6.204248	-0.814474	C	3.590669	-6.270329	0.474567
H	-0.781363	4.940932	1.415714	H	2.368105	-4.713991	2.374129
C	0.438320	2.562393	1.958667	C	1.080883	-2.308547	2.417874
H	-0.780361	1.017644	-3.055666	H	2.584707	-1.515096	-2.618328
H	0.895555	1.612080	-3.200277	H	1.029529	-2.337031	-2.909167
H	-0.437330	2.525245	-3.974795	H	2.558469	-3.164554	-3.335070
H	-2.663638	6.264588	-0.186799	H	2.970895	-6.976196	1.066801
H	-2.032849	6.463453	-1.853905	H	4.543529	-6.136253	1.031634
H	-1.056905	6.991710	-0.445244	H	3.835173	-6.756202	-0.491130
H	0.106801	3.234286	2.774908	H	1.253104	-2.891020	3.344195
H	1.552553	2.534432	1.984925	H	-0.015387	-2.133447	2.328293
H	0.057664	1.540380	2.172407	H	1.552683	-1.311463	2.550187
C	0.885828	-3.268441	-1.638832	C	0.366203	3.271191	-1.120848
C	1.117735	-3.293627	0.827679	C	-0.087334	2.725716	1.255056
C	0.697567	-4.665490	-1.604393	C	0.253210	4.640090	-0.793566
C	0.929540	-4.690393	0.797024	C	-0.197735	4.104846	1.514783
C	0.703840	-5.395530	-0.400976	C	-0.022478	5.080084	0.512855
C	0.521510	-6.897552	-0.398042	C	-0.100619	6.553702	0.844489
H	0.550749	-5.198363	-2.559037	H	0.379915	5.383976	-1.598356
C	1.391317	-2.605668	2.142882	C	-0.246477	1.738958	2.387869
H	0.956741	-5.242527	1.751885	H	-0.413295	4.425842	2.547995
C	0.907041	-2.549135	-2.963883	C	0.643134	2.877261	-2.552884
H	-0.072441	-2.051740	-3.150006	H	1.683299	2.508187	-2.679210
H	1.101185	-3.257662	-3.793389	H	0.497035	3.741466	-3.230804
H	1.677550	-1.752282	-2.988620	H	-0.011682	2.051817	-2.896876
H	2.451415	-2.277084	2.222754	H	-1.128192	1.067576	2.290742
H	1.199896	-3.293207	2.990057	H	-0.343783	2.274562	3.352405
H	0.740000	-1.715844	2.275671	H	0.648015	1.088277	2.460900
H	0.046633	-7.249169	0.540472	H	-0.253729	7.172142	-0.062871
H	1.499410	-7.421716	-0.484445	H	0.839815	6.901166	1.326183
H	-0.104956	-7.234978	-1.248466	H	-0.924776	6.771296	1.555407
C	-4.577899	-1.759155	0.071007	Cl	3.583787	0.931978	-2.320167
Cl	-2.209080	-1.114388	-2.549321	Cl	3.157763	1.994175	1.929478
Cl	-1.543395	-0.754131	2.146599	C	4.107560	-0.708018	0.452355
O	-5.904055	0.539942	-0.543654	H	5.213436	-0.537020	0.517867
C	-6.563938	1.668469	-1.169977	H	3.749518	-1.721291	0.719562
C	-8.084921	1.492272	-1.262662	C	-1.979446	0.643222	-1.553651
H	-6.161724	1.591898	-2.202649	H	-1.903535	1.750424	-1.605950
C	-6.101884	3.019744	-0.609262	H	-1.624688	0.261217	-2.539218
H	-6.510428	3.242170	0.395829	C	-4.286231	1.165885	-0.656915
H	-6.429680	3.830502	-1.292599	C	-3.932848	-0.975348	-1.750408
H	-4.995612	3.051292	-0.548640	C	-4.924248	0.463984	0.550053
H	-8.331783	0.494439	-1.678012	H	-5.080010	1.594815	-1.328277
H	-8.502499	2.259645	-1.947064	H	-3.731204	2.038155	-0.254860
H	-8.598847	1.596756	-0.286730	C	-4.539643	-1.714435	-0.550685
C	-6.066117	0.138999	0.747822	H	-4.694811	-0.880034	-2.572768
C	-5.347881	-1.052021	1.102723	H	-3.133375	-1.626293	-2.158882
C	-6.840394	0.804977	1.724154	H	-5.708571	1.085763	1.028910
C	-6.897798	0.314707	3.039312	H	-4.140582	0.168185	1.293158
C	-6.186729	-0.840564	3.405732	H	-5.025872	-2.666849	-0.840246
C	-5.424543	-1.507860	2.438789	H	-3.766669	-1.898499	0.238852
H	-7.507232	0.851486	3.784138	N	-3.383299	0.306465	-1.383775
H	-7.395195	1.715930	1.469663	N	-5.592339	-0.866233	0.169672

H	-4.873904	-2.419225	2.716425
H	-6.229093	-1.219805	4.438172
C	-2.349846	0.894733	-0.274313
C	-3.695194	-2.787454	0.263022
H	-4.757530	-1.427438	-0.964217
H	-3.258487	-3.302533	-0.607486
H	-3.436859	-3.169343	1.263175
H	-2.531892	1.465683	0.663980
H	-2.708499	1.357615	-1.220673
C	3.758552	-1.117783	-0.822663
H	3.761582	-2.219260	-0.638975
H	3.693619	-0.988161	-1.924180
C	5.601292	-0.984123	0.865375
C	5.885242	0.197135	-1.224980
C	6.261338	0.161570	1.633678
H	6.321281	-1.830303	0.668160
H	4.828473	-1.400312	1.544769
C	6.527278	1.381213	-0.499358
H	6.670397	-0.479453	-1.672880
H	5.322358	0.622616	-2.081192
H	6.819590	-0.193103	2.523817
H	5.482651	0.922538	1.910901
H	7.256305	1.923541	-1.131923
H	5.729185	2.075246	-0.123852
N	4.977979	-0.487444	-0.337464
N	7.259248	0.951046	0.774376
C	7.616978	2.202039	1.541073
H	8.125400	1.905210	2.478319
H	8.285632	2.827666	0.922319
H	6.652159	2.732681	1.749203
C	8.495188	0.103687	0.506640
H	8.922915	-0.109323	1.507884
H	8.140741	-0.860391	0.093462
C	9.546022	0.718599	-0.411466
H	9.932907	1.687718	-0.038761
H	10.407202	0.021568	-0.460731
H	9.181342	0.857460	-1.448338
Cl	4.338234	2.875149	1.565679
C	-5.955330	-1.572725	1.453111
H	-6.696771	-0.955612	1.995958
H	-6.382571	-2.563313	1.213146
H	-5.009938	-1.681755	2.040847
C	-6.835617	-0.599114	-0.668779
H	-7.497958	0.006599	-0.016922
H	-6.524971	0.051017	-1.508522
C	-7.569194	-1.827769	-1.194668
H	-7.903754	-2.510741	-0.388972
H	-8.478640	-1.481344	-1.726353
H	-6.967996	-2.406591	-1.923145
Cl	-2.691200	-1.360419	2.264132

Table S4. Coordinates data set, absolute energies (a.u.) for DFT all the optimized ammonium tagged complexes (AquaMet^{TM+}).

Precat			
102			
precatnocl_2 SCF Done: -2827.27562574 A.U.			
Ru	-2.060265	0.144218	-0.093212
C	-0.130029	0.287434	0.165466
N	0.517680	1.505660	0.264766
N	0.870381	-0.678845	0.111124
C	2.225674	-0.112459	0.286404
C	1.975508	1.399977	0.170586
H	2.467494	1.989911	0.972210
H	2.340886	1.798061	-0.805573
C	0.707005	-2.092842	0.336437
C	-0.064410	2.821792	0.385524
C	-0.295220	3.612365	-0.772506
C	-0.846094	4.899462	-0.597565
C	-1.120648	5.434749	0.674999
C	-0.789678	4.656924	1.802890
C	-0.253583	3.360957	1.688580
C	0.104986	3.153702	-2.155864
H	-1.047230	5.510093	-1.493896
C	-1.749927	6.800324	0.831872
H	-0.952581	5.072377	2.811516
C	0.105473	2.580356	2.930059
H	-0.177406	2.099707	-2.352001
H	1.205090	3.254017	-2.300477
H	-0.375805	3.780992	-2.932108
H	-1.598384	7.429712	-0.067804

TS_Open			
102			
PENJOLL-TSopen+ SCF Done: -2827.24323473 A.U.			
Ru	-1.992635	0.608443	-0.145316
C	-0.070178	0.545674	-0.148280
N	0.702837	1.682489	0.027551
N	0.813004	-0.528879	-0.163593
C	2.169955	-0.124673	0.271797
C	2.138598	1.388891	0.026369
H	2.266426	-0.328062	1.367479
H	2.663349	1.969840	0.811522
H	2.599296	1.652545	-0.956943
C	0.498938	-1.922069	-0.321048
C	0.278120	3.057834	-0.094992
C	0.206064	3.654828	-1.382164
C	-0.194729	5.001703	-1.468896
C	-0.492599	5.771187	-0.327835
C	-0.332513	5.168506	0.935705
C	0.064802	3.825033	1.083168
C	0.612545	2.916565	-2.638019
H	-0.277051	5.463300	-2.467074
C	-0.981180	7.195747	-0.454757
H	-0.516628	5.765152	1.844774
C	0.292347	3.249150	2.460443
H	0.392525	1.834243	-2.581517
H	1.701718	3.046648	-2.833889
H	0.075393	3.314473	-3.520439

H	-1.339951	7.342302	1.708592	H	-0.584803	7.687454	-1.366028
H	-2.847131	6.712959	0.991938	H	-0.696754	7.808576	0.424368
H	0.134679	3.242325	3.817651	H	-2.090803	7.223740	-0.526460
H	1.092965	2.080251	2.841467	H	0.122122	4.017581	3.239549
H	-0.652905	1.788389	3.110834	H	1.333805	2.877075	2.581330
C	0.680628	-2.989476	-0.763257	H	-0.385924	2.392546	2.658978
C	0.595446	-2.565456	1.674624	C	0.398003	-2.453270	-1.637199
C	0.582302	-4.371436	-0.489843	C	0.336225	-2.750622	0.820139
C	0.506749	-3.954099	1.888514	C	0.154948	-3.832904	-1.783331
C	0.508903	-4.878210	0.821717	C	0.094270	-4.124974	0.614397
C	0.435287	-6.365449	1.085353	C	0.001844	-4.689371	-0.672795
H	0.545736	-5.073944	-1.339484	C	-0.300173	-6.158335	-0.863212
C	0.480000	-1.606518	2.838013	H	0.070849	-4.249711	-2.801081
H	0.412056	-4.324323	2.923358	C	0.376650	-2.188093	2.222775
C	0.701148	-2.506064	-2.196068	H	-0.044971	-4.772317	1.496454
H	0.137466	-1.558737	-2.319405	C	0.471012	-1.560032	-2.854776
H	0.247520	-3.263636	-2.865201	H	-0.411621	-0.884987	-2.901828
H	1.737559	-2.339770	-2.565021	H	0.495255	-2.156895	-3.787086
H	1.325027	-0.886970	2.890606	H	1.360586	-0.896389	-2.845284
H	0.445140	-2.152262	3.800665	H	-0.227485	-1.259761	2.307831
H	-0.445701	-0.996247	2.754081	H	1.413256	-1.948093	2.551265
H	-0.264559	-6.599629	1.913475	H	-0.024409	-2.921547	2.949125
H	1.429005	-6.768113	1.381593	H	-1.386737	-6.317522	-1.038452
H	0.107375	-6.925924	0.187435	H	-0.022109	-6.755096	0.028251
C	-2.394396	-1.656546	0.170803	H	0.232150	-6.575922	-1.742068
Cl	-1.827385	0.269170	-2.443636	C	-2.513570	-1.091909	-0.589363
Cl	-2.747563	0.977685	1.998223	Cl	-2.465185	1.717374	-2.130895
O	-4.309097	0.023157	-0.540661	Cl	-2.131793	0.737131	2.183705
C	-5.107153	1.204887	-0.921898	O	-4.458222	-1.369341	1.473001
C	-5.675609	1.071657	-2.334344	C	-5.253074	-1.036422	2.647088
H	-4.307254	1.973089	-0.946667	C	-6.042542	0.263456	2.476176
C	-6.101330	1.586540	0.173750	H	-4.446067	-0.838861	3.382996
H	-6.957735	0.887786	0.249501	C	-6.069430	-2.227527	3.165129
H	-6.510455	2.593157	-0.051039	H	-6.976425	-2.438434	2.563733
H	-5.586853	1.630245	1.153858	H	-6.402932	-2.018905	4.202936
H	-4.878116	0.770439	-3.041621	H	-5.446263	-3.144354	3.186781
H	-6.066168	2.060097	-2.653276	H	-5.370369	1.072651	2.127325
H	-6.509788	0.346257	-2.405205	H	-6.463808	0.567445	3.456530
C	-4.778205	-1.249222	-0.366392	H	-6.885218	0.171105	1.762873
C	-3.744540	-2.161634	0.013369	C	-4.935147	-1.456283	0.206582
C	-6.103067	-1.689274	-0.522489	C	-3.949306	-1.371508	-0.828188
C	-6.401883	-3.047714	-0.302908	C	-6.284241	-1.698833	-0.146411
C	-5.402139	-3.967130	0.068409	C	-6.652525	-1.869200	-1.489369
C	-4.083468	-3.523302	0.224662	C	-5.687463	-1.819987	-2.511175
H	-7.442264	-3.387956	-0.425675	C	-4.349874	-1.580935	-2.173264
H	-6.904710	-0.998022	-0.809099	H	-7.709811	-2.057451	-1.735072
H	-3.284345	-4.223707	0.516277	H	-7.049827	-1.779283	0.635079
H	-5.657476	-5.024534	0.235662	H	-3.585196	-1.521230	-2.964173
H	-1.634971	-2.401715	0.472622	H	-5.976414	-1.962379	-3.563587
C	3.236507	-0.635313	-0.749425	H	-1.797727	-1.888100	-0.875838
H	2.594145	-0.375166	1.309460	C	3.290356	-0.859626	-0.478497
N	4.566028	-0.027329	-0.561042	H	3.175576	-1.965093	-0.351079
H	2.871956	-0.356540	-1.759029	H	3.182277	-0.649486	-1.562688
H	3.284111	-1.751631	-0.712986	C	5.049985	-0.895569	1.236041
C	5.356995	0.085516	-1.775545	C	5.662302	-0.639999	-1.062245
C	5.351851	-0.622765	0.510962	C	6.329027	-0.198907	1.694987
C	6.558008	0.251580	0.834222	H	5.166377	-2.013482	1.254821
H	5.668305	-1.678117	0.286563	H	4.279289	-0.663259	1.999990
H	4.744126	-0.680903	1.437754	C	6.949210	0.086306	-0.680742
C	6.582846	0.967017	-1.534496	H	5.857823	-1.732810	-1.240891
H	4.760194	0.589275	-2.564678	H	5.340672	-0.224212	-2.040060
H	5.655531	-0.909094	-2.206300	H	6.693614	-0.598366	2.661955
N	7.461861	0.474401	-0.379318	H	6.144851	0.888176	1.800021
H	6.215573	1.259568	1.140633	H	7.758158	-0.079842	-1.416550
H	7.182356	-0.174079	1.641978	H	6.752691	1.174102	-0.606565
H	6.254798	1.986040	-1.249914	N	4.627786	-0.397302	-0.066044
H	7.230573	1.032218	-2.431133	N	7.479327	-0.332370	0.690462
C	8.464913	1.547781	-0.050385	C	8.582931	0.608171	1.095885
H	9.106401	1.726137	-0.933639	H	8.960547	0.313824	2.092946
H	9.083442	1.226200	0.806175	H	9.399565	0.559980	0.353942
H	7.924430	2.475487	0.212643	H	8.181200	1.637142	1.136575

C	8.198163	-0.804769	-0.811572	C	8.001785	-1.778538	0.705841
C	9.041651	-1.486238	0.257735	H	8.354553	-1.941287	1.744430
H	8.820384	-0.494088	-1.675220	H	7.120260	-2.428465	0.553449
H	7.424156	-1.494942	-1.196056	C	9.092954	-2.108997	-0.303865
H	9.839502	-0.838857	0.672041	H	10.009766	-1.499362	-0.180839
H	9.549393	-2.347593	-0.221933	H	9.388964	-3.164421	-0.135803
H	8.439346	-1.897806	1.091415	H	8.750150	-2.039913	-1.355100
Act				TS_Ci1			
102				108			
PENJOLL-Act+ SCF Done: -2827.25391155 A.U.				PENJOLL-TS1+ SCF Done: -2905.77972796 A.U.			
Ru	-1.774054	1.201615	-0.576155	Ru	-1.513141	1.093843	-0.434447
C	-0.002532	0.776953	0.018710	C	0.123678	0.529143	0.389743
N	0.920441	1.753686	0.340005	N	1.091971	1.431855	0.796629
N	0.674020	-0.440331	0.049646	N	0.690092	-0.738141	0.508032
C	2.090980	-0.293777	0.446618	C	2.129439	-0.671052	0.842584
C	2.269563	1.232880	0.568552	C	2.306571	0.783188	1.304987
H	2.241177	-0.790695	1.435577	H	2.347311	-1.392263	1.660921
H	2.651114	1.549835	1.563372	H	2.377005	0.877366	2.413083
H	2.982699	1.623300	-0.193805	H	3.221596	1.242283	0.874081
C	0.097720	-1.759522	0.133209	C	0.031114	-2.017040	0.600967
C	0.695594	3.174370	0.468817	C	0.974907	2.869022	0.883931
C	0.942957	4.033146	-0.636593	C	1.446254	3.674138	-0.188718
C	0.747197	5.417336	-0.456855	C	1.341941	5.074809	-0.067604
C	0.353459	5.967116	0.778675	C	0.827302	5.691405	1.089004
C	0.191163	5.091189	1.869904	C	0.449687	4.863445	2.164895
C	0.364226	3.699655	1.746874	C	0.522002	3.459217	2.096001
C	1.436536	3.509458	-1.965418	C	2.090956	3.072097	-1.415153
H	0.921835	6.088377	-1.314497	H	1.690999	5.703302	-0.904069
C	0.103806	7.450222	0.927265	C	0.680702	7.192996	1.176425
H	-0.081172	5.503185	2.855944	H	0.084232	5.325083	3.097359
C	0.180346	2.809998	2.953069	C	0.115882	2.627115	3.288904
H	0.714019	2.804460	-2.428914	H	1.389716	2.414244	-1.972234
H	2.401837	2.966221	-1.859180	H	2.976425	2.454443	-1.141929
H	1.605210	4.343006	-2.674733	H	2.441346	3.866529	-2.102962
H	0.703819	8.043146	0.207867	H	1.360179	7.715488	0.473633
H	0.335820	7.805780	1.951585	H	0.884618	7.565970	2.200805
H	-0.965496	7.688483	0.735039	H	-0.356897	7.501224	0.920914
H	0.255331	3.395313	3.890528	H	0.016692	3.258942	4.192958
H	0.928227	1.991521	2.996704	H	0.847453	1.824224	3.515460
H	-0.824597	2.336840	2.922828	H	-0.866726	2.144917	3.098367
C	-0.024921	-2.568718	-1.027208	C	-0.114641	-2.860276	-0.529456
C	-0.303530	-2.242759	1.409792	C	-0.411193	-2.439542	1.889140
C	-0.513789	-3.882884	-0.868774	C	-0.672169	-4.144275	-0.333145
C	-0.773759	-3.566260	1.510407	C	-0.957873	-3.726813	2.026248
C	-0.874991	-4.410421	0.385795	C	-1.085973	-4.605184	0.927991
C	-1.351739	-5.839155	0.519973	C	-1.650712	-5.995470	1.113550
H	-0.626677	-4.511753	-1.768023	H	-0.796625	-4.800699	-1.211105
C	-0.304657	-1.339037	2.622525	C	-0.339103	-1.509275	3.078956
H	-1.088969	-3.942055	2.498409	H	-1.303354	-4.051937	3.022201
C	0.314340	-2.058710	-2.409398	C	0.255812	-2.432246	-1.931203
H	0.045598	-0.990474	-2.534357	H	0.450673	-1.346301	-2.007279
H	-0.231544	-2.639496	-3.178814	H	-0.576657	-2.658347	-2.628549
H	1.397494	-2.167992	-2.639332	H	1.140515	-2.991892	-2.308660
H	-0.955907	-0.454718	2.454827	H	-0.919873	-0.580307	2.897352
H	0.705094	-0.945511	2.870623	H	0.701538	-1.194489	3.310865
H	-0.678482	-1.874865	3.516340	H	-0.746867	-1.994756	3.986712
H	-1.978849	-5.981019	1.422771	H	-0.927042	-6.654474	1.641407
H	-0.492011	-6.539994	0.606576	H	-1.891000	-6.474493	0.143874
H	-1.939663	-6.158960	-0.364136	H	-2.574363	-5.981635	1.728635
C	-2.677204	-0.406872	-0.423619	C	-2.493919	-0.475455	-0.392375
Cl	-1.186555	1.282653	-2.846964	Cl	-0.541378	1.053160	-2.587865
Cl	-2.752423	2.318642	1.214238	Cl	-2.625161	2.184912	1.311484
O	-4.461963	-2.054647	0.824420	O	-4.547667	-1.940784	0.644273
C	-5.236821	-2.837416	1.774435	C	-5.515773	-2.625232	1.488141
C	-6.288472	-1.999985	2.510244	C	-6.680936	-1.719297	1.899747
H	-4.447116	-3.096369	2.511489	H	-4.900055	-2.802974	2.395237
C	-5.752865	-4.157719	1.188433	C	-5.922746	-4.000720	0.944761
H	-6.620428	-4.032072	0.511431	H	-6.629481	-3.948815	0.093497
H	-6.072965	-4.823791	2.016249	H	-6.417635	-4.579542	1.751843
H	-4.947710	-4.673232	0.627366	H	-5.027547	-4.566979	0.617738
H	-5.837204	-1.063048	2.893851	H	-6.300684	-0.750599	2.281214

H	-6.673023	-2.575864	3.377121
H	-7.155470	-1.730607	1.875919
C	-4.965512	-1.409985	-0.258943
C	-4.033780	-0.540145	-0.938231
C	-6.287906	-1.519043	-0.739953
C	-6.699468	-0.786198	-1.866087
C	-5.806218	0.064251	-2.541317
C	-4.492028	0.180532	-2.076783
H	-7.738056	-0.890395	-2.218657
H	-7.010031	-2.174662	-0.238723
H	-3.769724	0.812301	-2.618644
H	-6.131339	0.625122	-3.430462
H	-2.313189	-1.241175	0.203423
C	3.049806	-0.934199	-0.575705
H	2.770512	-2.004572	-0.736957
H	2.918304	-0.412380	-1.545711
C	4.866963	-1.752307	0.855341
C	5.405480	-0.802423	-1.273919
C	6.247380	-1.401259	1.406020
H	4.833529	-2.816143	0.493438
H	4.167308	-1.709570	1.715795
C	6.793425	-0.396899	-0.785978
H	5.446255	-1.783949	-1.821242
H	5.098635	-0.046532	-2.026704
H	6.598158	-2.143105	2.150488
H	6.216881	-0.400130	1.879163
H	7.539923	-0.388214	-1.602269
H	6.746527	0.613891	-0.334821
N	4.459291	-0.799511	-0.167156
N	7.322171	-1.315689	0.316450
C	8.560265	-0.702147	0.913660
H	8.928715	-1.353756	1.727873
H	9.334245	-0.598852	0.132857
H	8.307981	0.295345	1.317642
C	7.643194	-2.729995	-0.194742
H	8.026700	-3.271435	0.693725
H	6.674989	-3.190344	-0.466231
C	8.623545	-2.815412	-1.357090
H	9.615061	-2.374281	-1.133458
H	8.794544	-3.890932	-1.566378
H	8.230816	-2.369329	-2.291798

H	-7.252713	-2.208219	2.715215
H	-7.387919	-1.512061	1.072632
C	-4.799896	-1.428452	-0.586117
C	-3.728210	-0.639769	-1.149106
C	-5.993857	-1.597637	-1.319474
C	-6.140636	-1.007826	-2.586629
C	-5.106677	-0.240345	-3.151333
C	-3.920265	-0.057400	-2.432536
H	-7.082944	-1.158065	-3.137564
H	-6.820765	-2.188926	-0.908708
H	-3.088895	0.518548	-2.867647
H	-5.224395	0.206910	-4.150028
C	-2.688900	3.900597	-1.988593
C	-3.975060	3.526774	-1.860335
H	-2.280590	-1.272043	0.344657
H	-4.453079	3.450977	-0.869904
H	-4.595812	3.275880	-2.736759
H	-2.078965	4.164144	-1.107991
H	-2.196183	3.966028	-2.972520
C	2.990389	-1.008747	-0.398410
H	2.707033	-2.015809	-0.787292
H	2.737511	-0.273970	-1.190514
C	4.978603	-2.077271	0.565836
C	5.243279	-0.596214	-1.296837
C	6.408584	-1.809662	1.030526
H	4.919964	-3.018756	-0.045492
H	4.387645	-2.282501	1.482771
C	6.670227	-0.255760	-0.876521
H	5.239156	-1.404829	-2.077725
H	4.831349	0.307676	-1.792405
H	6.860453	-2.697699	1.515201
H	6.416743	-0.964383	1.746026
H	7.314394	-0.003975	-1.739885
H	6.656144	0.605397	-0.179550
N	4.435575	-0.920037	-0.129489
N	7.344827	-1.395705	-0.110850
C	8.631140	-0.890534	0.486656
H	9.114972	-1.710835	1.049270
H	9.300389	-0.538470	-0.318191
H	8.403765	-0.051967	1.170068
C	7.631570	-2.614992	-1.002417
H	8.112397	-3.352391	-0.328161
H	6.646913	-3.027140	-1.291435
C	8.487761	-2.358177	-2.235121
H	9.493493	-1.958501	-1.999590
H	8.643771	-3.334437	-2.737503
H	7.998593	-1.695643	-2.976053

TS_Con			
108			
PENJOLL-TSconc+ SCF Done: -2905.77136054 A.U.			
C	-0.071550	0.459862	0.006261
C	2.212074	-0.055549	0.382874
H	2.393523	0.013017	1.483307
C	2.111143	1.350763	-0.216099
H	2.660823	2.116059	0.366763
H	2.492654	1.382382	-1.265739
C	0.752642	-2.752826	1.338986
C	0.676867	-4.158231	1.251675
H	0.761259	-4.747530	2.180231
C	0.494326	-4.827040	0.025078
C	0.387094	-4.044110	-1.142518
H	0.254087	-4.544695	-2.116308
C	0.447780	-2.635217	-1.117134
C	0.624148	-1.995744	0.141558
C	0.965660	-2.088091	2.679530
H	0.743336	-2.791441	3.505922
H	0.312985	-1.195279	2.796323
H	2.022365	-1.761661	2.817161
C	0.383296	-6.333635	-0.034436
H	-0.676925	-6.656132	0.061019
H	0.944259	-6.820823	0.788353

Ci1			
108			
PENJOLL-CI1+ SCF Done: -2905.79069465 A.U.			
Ru	-1.813609	1.408301	-0.312015
C	0.080675	0.857063	0.094935
N	1.045974	1.819424	0.248030
N	0.717490	-0.364539	0.117143
C	2.168602	-0.241574	0.408494
C	2.408021	1.273178	0.279304
H	2.346413	-0.580930	1.458578
H	2.983591	1.702405	1.125354
H	2.956334	1.520888	-0.659372
C	0.107201	-1.664457	0.257291
C	0.848344	3.249404	0.329785
C	0.989494	4.060705	-0.830826
C	0.788190	5.449728	-0.695031
C	0.510320	6.053470	0.546527
C	0.489900	5.230157	1.689919
C	0.673769	3.836174	1.615076
C	1.428663	3.496794	-2.161535
H	0.871867	6.081224	-1.595328
C	0.248784	7.538264	0.651624
H	0.333968	5.686759	2.681509
C	0.704792	3.010238	2.877142

H	0.757652	-6.735571	-0.997663
C	0.318620	-1.851267	-2.398963
H	0.354279	-2.521808	-3.279349
H	1.121942	-1.091619	-2.509882
H	-0.637088	-1.279563	-2.434434
C	0.201884	2.967391	-0.321248
C	0.104690	3.788093	0.836707
C	-0.289790	5.129987	0.667529
H	-0.381776	5.768826	1.561933
C	-0.552993	5.680584	-0.603514
C	-0.372423	4.856071	-1.731520
H	-0.530454	5.277593	-2.738244
C	0.018412	3.505243	-1.623984
C	0.438686	3.256576	2.210202
H	0.286163	4.036121	2.982014
H	1.502504	2.935347	2.273639
H	-0.179915	2.369691	2.476173
C	-1.017177	7.111567	-0.749302
H	-0.747017	7.532668	-1.738363
H	-0.588079	7.764968	0.037228
H	-2.123637	7.177708	-0.657271
C	0.234672	2.678883	-2.867785
H	0.160347	3.308240	-3.775804
H	-0.527641	1.870717	-2.938960
H	1.233609	2.192270	-2.877156
C	-2.335515	-1.277435	0.342109
H	-1.788252	-1.858646	1.114658
C	-3.407836	-2.006230	-0.344540
C	-3.157484	-3.301488	-0.872278
H	-2.160208	-3.744591	-0.730577
C	-4.135779	-3.990167	-1.601595
H	-3.906893	-4.979641	-2.027446
C	-5.404864	-3.413098	-1.791907
H	-6.174811	-3.942389	-2.375120
C	-5.697038	-2.163854	-1.222226
C	-4.719714	-1.466842	-0.489026
N	0.833107	-0.572745	0.175368
N	0.666797	1.609090	-0.169377
Cl	-1.651829	0.396943	2.589508
Cl	-2.390034	0.489938	-2.249112
Ru	-2.032351	0.545393	0.136205
H	-6.689752	-1.704533	-1.340696
O	-5.037038	-0.263236	0.099644
C	-5.623454	-0.262363	1.459121
C	-3.411312	2.482031	-0.229278
C	-3.166007	2.528145	1.120520
H	-4.303129	1.985466	-0.642135
H	-2.801370	3.062417	-0.939671
H	-2.360390	3.146851	1.540724
H	-3.846712	2.068958	1.852706
C	-6.560634	0.941105	1.515270
H	-6.047530	1.869444	1.196305
H	-6.929627	1.091560	2.550519
H	-7.435750	0.786199	0.850592
C	-6.328399	-1.562938	1.839870
H	-4.766067	-0.110787	2.156013
H	-7.207190	-1.766449	1.194038
H	-6.689149	-1.470071	2.884903
H	-5.650851	-2.438317	1.795424
C	3.299692	-0.929194	-0.260638
N	4.632160	-0.310236	-0.141426
H	3.071650	-1.036183	-1.341206
H	3.278998	-1.958505	0.174407
C	5.587277	-0.764516	-1.142560
C	5.211743	-0.401932	1.191436
C	6.831993	0.117247	-1.121937
H	5.141541	-0.663816	-2.154207
H	5.863698	-1.848826	-1.033300
C	6.460504	0.470877	1.298293
H	5.428388	-1.461584	1.497424
H	4.495552	-0.014497	1.945557
H	0.882793	2.567952	-2.425965
H	2.520835	3.277141	-2.152603
H	1.257011	4.229924	-2.973900
H	0.753878	8.103852	-0.157118
H	0.585200	7.946736	1.626042
H	-0.839614	7.752318	0.568935
H	0.792535	3.660358	3.769468
H	1.557066	2.297872	2.887161
H	-0.230430	2.415320	2.967974
C	-0.094830	-2.481499	-0.888282
C	-0.218064	-2.128759	1.561181
C	-0.586939	-3.787275	-0.689746
C	-0.696631	-3.447583	1.698936
C	-0.877591	-4.298197	0.590983
C	-1.395434	-5.709430	0.757078
H	-0.757075	-4.423433	-1.574673
C	-0.140705	-1.220215	2.767138
H	-0.949806	-3.814306	2.707843
C	0.175360	-1.985782	-2.290832
H	-0.138631	-0.929797	-2.429052
H	-0.370380	-2.605618	-3.029001
H	1.253706	-2.053365	-2.555923
H	-0.885541	-0.394056	2.693915
H	0.850345	-0.731736	2.882520
H	-0.346208	-1.781853	3.699132
H	-1.543953	-5.970985	1.823446
H	-0.696135	-6.453168	0.318951
H	-2.367188	-5.843311	0.235673
C	-2.602339	-0.291389	-0.203499
Cl	-1.225770	1.402386	-2.657738
Cl	-2.364890	1.863429	1.992389
O	-4.290412	-2.037327	1.022233
C	-5.236566	-2.641771	1.950976
C	-6.631293	-2.016409	1.857223
H	-4.795240	-2.326185	2.919725
C	-5.212622	-4.174761	1.921787
H	-5.737814	-4.608266	1.047873
H	-5.710618	-4.564716	2.833463
H	-4.167749	-4.544171	1.919630
H	-6.563946	-0.911148	1.904747
H	-7.242391	-2.357287	2.718109
H	-7.171985	-2.293493	0.930828
C	-4.439221	-1.968886	-0.323070
C	-3.577413	-1.020638	-0.995718
C	-5.358015	-2.730079	-1.079561
C	-5.441081	-2.565698	-2.471542
C	-4.617087	-1.641470	-3.140727
C	-3.710061	-0.873364	-2.404119
H	-6.169457	-3.169305	-3.036844
H	-6.017648	-3.454526	-0.586443
H	-3.048374	-0.145110	-2.899510
H	-4.689748	-1.517594	-4.232067
C	-3.194081	3.131891	-0.921877
C	-4.097497	2.099684	-0.769576
H	-2.352020	-0.810971	0.743511
H	-4.585596	1.909865	0.198854
H	-4.473186	1.546965	-1.643510
H	-2.976443	3.812861	-0.079420
H	-2.853363	3.439462	-1.923646
C	3.044563	-1.081913	-0.535118
H	2.715779	-2.150484	-0.510682
H	2.890756	-0.715568	-1.570677
C	4.900273	-1.730502	0.938306
C	5.368652	-1.172096	-1.340265
C	6.313952	-1.343644	1.366478
H	4.817282	-2.837560	0.761549
H	4.242199	-1.518677	1.806850
C	6.787710	-0.736868	-0.984723
H	5.357539	-2.233654	-1.710871
H	5.048807	-0.545301	-2.198773
H	6.676801	-1.966341	2.208119

N	7.520723	0.133894	0.243315	H	6.334564	-0.278718	1.670434
H	6.947455	0.378571	2.289208	H	7.497566	-0.889463	-1.819273
H	6.189678	1.531065	1.126573	H	6.785056	0.336192	-0.709231
H	7.581961	-0.197537	-1.871637	N	4.476474	-0.945704	-0.212363
H	6.544974	1.167920	-1.324554	N	7.340790	-1.475101	0.235160
C	8.173527	-1.214378	0.592495	C	8.620202	-0.811088	0.669843
C	9.190944	-1.744800	-0.408819	H	9.012607	-1.331430	1.563574
H	7.345460	-1.935020	0.726997	H	9.359550	-0.858997	-0.149318
H	8.636037	-1.055236	1.587603	H	8.409956	0.246139	0.914670
H	8.744063	-2.005666	-1.388338	C	7.599267	-2.965058	-0.042229
H	9.607573	-2.683461	0.009679	H	8.020026	-3.359793	0.904602
H	10.048166	-1.062394	-0.571696	H	6.605807	-3.430888	-0.179266
C	8.564631	1.218688	0.250901	C	8.508074	-3.280583	-1.222433
H	8.075103	2.189045	0.049189	H	9.518437	-2.834924	-1.135345
H	9.315568	1.015228	-0.532893	H	8.647608	-4.380463	-1.246750
H	9.052420	1.244509	1.243329	H	8.068851	-2.995260	-2.198441
TS_MCy				MCy			
108				108			
PENJOLL-TSMCy+ SCF Done: -2905.78835366 A.U.				PENJOLL-MCy+ SCF Done: -2905.79854839 A.U.			
Ru	1.715351	1.508086	-0.045422	Ru	1.745369	1.355763	0.042698
C	-0.204639	0.888602	-0.252727	C	-0.228033	0.990815	0.030420
N	-1.227948	1.770000	-0.463051	N	-1.215384	1.908473	-0.151164
N	-0.695752	-0.377596	-0.429786	N	-0.788860	-0.256585	0.080609
C	-2.143046	-0.379159	-0.757792	C	-2.225289	-0.221653	-0.289415
C	-2.426989	1.113173	-1.012203	C	-2.548645	1.281534	-0.181068
H	-2.300317	-0.977798	-1.681247	C	-3.098610	-1.119681	0.599865
H	-2.533708	1.343655	-2.094889	H	-2.322238	-0.557995	-1.349760
H	-3.348036	1.461865	-0.498717	H	-3.138573	1.663388	-1.037757
C	0.016362	-1.624589	-0.313079	H	-3.113210	1.519021	0.751858
C	-1.197853	3.200260	-0.258639	C	-0.074257	-1.494793	0.291314
C	-1.513104	3.702369	1.034683	C	-1.098335	3.350514	-0.148335
C	-1.496709	5.095477	1.232054	C	-1.110378	4.044378	1.091344
C	-1.203170	5.996268	0.188406	C	-1.024462	5.451121	1.062204
C	-0.967858	5.465710	-1.094270	C	-0.954308	6.175298	-0.143461
C	-0.977091	4.079229	-1.353887	C	-1.011297	5.453410	-1.352489
C	-1.866293	2.779461	2.176074	C	-1.098452	4.047785	-1.386599
H	-1.724987	5.488810	2.236787	C	-1.213088	3.324212	2.413820
C	-1.137121	7.484689	0.443322	H	-1.022917	5.997123	2.020487
H	-0.778419	6.153341	-1.935428	C	-0.815220	7.680554	-0.141572
C	-0.808596	3.578921	-2.768345	H	-0.996112	6.001686	-2.309360
H	-0.966005	2.221329	2.514522	C	-1.204049	3.325004	-2.706978
H	-2.637696	2.034786	1.880625	H	-1.459569	4.033209	3.228102
H	-2.260041	3.352682	3.038167	H	-0.250989	2.824940	2.668103
H	-1.326778	8.069574	-0.478884	H	-1.994846	2.535285	2.403799
H	-0.129928	7.775559	0.814995	H	0.256704	7.977357	-0.158252
H	-1.868792	7.802123	1.214028	H	-1.263322	8.133671	0.765629
H	-0.451417	4.391594	-3.430696	H	-1.292100	8.138719	-1.031575
H	-1.778857	3.228145	-3.187102	H	-1.176952	4.041751	-3.550697
H	-0.081816	2.740755	-2.831595	H	-2.156216	2.754853	-2.790265
C	0.335940	-2.139499	0.974622	H	-0.371682	2.598064	-2.831024
C	0.318763	-2.354525	-1.493883	C	0.225735	-1.893478	1.625051
C	0.948903	-3.405530	1.047967	C	0.246421	-2.327259	-0.816827
C	0.921009	-3.622408	-1.355946	C	0.897850	-3.117152	1.814253
C	1.242054	-4.169578	-0.099505	C	0.907475	-3.544882	-0.561118
C	1.910514	-5.520537	0.022507	C	1.256997	-3.953922	0.740302
H	1.206406	-3.805489	2.042848	C	2.017777	-5.236959	0.980602
C	0.049750	-1.790638	-2.869603	H	1.145122	-3.425438	2.843560
H	1.158058	-4.193008	-2.269743	C	-0.096040	-1.941936	-2.236704
C	0.042767	-1.371371	2.242292	H	1.165029	-4.190315	-1.417437
H	0.480537	-0.350240	2.224189	C	-0.143403	-1.053333	2.822611
H	0.453155	-1.902893	3.122348	H	0.535603	-0.175310	2.917681
H	-1.048172	-1.245762	2.413719	H	-0.072971	-1.645958	3.755485
H	-1.037080	-1.722491	-3.103747	H	-1.170920	-0.640798	2.750424
H	0.504112	-2.431321	-3.650353	H	-1.189907	-2.007969	-2.437884
H	0.477369	-0.767344	-2.963734	H	0.400812	-2.622207	-2.955529
H	1.432627	-6.143765	0.806971	H	0.234019	-0.904107	-2.463637
H	2.978477	-5.410365	0.310304	H	1.713545	-5.723341	1.929755
H	1.877734	-6.083506	-0.931441	H	3.107344	-5.028639	1.057882
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Cl	1.848759	1.334672	-2.477952	Cl	1.903866	1.752801	2.409488

O 4.809311 -1.764770 -0.858787	Cl 1.553481 1.197434 -2.380770
C 5.898292 -2.438616 -1.555318	O 4.385068 -1.946054 -1.389778
C 7.277468 -1.905465 -1.157029	C 5.228937 -2.660239 -2.338691
H 5.701635 -2.108165 -2.597006	C 6.707193 -2.280119 -2.225487
C 5.764975 -3.966065 -1.537193	H 4.848046 -2.254523 -3.300326
H 6.064359 -4.425279 -0.574194	C 4.960358 -4.170628 -2.350823
H 6.415392 -4.397959 -2.325540	H 5.419287 -4.704433 -1.494400
H 4.720214 -4.263178 -1.757772	H 5.378725 -4.613230 -3.278585
H 7.299073 -0.798749 -1.215982	H 3.869523 -4.366808 -2.341148
H 8.037270 -2.296944 -1.864270	H 6.829971 -1.178555 -2.246068
H 7.583833 -2.204751 -0.135424	H 7.261423 -2.701383 -3.089174
C 4.655225 -1.682887 0.484761	H 7.180642 -2.664375 -1.300460
C 3.702278 -0.698381 0.959802	C 4.653262 -1.813965 -0.060241
C 5.341630 -2.492680 1.419128	C 4.168611 -0.616488 0.574928
C 5.122474 -2.336337 2.795844	C 5.342263 -2.783179 0.705042
C 4.214232 -1.374038 3.275156	C 5.563033 -2.585453 2.076656
C 3.517772 -0.576142 2.363152	C 5.089215 -1.423549 2.711965
H 5.675962 -2.977743 3.500820	C 4.397926 -0.463151 1.964382
H 6.054924 -3.250535 1.073733	H 6.105736 -3.353266 2.651318
H 2.815370 0.195536 2.714843	H 5.707552 -3.700132 0.225204
H 4.055790 -1.245643 4.356853	H 3.991162 0.430573 2.461540
C 3.022777 3.218967 -0.276367	H 5.253340 -1.269657 3.789570
C 3.958999 2.208889 0.043541	C 2.790955 3.015055 -0.236034
H 3.327586 -0.151225 -1.070815	C 3.936381 1.943763 -0.115883
H 4.614216 1.814016 -0.749921	H 3.560880 0.108652 -1.341075
H 4.308323 2.091833 1.081165	H 4.578402 2.106150 -1.005254
H 2.939109 3.571797 -1.317575	H 4.483077 2.076794 0.834935
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H -2.556538 -1.966903 0.688134	H -2.670948 -2.152396 0.632711
C -5.328881 -1.037946 1.146455	C -5.472986 -1.347817 1.216935
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C -6.765846 -0.897747 0.651695	C -6.883723 -1.051288 0.714642
H -5.111994 -0.134856 1.754605	H -5.279431 -0.644925 2.053924
H -5.232523 -1.911992 1.847334	H -5.416437 -2.379801 1.659546
C -6.128200 -2.171211 -1.369340	C -6.160924 -1.756067 -1.542956
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H -4.031064 -2.258992 -1.704160	H -4.050920 -1.788719 -1.796234
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H -6.238324 -1.266274 -1.998625	H -6.234137 -0.715156 -1.914241
H -7.493972 -0.849007 1.483068	H -7.650149 -1.211014 1.496202
H -6.859452 0.022386 0.041821	H -6.939882 -0.000033 0.369491
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H -6.281493 -3.661718 0.783969	H -6.430710 -3.760975 0.128349
H -7.626844 -4.111459 -0.296965	H -7.725043 -3.877574 -1.092978
H -7.907981 -2.761875 2.507985	H -8.134661 -3.316242 1.954444
H -8.268555 -4.443893 2.060543	H -8.479644 -4.813266 1.060964
H -9.295142 -3.142550 1.417793	H -9.468089 -3.371558 0.739186
C -8.505437 -1.701722 -0.907017	C -8.553349 -1.373722 -1.075868
H -8.393970 -0.760908 -1.476486	H -8.401532 -0.322369 -1.381679
H -9.272849 -1.569712 -0.123878	H -9.352697 -1.423884 -0.315402
H -8.799541 -2.520404 -1.590149	H -8.829924 -1.983113 -1.956534
TS_Ci2	Ci2
108	108
PENJOLL-TS2+ SCF Done: -2905.78053899 A.U.	PENJOLL-CI2+ SCF Done: -2905.78910674 A.U.
Ru 1.542377 1.397409 0.300703	Ru -1.441567 -0.648451 -0.152995
C -0.204385 0.856811 -0.516028	C 0.367956 -0.157399 0.486504
N -1.312373 1.643506 -0.671663	N 0.867764 1.040679 0.912069
N -0.540959 -0.425464 -0.874135	N 1.405502 -1.064988 0.463601
C -1.999111 -0.557746 -1.109643	C 2.705650 -0.428850 0.767467
C -2.429524 0.904858 -1.290715	C 2.277196 0.938905 1.331775
H -2.168127 -1.161042 -2.027535	H 3.240038 -1.037475 1.529756
H -2.539783 1.193848 -2.360603	H 2.357345 0.989947 2.441490
H -3.390713 1.118574 -0.779497	H 2.886092 1.766784 0.912101
C 0.341656 -1.536202 -1.157882	C 1.260028 -2.500861 0.358117
C -1.423817 3.072809 -0.514790	C 0.146423 2.261953 1.154318
C -2.087202 3.594617 0.628199	C 0.204673 3.296289 0.184787

C	-2.227787	4.991730	0.737417	C	-0.460797	4.507063	0.463132
C	-1.746128	5.874205	-0.251000	C	-1.164314	4.714617	1.666393
C	-1.135097	5.317827	-1.391371	C	-1.180831	3.671393	2.614648
C	-0.972151	3.926689	-1.558319	C	-0.532052	2.440623	2.391305
C	-2.627725	2.689451	1.709089	C	0.930778	3.101167	-1.124937
H	-2.732741	5.402196	1.628115	H	-0.427495	5.313667	-0.288416
C	-1.873151	7.371351	-0.083686	C	-1.894736	6.011603	1.932893
H	-0.780835	5.986665	-2.193493	H	-1.712639	3.818966	3.569594
C	-0.340202	3.382691	-2.815197	C	-0.573774	1.352114	3.436627
H	-1.814113	2.063115	2.138950	H	0.502135	2.243197	-1.691891
H	-3.410128	2.001715	1.314233	H	2.012280	2.886546	-0.969069
H	-3.088361	3.281132	2.524419	H	0.860756	4.009620	-1.754876
H	-1.842707	7.897748	-1.058531	H	-1.740327	6.360031	2.974963
H	-1.038490	7.773418	0.531870	H	-2.991179	5.886015	1.796647
H	-2.815466	7.648547	0.431365	H	-1.566739	6.817612	1.246803
H	-0.196405	4.187080	-3.562417	H	-1.053823	1.716725	4.365396
H	-0.966291	2.595608	-3.286840	H	0.443186	0.993615	3.704768
H	0.651264	2.917958	-2.609785	H	-1.140957	0.462332	3.080443
C	0.736988	-2.450882	-0.147526	C	1.281778	-3.156565	-0.903459
C	0.722016	-1.735568	-2.518267	C	1.136528	-3.245954	1.568741
C	1.486638	-3.583978	-0.537515	C	1.132798	-4.561808	-0.921330
C	1.455387	-2.888302	-2.847013	C	1.013007	-4.643514	1.486312
C	1.834862	-3.838038	-1.874636	C	0.995368	-5.324515	0.251143
C	2.571097	-5.098773	-2.268949	C	0.808886	-6.823503	0.198102
H	1.802683	-4.293214	0.245880	H	1.131947	-5.074387	-1.898053
C	0.398790	-0.714276	-3.581504	C	1.079359	-2.566383	2.914975
H	1.748485	-3.044333	-3.898774	H	0.908698	-5.218733	2.421464
C	0.396436	-2.285048	1.316720	C	1.493877	-2.436937	-2.216934
H	0.027487	-1.273960	1.573918	H	1.112619	-1.396607	-2.210615
H	1.299817	-2.458297	1.936947	H	0.971678	-2.969372	-3.036862
H	-0.356065	-3.038507	1.640771	H	2.572199	-2.423503	-2.494059
H	-0.680667	-0.454747	-3.621074	H	1.881031	-1.811479	3.057243
H	0.693385	-1.079374	-4.584444	H	1.162101	-3.306076	3.734822
H	0.959294	0.224766	-3.373012	H	0.101415	-2.043973	3.018733
H	1.857757	-5.890168	-2.589586	H	1.067694	-7.236381	-0.797006
H	3.160133	-5.512510	-1.426289	H	-0.248305	-7.097239	0.407114
H	3.259038	-4.923807	-3.120894	H	1.429071	-7.339319	0.960154
C	3.715858	1.074716	1.014238	C	-3.739875	-1.226168	-1.275039
Cl	0.445850	1.105844	2.461004	Cl	-0.842032	0.168379	-2.362932
Cl	2.606410	1.606850	-1.854347	Cl	-2.148659	-1.623165	1.929084
O	5.003284	-1.012910	-0.164808	O	-5.230914	1.012983	-1.660719
C	6.154937	-1.626200	-0.812413	C	-5.922674	2.133945	-2.281310
C	7.430537	-1.524522	0.027746	C	-7.135415	1.695650	-3.108025
H	6.272627	-0.957937	-1.691421	H	-5.143543	2.483334	-2.991469
C	5.854128	-3.028906	-1.352447	C	-6.188016	3.284398	-1.302068
H	5.853713	-3.810525	-0.566193	H	-7.021439	3.083040	-0.600902
H	6.627718	-3.309497	-2.096949	H	-6.448327	4.198396	-1.874954
H	4.868737	-3.038182	-1.858935	H	-5.278028	3.502756	-0.707849
H	7.601236	-0.479393	0.355680	H	-6.857673	0.874089	-3.798442
H	8.299827	-1.834227	-0.588075	H	-7.488444	2.550641	-3.720498
H	7.407841	-2.171245	0.927473	H	-7.986166	1.353336	-2.486820
C	4.595623	-1.259774	1.106351	C	-5.786922	0.121697	-0.797782
C	3.853687	-0.204491	1.742923	C	-4.987602	-1.042975	-0.533039
C	4.832780	-2.465483	1.807294	C	-7.026859	0.279445	-0.139382
C	4.358303	-2.633062	3.117190	C	-7.467464	-0.687535	0.778307
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H	4.560210	-3.579059	3.645081	H	-8.437668	-0.544067	1.280323
H	5.386466	-3.280434	1.324826	H	-7.650482	1.161669	-0.326991
H	2.802762	0.381479	3.549369	H	-4.846293	-2.874832	0.623694
H	3.264880	-1.736671	4.780350	H	-7.034658	-2.572477	1.788311
C	1.486591	3.222087	0.500312	C	-2.347544	0.895714	0.193930
C	3.342358	2.322400	1.561354	C	-2.794897	-2.232644	-1.085962
H	4.262990	1.099171	0.058695	H	-3.590801	-0.544175	-2.127420
H	3.782758	3.226354	1.110957	H	-2.086325	-2.436461	-1.908188
H	2.993825	2.412144	2.602376	H	-2.935631	-3.022479	-0.331755
H	1.927548	3.903692	-0.261633	H	-3.110487	0.936119	1.004155
H	1.006527	3.702632	1.383012	H	-2.225341	1.802701	-0.437366
C	-2.666886	-1.232814	0.113056	C	3.570023	-0.309109	-0.510177
H	-2.201210	-2.233444	0.282706	H	3.735705	-1.325094	-0.942772
H	-2.433496	-0.613776	1.003952	H	2.989069	0.269354	-1.257842

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H -4.085901 -2.353706 -1.853945	H 5.437765 -0.868039 1.312368
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H -6.460392 -3.150831 -1.739616	H 7.838422 -0.145496 1.296137
H -6.301043 -1.355197 -1.658928	H 6.679983 1.210209 1.569278
H -6.891529 -1.209647 2.014889	H 6.983552 2.493305 -1.922915
H -6.530467 -0.224912 0.552201	H 6.152375 2.738822 -0.345558
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H -7.358588 -4.331728 0.049434	H 9.244207 -0.119378 -0.570513
H -5.845908 -3.942711 0.911316	H 7.759528 -0.539347 -1.464679
C -7.629103 -3.778232 2.144681	C 9.027441 0.897815 -2.491076
H -8.706772 -3.526700 2.091965	H 9.713926 1.746910 -2.303233
H -7.565859 -4.839814 2.459038	H 9.627094 0.108927 -2.988947
H -7.156352 -3.180922 2.949146	H 8.251789 1.211929 -3.216685
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C -0.046002 -0.453910 -0.166615	C 1.239334 -0.011777 0.030316
N -0.634707 -1.688559 0.007163	N 0.736590 -1.210314 0.479859
N -1.078517 0.471985 -0.217828	N 0.256120 0.952236 0.246161
C -2.370994 -0.125968 0.190802	C -1.004058 0.352780 0.734462
C -2.099818 -1.624433 0.003152	C -0.564156 -1.061041 1.151655
H -2.536679 0.092287 1.274916	H -1.370101 0.941275 1.603793
H -2.526962 -2.248400 0.813817	H -0.453316 -1.170963 2.254853
H -2.513656 -2.000032 -0.964946	H -1.282147 -1.836199 0.810181
C -0.980480 1.898136 -0.402926	C 0.457757 2.383192 0.342495
C -0.011240 -2.982243 0.019474	C 1.371021 -2.501323 0.500722
C 0.216044 -3.666020 -1.209389	C 1.126990 -3.410014 -0.558852
C 0.718899 -4.980818 -1.150134	C 1.719696 -4.687414 -0.488505
C 0.978316 -5.631853 0.072729	C 2.531056 -5.078967 0.594752
C 0.705034 -4.937143 1.270689	C 2.742819 -4.149352 1.635027
C 0.202213 -3.623689 1.274489	C 2.177879 -2.859345 1.613390
C -0.035974 -3.000696 -2.539777	C 0.279849 -3.019694 -1.747680
H 0.908756 -5.515168 -2.095986	H 1.541357 -5.398434 -1.312493
C 1.552504 -7.029286 0.105113	C 3.181524 -6.442994 0.632862
H 0.888035 -5.435553 2.237344	H 3.375905 -4.433971 2.492080
C -0.070260 -2.898905 2.569212	C 2.477503 -1.869901 2.715991
H 0.707426 -2.193565 -2.734718	H 0.702938 -2.137446 -2.275444
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H 2.653904 -6.998577 0.257177	H 3.152366 -6.881289 1.651471
H 1.367798 -7.572932 -0.842733	H 4.252461 -6.378869 0.340600
H 1.129952 -7.627074 0.938328	H 2.691971 -7.151852 -0.063899
H 0.157077 -3.543098 3.440684	H 3.096133 -2.333412 3.508437
H -1.134198 -2.585525 2.652411	H 1.555705 -1.479783 3.197627
H 0.540895 -1.970049 2.644181	H 3.030489 -0.990379 2.321532
C -0.986087 2.418497 -1.728804	C 0.192114 3.246823 -0.751502
C -1.021447 2.763801 0.725898	C 0.870035 2.909913 1.602754
C -1.001758 3.819012 -1.893974	C 0.378328 4.635390 -0.563183
C -1.048490 4.155023 0.496980	C 1.024428 4.298829 1.734825
C -1.030618 4.706690 -0.799259	C 0.793259 5.184675 0.660665
C -1.009555 6.203276 -1.010367	C 1.018902 6.669988 0.822806
H -0.999063 4.226608 -2.918719	H 0.189814 5.307969 -1.416914
C -1.005822 2.235411 2.141015	C 1.186837 2.004101 2.769047
H -1.069977 4.830152 1.369154	H 1.355317 4.703172 2.706006
C -0.961929 1.520110 -2.940506	C -0.300824 2.770017 -2.099580
H 0.035240 1.035423 -3.052070	H 0.237385 3.293150 -2.915778
H -1.175649 2.093345 -3.863533	H -1.380085 3.007548 -2.234441
H -1.697468 0.692617 -2.865001	H -0.146022 1.687132 -2.255651

H	-1.955868	1.723151	2.415064
H	-0.870036	3.062472	2.865060
H	-0.177575	1.506092	2.291779
H	-1.495211	6.744443	-0.173524
H	-1.514605	6.492968	-1.954036
H	0.036215	6.576174	-1.075893
C	3.427942	2.459548	-0.365182
Cl	2.180902	-0.048464	-2.571900
Cl	1.937854	0.173432	2.188770
O	4.619063	0.059838	-0.165790
C	5.424255	-0.758186	-1.084973
C	6.479039	0.074066	-1.811690
H	4.651355	-1.066261	-1.820353
C	5.983722	-2.009649	-0.401862
H	6.849161	-1.787588	0.255264
H	6.330721	-2.726940	-1.174765
H	5.203443	-2.511609	0.204681
H	6.017515	0.943882	-2.320168
H	6.968613	-0.551641	-2.585939
H	7.268298	0.444603	-1.126233
C	5.177607	1.026023	0.645977
C	4.513476	2.278539	0.618718
C	6.246652	0.799733	1.531869
C	6.660730	1.831059	2.393184
C	6.000126	3.072387	2.392196
C	4.927363	3.288657	1.513068
H	7.499486	1.651961	3.084392
H	6.733928	-0.183538	1.572603
H	4.418298	4.265226	1.486422
H	6.325893	3.873622	3.073338
C	2.343301	-1.801655	-0.075993
C	2.235460	3.053126	-0.111655
H	3.615992	2.076119	-1.384173
H	1.502617	3.214521	-0.916281
H	1.977548	3.412633	0.897387
H	2.542380	-2.284473	0.906538
H	2.644461	-2.384570	-0.976075
C	-3.571845	0.405583	-0.605496
H	-3.554709	1.523396	-0.619027
H	-3.479534	0.071656	-1.659682
C	-5.298665	0.576248	1.127186
C	-5.918123	-0.154513	-1.064386
C	-6.492791	-0.141294	1.749384
H	-5.527333	1.661479	0.944252
H	-4.494633	0.567605	1.892196
C	-7.121944	-0.914066	-0.512001
H	-6.223651	0.862916	-1.433192
H	-5.574966	-0.713288	-1.960118
H	-6.877669	0.392259	2.640811
H	-6.201858	-1.169324	2.041449
H	-7.955267	-0.962833	-1.237622
H	-6.818348	-1.945851	-0.245976
N	-4.848531	-0.110738	-0.076682
N	-7.667055	-0.299347	0.777097
C	-8.670233	-1.243635	1.384389
H	-9.050086	-0.809428	2.328122
H	-9.504905	-1.398663	0.678036
H	-8.175488	-2.210572	1.589677
C	-8.325026	1.071676	0.546879
H	-8.687888	1.383388	1.547193
H	-7.510610	1.763981	0.263130
C	-9.445874	1.110407	-0.483372
H	-10.295096	0.441712	-0.240164
H	-9.848587	2.143580	-0.494729
H	-9.098637	0.894161	-1.512980
H	0.358442	1.304941	3.013001
H	1.403572	2.594746	3.680060
H	2.085710	1.392935	2.541559
H	0.548110	7.250753	0.005083
H	2.105530	6.905345	0.814089
H	0.618349	7.041320	1.788701
Cl	1.883585	0.195256	-3.029845
Cl	3.947694	1.821972	0.541511
C	3.841939	-1.121494	-0.790828
H	4.808093	-1.068570	-1.356195
H	3.642410	-2.060309	-0.239578
C	-2.077392	0.343491	-0.379520
H	-2.220042	1.380445	-0.766230
H	-1.686184	-0.262785	-1.222551
C	-4.171530	0.662785	0.850429
C	-4.137913	-0.839444	-1.012355
C	-5.360748	-0.067022	1.470622
H	-4.510654	1.556769	0.259534
H	-3.581062	1.072420	1.696285
C	-5.304808	-1.638133	-0.438245
H	-4.501302	-0.084414	-1.761626
H	-3.508936	-1.555486	-1.581616
H	-6.024457	0.624220	2.026633
H	-5.001503	-0.854651	2.161547
H	-5.925685	-2.103091	-1.226626
H	-4.916543	-2.434201	0.227382
N	-3.351904	-0.247878	0.062963
N	-6.228601	-0.786284	0.432891
C	-7.190626	-1.691661	1.155509
H	-7.842701	-1.080035	1.806711
H	-7.802723	-2.242791	0.419633
H	-6.616799	-2.409725	1.769554
C	-7.017711	0.254791	-0.380962
H	-7.674873	0.753121	0.360186
H	-6.282481	1.006182	-0.724316
C	-7.821652	-0.286259	-1.555761
H	-8.571159	-1.048544	-1.264910
H	-8.385426	0.563897	-1.990639
H	-7.186082	-0.693810	-2.366405

Table S5. Coordinates data set, absolute energies (a.u.) for DFT optimized ionic complex (Cluster (Cr)Mil-101-AquaMet™).

Precat				Act			
217				217			
i =	23, E = -1494.8902351452			i =	35, E = -1494.8869603544		
Cr	25.9581117390	15.1123496912	17.2249211851	Cr	26.2350053249	15.0232330053	17.2103892519
Cr	22.6555799042	15.8258554551	17.5411141837	Cr	22.9488399220	15.7428922288	17.5391488394
Cr	24.9369341985	17.4449566438	19.4176482615	Cr	25.1802400524	17.3798048867	19.4298083870
O	24.5053460519	16.1686661675	18.1271417049	O	24.7199311967	16.1099847309	18.1282674957
O	25.1149495996	13.3773448835	17.7338241388	O	25.3591266146	13.3017690199	17.7332432076
O	25.1177221428	15.0913510514	15.4261228066	O	25.3618465164	15.0137333071	15.4164065848
O	26.8423664693	16.8048429489	16.7038022144	O	27.1455662537	16.7233746967	16.7140035758
O	26.9953246749	14.9376097809	18.9050289019	O	27.2308220053	14.8600407208	18.9092483136
O	23.1773150802	16.2472742430	15.7064518709	O	23.4183496222	16.1666208143	15.6987758204
O	22.1765590747	15.4064460082	19.4400065558	O	22.4747617481	15.3189658528	19.4414890307
O	22.9278870151	13.8677348250	17.3331201695	O	23.1714037545	13.7848632903	17.3333059573
O	25.8951160724	16.0950077613	20.5296426524	O	26.1306279903	16.0227082467	20.5298084394
O	26.5962141928	18.0467012485	18.5902928794	O	26.8365650718	17.9729223477	18.5880111155
O	23.3296071214	17.0328676964	20.5375511377	O	23.5721294509	16.9757343022	20.5423559453
C	23.8868828627	13.0690205297	17.6158777065	C	24.1352518858	12.9883387876	17.6169307070
C	23.5223256959	11.6311099158	17.8112260484	C	23.7759773554	11.5515396872	17.8156345775
C	22.1775808745	11.2319401845	17.7432928730	C	22.4310794980	11.1500539368	17.7770981524
C	24.5200684778	10.6798386960	18.0732809235	C	24.7840254508	10.6034989354	18.0488586101
C	24.1746586782	9.3416868818	18.2619421945	C	24.4485497685	9.2632216925	18.2364529134
C	22.8294494114	8.9376653023	18.1944283254	C	23.1035245899	8.8576362743	18.1978942660
C	21.8350698899	9.8982503079	17.9405803406	C	22.0988289160	9.8146978471	17.9752391496
H	25.5556439251	11.0074070625	18.1291835918	H	25.8188656979	10.9367118475	18.0811729760
H	21.4208454218	11.9859747385	17.5388267997	H	21.6671362512	11.9026017124	17.5949217558
C	27.3905992567	14.3763204450	21.1612618070	C	27.6445162092	14.3156987098	21.1636600355
C	28.1424246516	13.2603391648	20.7655216975	C	28.4072648329	13.2072550404	20.7658580832
C	27.2506333826	14.6804865887	22.5253324596	C	27.5042875648	14.6175905289	22.5281047571
C	28.7552021187	12.4590693060	21.7247476499	C	29.0220970737	12.4060478051	21.7237998596
C	28.6147666020	12.7581374811	23.0899712123	C	28.8719316900	12.6966374296	23.0901179375
C	27.8511066856	13.8696131710	23.4836526893	C	28.1066016127	13.8061791936	23.4849612941
C	29.2207574950	11.9093356497	24.1571984298	C	29.4636942125	11.8375407754	24.1572920741
H	26.6645908336	15.5507056508	22.8118938482	H	26.9147820350	15.4845814026	22.8170707404
C	26.7088771368	15.2012529764	20.1205799875	C	26.9533092995	15.1306927124	20.1215830307
C	22.4803551378	16.0791378058	20.4812780308	C	22.7537670297	15.9950646666	20.4821043280
C	21.7614868096	15.7085651434	21.7409087697	C	22.0492278150	15.6088709317	21.7415711207
C	22.1090562823	16.3019211244	22.9637682085	C	22.4106812013	16.1971209830	22.9621598591
C	21.4413237533	15.9363137198	24.1329339331	C	21.7519671931	15.8295571167	24.1343731897
C	20.4108999845	14.9798278441	24.0960521263	C	20.7178219325	14.8784582375	24.0986618962
C	20.0535279478	14.4038812938	22.8651771816	C	20.3498139207	14.3031682085	22.8707799808
C	20.7278720571	14.7566537011	21.7003752995	C	21.0166270277	14.6567013128	21.7024223877
H	22.9014318687	17.0460184969	22.9853276965	H	23.2054711722	16.9385144231	22.9773604568
H	20.4681662116	14.3080149226	20.7446247606	H	20.7508995253	14.2119819638	20.7461807408
C	19.6499571293	14.5486786734	25.3129625481	C	19.9571731802	14.4602546827	25.3167497364
O	22.1590313976	17.7176011544	17.7339239960	O	22.3948111423	17.6274472081	17.7331747582
O	23.9591671265	18.8944019550	18.4332304509	O	24.1875658594	18.8199854120	18.4317919978
H	28.2191405160	13.0279428999	19.7065334730	H	28.4889277905	12.9787141231	19.7061138467
C	24.0996463227	15.7146681112	14.9916773772	C	24.3458711072	15.6377493295	14.9828502878
C	23.9626965921	15.8211895332	13.5100636900	C	24.2072176782	15.7489144704	13.5027131358
C	24.9603981896	15.2615243231	12.6962198700	C	25.1984441835	15.1780626665	12.6888629472
C	24.8323975458	15.3103141064	11.3104923853	C	25.0677784401	15.2247143642	11.3037145301
C	23.7014704385	15.9062018547	10.7251823798	C	23.9411306292	15.8306345070	10.7207104384
C	22.7060411811	16.4626817099	11.5475194665	C	22.9545307998	16.4020919048	11.5426990096
C	22.8375463467	16.4351321977	12.9344206637	C	23.0884762216	16.3761257539	12.9290602828
H	22.0846302207	16.8779436729	13.5875803113	H	22.3422414104	16.8300966226	13.5823553545
H	25.8164330225	14.7841024436	13.1686912174	H	26.0502229665	14.6939550315	13.1625022525
C	22.7807408332	18.8044419036	17.9441512341	C	23.0079648035	18.7182269575	17.9421452307
C	22.0617650067	20.0855603906	17.6395546165	C	22.2749181913	19.9940523305	17.6347149570
C	20.7919817602	20.1823016934	17.0092611308	C	20.9965807091	20.0930268583	17.0142054985
C	20.2414419535	21.4580239187	16.8246010703	C	20.4473202046	21.3714871549	16.8400996778
C	20.8929472526	22.6265274237	17.2422192570	C	21.1090953612	22.5398470255	17.2457205023
C	22.1378234919	22.5221196776	17.8783414993	C	22.3620739441	22.4330056386	17.8635325840
C	22.7067173229	21.2679320544	18.0597459042	C	22.9257212048	21.1766728794	18.0443069181
S	19.7480886510	18.8189994453	16.3523186356	S	19.9568444151	18.7398392977	16.3138378092
C	27.0895658931	17.8175693238	17.4322203849	C	27.3611689378	17.7417673622	17.4406868453
C	28.0493647965	18.8295455551	16.9087413436	C	28.3237841023	18.7652345312	16.9307321817
C	28.3491922622	19.9711012759	17.6709150618	C	28.5979745370	19.9198449165	17.6834934684
C	29.2315610152	20.9230714602	17.1733540819	C	29.4697916496	20.8847970008	17.1868175814
C	29.8318016276	20.7423153799	15.9159039193	C	30.0889355591	20.7091179053	15.9372081582
C	29.5266676171	19.6000716657	15.1566674406	C	29.8168045242	19.5475705431	15.1922738767

C	28.6391073140	18.6462725383	15.6494504173	C	28.9413637227	18.5806362912	15.6841262189
H	28.3838014297	17.7597131655	15.0738005204	H	28.7157086717	17.6817069528	15.1146188369
H	27.8769625752	20.0922864781	18.6435139043	H	28.1132999600	20.0432258365	18.6498635196
O	20.9252661243	15.5561148917	17.1148490649	O	21.2240006706	15.4772292393	17.1204376757
O	27.3287080897	14.1546618269	16.4149823679	O	27.6159599997	14.0734501155	16.4023281614
O	25.3469815400	18.6719291182	20.6981290585	O	25.5802236382	18.6600839671	20.6862332648
H	24.6205019183	18.7773104691	21.3385378933	H	24.8315188664	18.7742837795	21.3006686093
H	28.1120721968	14.1529524600	16.9916685406	H	28.3739342818	14.0162996279	17.0063218156
H	20.4033624452	16.3980239942	17.2378818124	H	20.6847007350	16.3160066764	17.2135365484
H	27.7441501758	14.0748134751	24.5467118512	H	27.9974701275	14.0074588718	24.5485180682
H	29.3020173351	11.5734094182	21.4020251406	H	29.5762451928	11.5259425240	21.3978098993
O	28.7778522556	11.8219223315	25.2852397309	O	29.0115884677	11.7451082308	25.2816805357
O	30.3407272048	11.1949821005	23.8036565663	O	30.5785031059	11.1154546310	23.8056875728
H	30.6322480083	11.4666415879	22.9141557701	H	30.8831987770	11.3936073222	22.9226337624
H	29.4729004988	21.8216450842	17.7370723090	H	29.6860011906	21.7915320386	17.7478499004
H	29.9447948405	19.4624368280	14.1594782536	H	30.2508255500	19.4007806609	14.2029989299
C	30.7510592638	21.8159488417	15.4379482254	C	30.9883755615	21.8011822503	15.4490060005
O	30.7273942148	22.9536974765	15.8650975602	O	30.9555834579	22.9432517586	15.8671022313
O	31.6588964982	21.4690094891	14.4645287878	O	31.8911933448	21.4669285535	14.4653106933
H	31.6203919367	20.5069915766	14.3129989674	H	31.8689462186	20.5039391311	14.3159665792
C	23.4983661901	15.9366781641	9.2454294581	C	23.7341897969	15.8589298136	9.2427126031
H	21.8370201471	16.9150107256	11.0750153124	H	22.0909529752	16.8643146691	11.0698409518
H	25.5958760701	14.8379778455	10.6922772033	H	25.8247984166	14.7427710218	10.6850859885
O	22.4050768516	15.9477634640	8.7102308530	O	22.6394967109	15.8701998207	8.7096447558
O	24.6416006308	15.9445274712	8.4749167812	O	24.8766690061	15.8667211754	8.4723127667
H	25.4186506895	16.0427578350	9.0555933057	H	25.6541111741	15.9605176372	9.0532972836
H	20.7988430049	9.5698483044	17.9050243653	H	21.0641795421	9.4796102231	17.9648272513
H	24.9628049743	8.6271337041	18.5008679544	H	25.2445282534	8.5491623578	18.4495332585
C	22.3798950912	7.5262872810	18.4074854745	C	22.6568442197	7.4481909168	18.4096688851
O	21.2471449808	7.2289032660	18.7400873710	O	21.5276184729	7.1507552635	18.7475158688
O	23.3190609749	6.5371852310	18.2027948184	O	23.5798932698	6.4530325128	18.1988202571
H	24.1357191790	6.9352245774	17.8491750497	H	24.4046634964	6.8387297299	17.8497562886
H	21.7089328648	16.4329507591	25.0657071470	H	22.0272754138	16.3216077843	25.0671745067
H	19.2448862102	13.6764543816	22.8496773675	H	19.5379220722	13.5791059453	22.8612992786
O	20.2934020541	14.6985438648	26.5212415082	O	20.6006130550	14.6194914622	26.5232519809
H	21.2167241172	14.9708972459	26.3673623600	H	21.5272657083	14.8782914581	26.3664765871
O	18.5257968386	14.0830205337	25.2789088423	O	18.8300068446	14.0024997292	25.2816458634
C	20.3028441296	23.9895668501	17.0490928876	C	20.5290773189	23.9078624885	17.0500214089
H	19.2551172933	21.4844698448	16.3631598788	H	19.4559172727	21.4039389878	16.3895940325
H	22.6400569288	23.4258234619	18.2169501662	H	22.8760875086	23.3354738085	18.1877528113
O	19.3733844201	24.1153002642	16.0368158946	O	19.6050672164	24.0374232495	16.0341690159
H	19.3106306754	23.2678716366	15.5573120848	H	19.5410430955	23.1905086071	15.5538939490
O	20.6059248333	24.9588464588	17.7213698386	O	20.8383318484	24.8769166087	17.7199947395
O	19.3687867999	17.9563394150	17.4984629205	O	19.6045828718	17.8069925223	17.4170122151
O	20.5389239724	18.1289908361	15.3173865474	O	20.7671106119	18.1266286657	15.2443087569
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H	23.6754101489	21.1667020613	18.5435465106	H	23.8995412560	21.0732880966	18.5171549875
Ru	9.6145881558	23.5839923346	14.6205048109	Ru	10.0939425619	23.5507920020	14.7080076611
H	8.0432926419	25.6314098322	17.8341559319	Cl	10.2063042760	23.2941631688	16.9954491288
H	8.1354617223	27.4061691617	17.7060945600	C	13.5181811659	23.9251266829	16.9565634305
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C	13.1290468631	23.9941022283	16.9101130056	H	15.4663268190	14.6877981005	16.0965039771
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C	15.6455276611	17.5363889520	15.4022097206	H	15.7145343156	13.3474349292	14.9718700770
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H	16.2433229580	18.4452238714	15.5631824562	H	12.5927846510	19.8364538941	15.5349751748
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H	13.5789360700	16.9435765890	15.0052219496	N	16.6087976753	16.6403643071	14.2383709715
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C	15.7723410281	15.3882304030	14.0439150240	C	10.1768105883	20.0490561561	13.8700756253
C	6.7016598194	24.5516502461	14.9421153383	H	14.9802022208	15.3739301551	13.7304547480
C	12.3736197245	20.3115821455	14.4819233364	C	13.0073870993	19.0005197204	13.5805398434
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C	13.3218054299	21.5027472898	14.3531897847	H	12.2629228955	18.1897319146	13.6783590819
C	7.7946910780	27.5082071027	14.8676681101	C	8.0225127967	18.3507599567	13.2123386817
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C	4.3444170893	23.2289176419	14.2095167742	C	13.6016885991	24.3997239732	13.1306619416
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H	18.2936156974	16.1343850107	13.7592058486	H	14.3558077472	16.9033944768	12.4565839133
C	8.0823634462	22.6668487083	14.1329587139	C	14.1397905794	25.6887160569	13.0744665713
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H	16.3597488624	14.9834990195	13.2103407130	C	10.4368242851	20.7023044530	11.4134945250
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C	7.7924155422	18.4665999844	13.1615346333	H	4.4123839477	20.1937981352	15.7634787869
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H	8.0822827598	21.6767579232	13.6697060508	C	6.1989140735	25.6299266418	15.4964586774
H	5.6346488867	21.6309897073	13.5345283839	C	7.3258781771	24.8735640853	15.2037250837
C	14.6772196736	27.8990740819	14.1494937860	H	3.2524511849	21.4637196176	15.3215278841
H	16.7188071034	18.5454307572	13.1817749582	C	4.9325119787	25.0649527450	15.3037687537
C	14.6905528975	17.9605857549	12.7230905064	H	8.3084698220	25.3286318017	15.3478719857
H	13.8704949773	21.4864217536	13.3993908519	C	3.8149512899	20.6051284546	14.9392774816
C	6.6421842713	17.5633334511	12.8024526962	H	4.0371461104	25.6444379705	15.5200048084
H	8.1887354151	27.3148554233	13.8612073569	C	7.2440056935	23.5432452049	14.7185006848
C	13.2898046432	24.4975990301	13.0847335083	C	4.7984806470	23.7543650621	14.8412373345
C	9.5651667622	20.0128529236	12.4793694728	C	5.9334175144	22.9800934434	14.5573038694
H	14.1149567438	17.0584084295	12.4375455250	H	3.0871282765	19.8411598814	14.6310833235
C	13.8366414109	25.7820176925	13.0501716331	H	3.8066279837	23.3383860817	14.7128241000
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C	10.2525363115	20.7699369814	11.3636711837	C	8.4351189062	22.7826103774	14.3994909808
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Cr	23.1440442119	16.0135506291	17.5362960339	Cr	23.4785661466	16.0178292064	17.5495297196
Cr	25.3896483224	17.6367247548	19.4225648940	Cr	25.7141530047	17.6875625950	19.4495648839
O	24.8954734109	16.3936507094	18.1199600818	O	25.2058108713	16.3900153398	18.0797152423
O	25.5726972210	13.5373849566	17.7318836056	O	25.8962775099	13.6038577575	17.7358492373
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O	23.6306825026	16.3971787419	15.6992810070	O	23.8956813004	16.3927304124	15.6726021837
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O	27.0495738254	18.2570131337	18.5791464729	O	27.3787028079	18.2824878251	18.5886868809
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C	24.3395083128	13.2533680092	17.6158921948	C	24.6725027577	13.2800451750	17.6200490606
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C	27.8014042204	14.5276105796	21.1574471066	C	28.1662878393	14.5812641149	21.1591696025
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C	20.5498707792	14.5642863851	22.8634879612	C	20.8616220758	14.5887634137	22.8673756042
C	21.2207861918	14.9197528243	21.6971683099	C	21.5434599840	14.9349546603	21.7045402848
H	23.3887890839	17.2170346157	22.9785552967	H	23.7249250810	17.2139168398	22.9928540231
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C	20.1494956514	14.7224010278	25.3101553747	C	20.4397068057	14.7635723350	25.3129924489
O	22.6158745326	17.8963052690	17.7299132036	O	22.9463762667	17.9072245368	17.7362050942
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C	20.6974808828	21.6697303711	16.8476238453	C	21.0007495269	21.6807034611	16.8770715138
C	21.3509765014	22.8352892651	17.2742972940	C	21.6690287970	22.8464219876	17.2765212420
C	22.5962739194	22.7139273675	17.9084960243	C	22.9193671093	22.7301034708	17.9002537277
C	23.1608565271	21.4541310009	18.0806415145	C	23.4781544234	21.4705164119	18.0810967538

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C	27.5646111407	18.0038521924	17.4298002176	C	27.9009223779	18.0504458016	17.4456812195
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C	28.7637105926	20.1973329217	17.6374084642	C	29.1339293116	20.2277630427	17.6736031896
C	29.6371221639	21.1580183206	17.1393398218	C	30.0034307631	21.1931033298	17.1743194397
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C	29.9958212911	19.8039348340	15.1554024190	C	30.3490685792	19.8550369521	15.1804561428
C	29.1186619014	18.8407110961	15.6495718995	C	29.4745397975	18.8876261348	15.6751273449
H	28.8943342356	17.9376787161	15.0857374628	H	29.2461302885	17.9895502034	15.1053015482
H	28.2704961498	20.3257773249	18.5989888037	H	28.6488260242	20.3513997512	18.6396335615
O	21.3894060575	15.7774083273	17.1922260131	O	21.7309261231	15.7915542358	17.1996309118
O	27.8337755347	14.3067792371	16.4097532258	O	28.1346766079	14.3942883408	16.4066675803
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H	25.0618070789	19.0019724062	21.3103364360	H	25.3243973110	19.0317207627	21.3281709363
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H	28.1553241893	14.1925435975	24.5405579047	H	28.5218964611	14.2500499786	24.5435963360
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O	30.7906759720	11.3476160266	23.7964922210	O	31.1089339809	11.3562314879	23.8069336489
H	31.0647480890	11.5983586643	22.8949494874	H	31.4079080536	11.6105795073	22.9147342567
H	29.8477044572	22.0708324480	17.6928775212	H	30.2179827508	22.1013051609	17.7332589554
H	30.4331273496	19.6543296550	14.1677412254	H	30.7796668855	19.7071415796	14.1897211051
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O	31.1805206766	23.1743767595	15.8627669165	O	31.4995358468	23.2502063185	15.8670748365
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H	32.0559379191	20.7336677156	14.2934743364	H	32.4092433465	20.8140686021	14.3093706348
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H	26.0046476686	14.9648640258	10.6724565381	H	26.3591186288	15.0072708148	10.6803073011
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O	25.0932293778	16.1709473597	8.4761448129	O	25.4243885436	16.1767615853	8.4733472401
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H	25.3806768072	8.8106578701	18.4571268000	H	25.7393876358	8.8258021128	18.4742346121
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O	23.7800432786	6.7541232656	18.1991765717	O	24.1106865752	6.7579997209	18.2004532902
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H	22.1998860943	16.5986435206	25.0614296490	H	22.5241959033	16.6078760604	25.0705476482
H	19.7423910394	13.8346829729	22.8514208738	H	20.0467640298	13.8681834172	22.8499362698
O	20.7596287473	14.9277921913	26.5239525345	O	21.0729437252	14.9305319690	26.5237877789
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O	19.0390870470	14.2248253830	25.2752418183	O	19.3082056130	14.3153486625	25.2781759975
C	20.7636690294	24.2051251294	17.0855912395	C	21.0865345274	24.2133547519	17.0768387304
H	19.7104608807	21.6960919797	16.3871458770	H	20.0115780956	21.7096759172	16.4221331190
H	23.1044999466	23.6125026296	18.2534684677	H	23.4375578567	23.6286774284	18.2288580259
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H	19.7301437104	23.4918448613	15.6149014707	H	20.0899718178	23.4970857664	15.5860785422
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O	19.8991591228	18.1103816476	17.4425856226	O	20.1535776871	18.1236298305	17.4957966038
O	20.9869361283	18.4345303563	15.2408645314	O	21.3097152647	18.4344756280	15.3174457866
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H	15.5172077157	15.2109835652	17.8857170621	Ru	9.2382494606	22.4880133808	14.7479610958
H	15.8537517300	17.3479992375	17.4955912931	C	11.0373655620	21.5508531312	14.7211796072
H	17.1668412668	14.7216034473	17.4197703886	N	12.2663528517	22.1120860017	14.7109447555
C	16.1133233505	14.7052962355	17.1166647969	N	11.1652919592	20.2035916342	14.8624303954
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H	5.0484998633	23.7255149001	17.8621202844	C	13.3399216446	21.1025259830	14.8335469607
C	9.6093313307	19.5914782850	17.1603232056	H	14.0527463798	21.4051728481	15.6096234742
H	15.7941558860	13.6530238651	17.0991281320	H	13.8860514743	21.0074099998	13.8835140164
C	15.7182437919	17.7087299088	16.4702400289	C	10.1340073206	19.1933543237	14.8644439085
C	12.8099047705	24.2526044747	16.4409885469	C	12.6193356661	23.4782526515	14.4105837701
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C	5.1673917070	23.0287078664	17.0355430418	C	13.3373516074	25.6673194679	15.1202834208
C	17.8804632203	16.7691235165	15.7749404817	C	12.9634071009	24.3579222372	15.4577496716
C	14.2453335065	17.9063497375	16.1306317850	C	12.5916633452	22.8710487819	11.9292994658
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H	18.2220673061	17.7754872629	15.5060635887	C	9.6838912226	18.6867891331	13.6207428474
C	4.0991094030	22.2229906956	16.6256872732	C	9.7341858627	18.5958373619	16.0801275614
C	15.8947512129	15.2845949143	15.7252272070	C	8.8696041852	17.5460428941	13.6268760428
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H	12.2199234241	19.8864975092	16.1415176322	C	8.5196340403	16.8850718274	14.8100627023
N	16.3946920345	16.7130971995	15.5408510180	H	8.5350967762	17.1442719209	12.6717300780
H	8.0231892621	17.4694728407	16.7194182507	C	10.1595030488	19.1040932481	17.4357880879
C	9.2849468027	18.9627956273	15.8273622244	H	8.6303408079	16.9765095173	16.9576514161
H	13.4949461318	26.5521288139	15.2737273776	C	10.0818126026	19.3003149788	12.3045275427
H	18.3718900125	16.0087729087	15.1590283454	C	7.3087818342	21.9045381694	14.8652019655
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C	8.4230390439	17.8553380723	15.7822030382	Cl	9.7447587173	22.6366067210	17.0846322886
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C	12.8268246091	24.5358705932	14.9603858105	C	4.6502414782	18.8011265614	14.1048388376
H	14.8330713452	15.2723561563	15.4590810389	C	4.6425571068	17.3722721561	14.6507847637
C	12.2353498711	20.0027035274	15.0467270313	H	4.9373470078	18.7409838516	13.0468088796
H	16.4361267824	14.7012840927	14.9701727717	C	3.3043851318	19.5163461701	14.1873262845
C	13.2634265674	25.7962181638	14.5243800500	H	2.9435549778	19.6262301436	15.2159387045
C	4.2550251904	21.3085035955	15.5832227476	H	2.5585418902	18.9323026919	13.6298035152
N	14.0873558501	18.3773727268	14.7520145478	H	3.3663415469	20.5136172158	13.7331628874
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C	13.0838022085	21.2126174857	14.6424278989	H	3.9511613825	16.7589781160	14.0557597957
C	8.8114176255	25.3492435874	14.4968133498	H	4.3258504297	17.3028730579	15.6970701731
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C	16.1384093092	17.1867022654	14.1179260417	C	6.5922785785	21.3349697936	16.0276874772
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C	12.6945655762	18.6930422294	14.3972467166	C	5.0421301539	20.3838954701	18.1883787170
Ru	9.2639198920	23.1449086873	14.3338536856	C	5.8598626111	21.5045224442	18.3620983147
C	10.7940252874	21.7693597076	14.3861254996	C	6.6149634608	21.9619962878	17.2890075396
C	9.8131480496	19.4485286411	14.6134316766	H	4.4400821719	20.0106151916	19.0142056316
C	5.4869045885	21.1800511463	14.9235875180	H	4.3466667621	18.8701833246	16.8421392645
H	6.7698142431	24.7181049264	14.7010610935	H	7.2721499815	22.8169181054	17.4234876172
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H	11.9992454214	17.8730155842	14.6530228049	H	7.0508389434	21.4101907269	13.9251979479
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H	16.6877328615	18.1314763865	14.0221099450	N	14.4713130307	18.3240287070	14.6304452813
H	5.2316914796	18.0761233210	15.2411307431	H	12.9161995103	18.7993632197	13.3309837546
H	3.5668849496	18.6934584041	15.2410225134	H	12.4036452272	17.7208954719	14.6399315552
C	8.0767262180	17.2306932734	14.5787758500	C	15.0258362587	17.4821434137	13.5698232643
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C	7.6110222172	24.8612359438	14.0287335032	C	16.2564856142	17.5887420893	16.1612163153
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C	13.4402145452	26.0970791384	13.1703018235	C	16.5306608660	17.3374274424	13.7415895263
H	14.1069317887	16.4489305530	13.8060068115	H	14.8614145496	17.9786061593	12.6015773050
C	7.2221087599	15.9847125050	14.5653070974	H	14.5293017023	16.4944449496	13.5054069942
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H	12.6576418698	18.8198526768	13.3065478590	H	18.9029089452	16.2392217185	14.4683059764
H	4.0116205928	17.3710355474	14.1530020291	H	18.7418153740	16.6266019180	16.2218029394
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H	14.6017288420	17.8178538805	12.8011632428	H	17.0909688386	14.8074299370	14.3220385387
C	13.2074209662	25.0801377393	12.2355453489	H	15.4779634828	15.1959691820	14.9421506579
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H	2.8879916105	20.3753879665	13.2994990096	H	16.6670569683	13.5156529170	16.3646533699
Cl	9.2839349241	23.2025446247	11.9635861004	H	16.2946074019	14.9598293222	17.3126452414
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H	5.4252486756	18.7063616985	12.7913705074	C	7.7875984678	15.5643880962	14.7805270246
C	9.9333437853	19.4264653463	12.0596543204	C	8.5152332701	24.3407294701	14.8768742270
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H	9.7532128480	20.3489467942	12.2243170516
H	7.3633858241	15.3563402667	13.7898500761
H	6.9747302499	15.5279165866	15.5184099945
H	8.4735991517	14.7393573455	15.0246597645

Ci2

223

i = 16, E = -1508.6061006353

Cr	26.1593888107	15.0119937981	17.2143948774
Cr	22.8383848657	15.7220288634	17.5462033639
Cr	25.1026255887	17.3608651752	19.4279042608
O	24.6020440042	16.0975985747	18.1296228530
O	25.2383063377	13.3015432795	17.7364799960
O	25.3131368564	15.0042103069	15.4164875564
O	27.0831475395	16.7085193519	16.7246568792
O	27.1675207955	14.8527547685	18.9149994355
O	23.3338405948	16.0867517459	15.6991448371
O	22.3480301513	15.3141728157	19.4473084897
O	23.0424899705	13.7674609835	17.3425382287
O	26.0720508320	16.0149131685	20.5345965838
O	26.7667958209	17.9644325787	18.5941899596
O	23.4957505638	16.9499740684	20.5445413587
C	24.0169922825	12.9791489352	17.6227572841
C	23.6665679078	11.5416317815	17.8229476854
C	22.3207093864	11.1451013510	17.7895109808
C	24.6709100241	10.5882555077	18.0535719804
C	24.3278962858	9.2492046113	18.2427300997
C	22.9801526012	8.8502845856	18.2085105811
C	21.9802925203	9.8126817091	17.9885421677
H	25.7083628502	10.9135872618	18.0847173316
H	21.5616977112	11.9034362331	17.6110156967
C	27.5565469606	14.2803779226	21.1676896458
C	28.3137704403	13.1691689750	20.7675468237
C	27.4100191469	14.5703800597	22.5335584836
C	28.9396995441	12.3699011095	21.7219862096
C	28.8029336910	12.6603475119	23.0894987679
C	28.0230867489	13.7609393563	23.4865325778
C	29.4164647072	11.8169390542	24.1568736052
H	26.8158760608	15.4321154988	22.8310265749
C	26.8862499271	15.1151423229	20.1274209285
C	22.6549329511	15.9850048746	20.4849329612
C	21.9411682323	15.6064258802	21.7433629554
C	22.2990541928	16.1909199092	22.9660644450
C	21.6395137773	15.8211492403	24.1386044138
C	20.6039765349	14.8701630034	24.1026120424
C	20.2386533018	14.2987998119	22.8719838108
C	20.9058191214	14.6555131061	21.7040527566
H	23.0947429250	16.9317841388	22.9799846899
H	20.6380079827	14.2117447081	20.7478554812
C	19.8330262483	14.4529747486	25.3176344523
O	22.3138732617	17.6099775949	17.7352533340
O	24.1100713229	18.8092990134	18.4309654051
H	28.3928656615	12.9427394300	19.7072607550
C	24.2748215694	15.5915592727	14.9849959512
C	24.1279650155	15.7109059435	13.5063961497
C	25.1103648531	15.1427818244	12.6811444887

I14e

197

i = 112, E = -1421.7167583376

Cr	24.9697534923	15.0979232345	17.2067523356
Cr	21.6544235467	15.7919158778	17.5408426571
Cr	23.9264329623	17.4508571926	19.4227619827
O	23.4154808682	16.1893891248	18.1237182771
O	24.0461862832	13.3819879066	17.7312296119
O	24.1111827691	15.0918563710	15.4105004627
O	25.8951770039	16.7976552526	16.7135215127
O	25.9756248163	14.9359748424	18.9044235016
O	22.0940560776	16.1067729114	15.6906574985
O	21.2262235966	15.3922897545	19.4490334707
O	21.8542413041	13.8504787349	17.3376228802
O	24.8790053380	16.1006128236	20.5252182726
O	25.5864001400	18.0492934832	18.5846182704
O	22.3228702482	17.0529419360	20.5435435419
C	22.8254720836	13.0598928841	17.6166894374
C	22.4637755644	11.6246366393	17.8117630244
C	21.1161450829	11.2311514050	17.7827151095
C	23.4693386992	10.6729385480	18.0353617816
C	23.1271713405	9.3345993242	18.2232167331
C	21.7799666587	8.9354370509	18.1940285325
C	20.7782141793	9.8977000847	17.9806168539
H	24.5060321963	11.0008503312	18.0607980365
H	20.3552357326	11.9885427513	17.6088617067
C	26.3524872388	14.3629716184	21.1578330185
C	27.1028089973	13.2472027021	20.7582950229
C	26.2030605074	14.6585230261	22.5220378776
C	27.7152429972	12.4436512266	21.7157655208
C	27.5756852171	12.7396037591	23.0819703254
C	26.8036951715	13.8449820197	23.4777816845
C	28.1977803172	11.9025026322	24.1518416099
H	25.6131181564	15.5254543994	22.8107415255
C	25.6888886338	15.1970798455	20.1166670897
C	21.5011680106	16.0741597373	20.4860908282
C	20.7876254910	15.6927389140	21.7437350455
C	21.1439608300	16.2793210495	22.9668483974
C	20.4799872167	15.9115641217	24.1367397571
C	19.4449991182	14.9619283660	24.0979402806
C	19.0793715201	14.3903592754	22.8670110832
C	19.7508744107	14.7441295956	21.7008466745
H	21.9394055107	17.0198837182	22.9869150932
H	19.4851714189	14.3021767126	20.7431396269
C	18.6783579329	14.5411559047	25.3127864832
O	21.1468574472	17.6716795356	17.7303026259
O	22.9280490142	18.8915214134	18.4271878234
H	27.1818202303	13.0189914738	19.6982981407
C	23.0561459442	15.6449290052	14.9749614372
C	22.9135925345	15.7604661476	13.4963435381
C	23.9085421893	15.1950760999	12.6832683108

C	24.9671245710	15.1916372883	11.2965925271	C	23.7894352207	15.2612018207	11.2983835317
C	23.8348134920	15.7995389941	10.7246695431	C	22.6732842415	15.8846737939	10.7165009224
C	22.8604724224	16.3758540253	11.5584405207	C	21.6802805076	16.4479631319	11.5366487102
C	23.0074333610	16.3450432866	12.9439544476	C	21.8004331023	16.3991531984	12.9234134344
H	22.2677708570	16.8017597441	13.6029374351	H	21.0507654667	16.8494917784	13.5754076783
H	25.9641786479	14.6568401210	13.1482169816	H	24.7550666901	14.7020390507	13.1564371553
C	22.9269537985	18.7005160995	17.9469552739	C	21.7468336981	18.7705648521	17.9402118204
C	22.1881351418	19.9789231416	17.6532066070	C	20.9951871689	20.0361199816	17.6372895506
C	20.9157268033	20.0834204660	17.0227261963	C	19.7174959110	20.1254050638	17.0121980308
C	20.3661090361	21.3621407845	16.8506813903	C	19.1662765399	21.4018132079	16.8232498899
C	21.0214547095	22.5280004200	17.2742990910	C	19.8236019672	22.5700082679	17.2337670130
C	22.2631740032	22.4152949001	17.9153726410	C	21.0668796719	22.4713256192	17.8706060623
C	22.8264641949	21.1578016324	18.0890645567	C	21.6360954431	21.2207512803	18.0552695425
S	19.8949735196	18.7304300116	16.3132014054	S	18.6967978583	18.7630928509	16.3021891290
C	27.2850597909	17.7323989400	17.4445399506	C	26.1029571214	17.8231468835	17.4317861750
C	28.2235299242	18.7656456759	16.9228368137	C	27.0475051731	18.8569485312	16.9105073124
C	28.4805813062	19.9225228575	17.6748390610	C	27.3079969286	20.0203607007	17.6539870766
C	29.3475362659	20.8872205256	17.1776029432	C	28.1784717851	20.9855662712	17.1554466445
C	29.9659189043	20.7061964241	15.9299029806	C	28.8105212018	20.8018259066	15.9131123511
C	29.7034369181	19.5452780928	15.1820121849	C	28.5415096764	19.6373005578	15.1720680657
C	28.8329987800	18.5773107567	15.6739575866	C	27.6672088874	18.6700272838	15.6653993248
H	28.6054684790	17.6755854677	15.1104891240	H	27.4473994396	17.7679468978	15.0990940742
H	27.9893512355	20.0428948925	18.6379033090	H	26.8169786054	20.1500846187	18.6162013479
O	21.1029299963	15.4736608428	17.1238695134	O	19.9153164051	15.5553735918	17.1982077044
O	27.5476007018	14.0622300616	16.4111160953	O	26.3558120734	14.1500825935	16.4030773164
O	25.4564992051	18.6508903076	20.6915176848	O	24.3234675241	18.7317396743	20.6773619879
H	24.6980530140	18.7475151646	21.2959784259	H	23.5788270917	18.8335636347	21.2988927786
H	28.2952344966	14.0005022854	17.0276145153	H	27.1024119456	14.0979904634	17.0201061352
H	20.5686046779	16.3182388714	17.2236952270	H	19.3707423850	16.4071380815	17.2561309059
H	27.9145670903	13.9577824297	24.5518459979	H	26.6924524160	14.0453733544	24.5410429316
H	29.4947597580	11.4914945718	21.3910382641	H	28.2640609843	11.5604716842	21.3897190446
O	28.9601693445	11.7320397560	25.2830672379	O	29.3244787408	11.1973668838	23.7997675752
O	30.5549962773	11.1186760477	23.8165914901	H	29.6035663879	11.4579373436	22.9027220802
H	30.8301811363	11.3738240863	22.9169068875	H	28.3870080591	21.8974575182	17.7109827307
H	29.5632052094	21.7967346919	17.7319465191	H	28.9805503598	19.4865842940	14.1855287136
H	30.1405934659	19.3993238288	14.1945816013	C	29.7303531997	21.8846003319	15.4385526933
C	30.8549678947	21.8021184270	15.4440263740	O	29.7096279660	23.0226432076	15.8661040288
O	30.8223174161	22.9416348005	15.8668739269	O	30.6431897624	21.5446095259	14.4654699325
O	31.7588875185	21.4702529343	14.4636393416	H	30.6026468151	20.5848233247	14.3003280986
H	31.7490967552	20.5070913005	14.3223195953	C	22.4798067961	15.9317507562	9.2388508115
C	23.6124084950	15.8424972660	9.2487020688	H	20.8238358162	16.9226656936	11.0631337675
H	21.9932545997	16.8388168748	11.0914931531	H	24.5463478709	14.7829894437	10.6770165314
H	25.7167225357	14.7027796051	10.6726415687	O	21.3868967353	15.9488364356	8.7039741319
O	22.5153394368	15.8637286009	8.7181716270	O	23.6248176290	15.9448427411	8.4724328549
O	24.7476574046	15.8607558349	8.4709472223	H	24.4000843805	16.0382111327	9.0561925098
H	25.5308234006	15.9400686964	9.0455054925	H	19.7416449247	9.5694905245	17.9775432997
H	20.9437034213	9.4841671154	17.9806334526	H	23.9208501194	8.6162813154	18.4292734536
H	25.1203328101	8.5302992792	18.4540957975	C	21.3305219419	7.5263195619	18.4068557092
C	22.5249398290	7.4420576218	18.4159799024	O	20.2008832039	7.2297437210	18.7462535707
O	21.3922249865	7.1466618870	18.7505869605	O	22.2528842718	6.5310010385	18.1976100753
O	23.4445364106	6.4427400528	18.2022380135	H	23.0753007659	6.9153299823	17.8419574915
H	24.2708889489	6.8294920791	17.8572467893	H	20.7529888540	16.4019270979	25.0709500235
H	21.9168506690	16.3132319693	25.0709540373	H	18.2650536116	13.6690681518	22.8523913301
H	19.4276032860	13.5736527822	22.8602575873	O	19.2959009381	14.7022870916	26.5275878364
O	20.4688209580	14.6119879343	26.5291049360	H	20.2217209062	14.9767193311	26.3939773787
H	21.3984549728	14.8662909226	26.3829491256	O	17.5576487666	14.0733978432	25.2730963575
O	18.7029135273	14.0011899680	25.2820464317	C	19.2639478225	23.9428616235	17.0427111820
C	20.4446314109	23.8970959671	17.0621886746	H	18.1814080887	21.4317914680	16.3578353888
H	19.3795796008	21.3941585090	16.3908041267	H	21.5655087511	23.3785329807	18.2040725440
H	22.7751167301	23.3117100485	18.2568472694	O	18.3528361677	24.1104905637	16.0245125481
O	19.5449040852	24.0297678981	16.0263132858	H	18.2590116518	23.2706764756	15.5363039019
H	19.4860995850	23.1828927463	15.5465387519	O	19.5922047793	24.8934729251	17.7272379532
O	20.7285404677	24.8711657925	17.7343492445	O	18.3611547754	17.8110439120	17.4014776371
O	19.5423222079	17.7980384485	17.4202112685	O	19.5271697740	18.1898058489	15.2324745292
O	20.7108374301	18.1194049597	15.2494190949	O	17.4810864857	19.4460983123	15.7893959044
O	18.6875285987	19.4336400985	15.7908943631	H	22.6056329185	21.1236954626	18.5368201483
H	23.7921835814	21.0469894074	18.5767111789	Ru	8.5357477772	23.4849204244	14.4920743920
Ru	9.6463188641	23.2916307770	14.3809285770	Cl	7.9316504813	22.8257960914	16.6024350462
Cl	9.4814305915	22.7652466509	16.6902734235	C	12.1982438925	23.8771878778	16.9440108528
C	13.2739390484	23.9334207205	16.9626584182	C	8.4269407397	19.5638642292	16.3485624184
C	9.8242242114	19.4479916530	16.3853605231	H	14.5085970123	16.7457164248	16.2410382163

H	15.9833959174	16.8200200914	16.2911483188	H	13.8558504879	14.6379051738	16.0730347310
H	15.3784301716	14.6998902791	16.1316389867	H	15.4669388227	14.0577042609	15.5731563393
H	17.0157514817	14.1864572855	15.6488100108	C	14.4452335616	14.2574516255	15.2302870191
C	15.9887665807	14.3366409257	15.2964835322	H	12.6259430066	18.3350968790	15.9124623489
H	14.0846414651	18.3847034819	15.9446859993	C	14.4094332904	17.3495478790	15.3323496317
C	15.8878171763	17.4226451457	15.3810961328	H	16.6768099700	15.9173676606	15.3860448253
H	18.1826230716	16.0609196271	15.4582934349	H	15.0442088214	18.2402344528	15.4451720373
H	16.5178109431	18.3168001137	15.5023656228	H	13.3358024882	26.2552017939	16.3853449627
H	14.2866348874	26.3663059024	16.4180022037	H	14.0038323579	13.2920585393	14.9392070728
H	15.5928373463	13.3504927954	15.0116367598	C	12.9568138661	17.7250560125	15.0594405525
C	14.4334585463	17.7814356646	15.0941165646	H	11.1066596667	19.8730170235	15.5324509016
H	12.4910896837	19.8317617214	15.5547001465	H	6.3682451072	18.2139127504	15.3555074249
H	7.9210737895	17.8794945813	15.4003340248	C	12.4455982141	24.4719403437	15.5797243775
C	13.4760321759	24.5507932376	15.6012060977	C	16.5067792108	16.4198730061	14.4289030757
C	17.9993979251	16.5146835258	14.4794470058	C	8.0142627809	19.5137408761	14.8978430842
C	9.4472310082	19.3141598073	14.9315348839	H	12.3065070638	16.8275655418	15.0468853384
H	13.7935547847	16.8760659769	15.0720199305	C	13.0499023848	25.7337115348	15.4728114778
C	14.0395310377	25.8321700019	15.5016389681	H	12.9665689723	21.3160115673	15.1497706709
H	14.2342857346	21.4301988178	15.2547243721	H	16.9530180075	17.4220720833	14.4790629787
H	18.4338208638	17.5209700815	14.4818088006	C	6.8997268213	18.7316893943	14.5580879475
C	8.4162511329	18.4241875261	14.5973935671	N	15.0209570099	16.5525703595	14.1875227282
N	16.5129608567	16.6297710296	14.2409059826	C	14.3902784872	15.1701867304	14.0135188626
C	15.9057409408	15.2382607317	14.0727280319	C	11.1734444828	20.2151248879	14.4864818412
C	12.5624940475	20.1904327755	14.5154726799	C	12.2071045843	21.3368215920	14.3588673682
C	13.5188219683	21.3863457896	14.4251169274	N	11.3853552820	22.5527025344	14.4673781814
N	12.6024938433	22.5452434878	14.4708558736	C	10.0442186196	22.2992789280	14.3122548989
C	11.3049775158	22.1788788772	14.2820927759	N	9.9134827575	20.9248700772	14.1489140018
N	11.2603256763	20.8177909609	14.1587679404	N	12.8417648725	18.5105834909	13.8276938802
N	14.3171507791	18.5669235548	13.8591340755	C	12.0475438267	23.8240992771	14.3939245327
C	13.1505613437	23.8723965743	14.4073408143	H	16.9412738898	15.8371014383	13.6096819286
H	18.4350851474	15.9029242334	13.6826222635	C	8.7029745483	20.1918236388	13.8665173620
C	10.0896579129	20.0186509644	13.8881347381	H	13.3521441257	15.3322073040	13.7072448343
H	14.8635393350	15.3757078374	13.7682090397	C	11.4804474532	19.0187557211	13.5785091964
C	12.9448674377	19.0290271064	13.5940828999	C	13.2681168882	26.3499351965	14.2346721403
C	14.3024741265	26.4344956239	14.2660517195	H	14.9199637865	14.7243316191	13.1621999608
H	16.4443392263	14.7991709905	13.2235351807	H	10.7076953644	18.2368801194	13.6901528809
H	12.1990961357	18.2164573472	13.6768893804	C	6.4555484031	18.5964643473	13.2395518221
C	8.0206788767	18.2013808446	13.2753082112	C	14.8111429740	17.3606570263	12.9135769895
C	16.3045953788	17.4368937730	12.9683651688	C	13.8527518330	27.7389991825	14.1528941831
C	14.8882879564	27.8236896461	14.1882379766	H	15.4269068121	18.2609238105	13.0287399683
H	16.9015695663	18.3480182015	13.0979841247	C	13.3522437440	17.7470095592	12.6905332637
C	14.8446891088	17.8021947037	12.7293878674	H	12.7263800604	21.2971264134	13.3881178038
H	14.0880042655	21.3786069389	13.4831614076	C	5.2630574996	17.7319698968	12.9067910824
C	6.9645879567	17.1698217702	12.9565796819	C	12.3116014382	24.3852463251	13.1262663836
C	13.4590343853	24.4250765415	13.1426222143	C	8.2904743870	20.0567560853	12.5166815573
C	9.6885537370	19.8439619078	12.5394340710	H	12.7326903262	16.8599523377	12.4530845485
H	14.2366064843	16.9058376465	12.4960439047	C	12.9136671955	25.6481920833	13.0748667698
C	14.0194743353	25.7066907402	13.1025118287	Cl	7.7160355229	23.6874031668	12.3586250040
Cl	9.6120534794	23.9217966897	12.0793032542	C	7.1634996157	19.2716825355	12.2387838459
C	8.6521662379	18.9394188110	12.2677015130	H	11.4438220317	19.3608470178	12.5356598620
H	12.9130964147	19.3888701470	12.5566092291	H	15.2014457662	16.7614405824	12.0811828779
H	16.7173547433	16.8501859422	12.1382291527	H	13.3281856262	18.3861896458	11.7947237139
H	14.8168805477	18.4358857371	11.8299007856	C	11.9470637491	23.6706531184	11.8486200053
C	13.2224174908	23.6686931256	11.8609658121	C	9.0263736446	20.7021380227	11.3701209558
C	10.3459123265	20.5711443796	11.3957997401	H	13.0987426322	26.1005555910	12.1019211625
H	14.2468100480	26.1462304349	12.1327876166	H	6.8406925761	19.1743503360	11.2035963162
H	8.3530416249	18.7923286566	11.2308171043	C	9.2796511923	25.1092025959	14.7852341476
H	5.5809408937	19.0269599392	11.6892984086	H	8.5396406583	25.8981545332	15.0113139857
H	4.8082123315	21.9692715400	17.7935132821	H	10.3270718565	25.4152557851	14.7679970565
C	5.0048005632	21.9034841424	16.7267166245	H	11.6754897137	22.9169568560	16.8853167471
C	6.0623504700	22.6067312288	16.1634857451	H	11.5769002865	24.5484667288	17.5540782226
H	3.9384829668	19.4100655982	12.2502579646	H	13.1460308285	23.7317565667	17.4820596859
C	4.1737655317	21.1402810245	15.8975366925	O	27.7641229523	11.8223309120	25.2838733390
H	6.7043432493	23.2165836142	16.7938535579	H	9.2263174360	20.2847554710	16.5399889914
C	4.7105400090	19.6701687015	11.5174217505	H	8.7423373512	18.5694978954	16.6966302664
H	3.3021010735	20.6350919703	16.3094166112	H	7.5758798681	19.8758041165	16.9701005051
C	6.3339704984	22.5537963108	14.7803911452	H	5.0582947168	17.7255263759	11.8289226327
C	4.4623551762	21.0003365786	14.5394670517	H	4.3568594645	18.0857221372	13.4196300325
C	5.5713414538	21.6532182241	13.9730038385	H	5.4258472418	16.6916790559	13.2246088123
H	4.3047674409	19.4406077964	10.5210901471	H	8.5618460669	20.4221414731	10.4165893619
H	3.8257437320	20.3787363254	13.9210079633	H	10.0820790965	20.4021493097	11.3319865676

O	6.0061456861	21.4728196439	12.6873431437	H	8.9968447998	21.7975593956	11.4474996487
C	5.1247163197	21.1438775519	11.5613542065	H	12.2009236349	24.2864621690	10.9770824712
C	3.9647706548	22.1244902662	11.4333105525	H	10.8733158934	23.4394754476	11.8031791922
H	3.2411028064	22.0247371465	12.2505373498	H	12.4943923752	22.7215581428	11.7469119130
H	3.4335431762	21.9356430508	10.4904685499	H	13.9810636736	28.0597205805	13.1116479828
H	4.3327038851	23.1585509433	11.4153082165	H	14.8313295184	27.7947781673	14.6504930739
C	7.1965180914	23.5354390013	14.1139837922	H	13.1959676911	28.4689579254	14.6488086487
H	7.2464086965	23.4446108630	13.0291490374				
H	5.8163392642	21.3110137486	10.7251516966				
C	10.3461910353	24.9209438901	14.8178226216				
C	7.6700716800	24.7143773873	14.6617352799				
H	10.5233864621	25.6951350186	14.0608644568				
H	10.5386549403	25.1828253409	15.8662651144				
H	7.9415828083	25.5287963179	13.9945730830				
H	7.5376815608	24.9530801249	15.7153504958				
H	12.7547756020	22.9710091710	16.9105412893				
H	12.6765944672	24.5896322897	17.6111353647				
H	14.2451080136	23.7873105564	17.4592585623				
H	10.5724548830	20.2247564135	16.5633021101				
H	10.1838219676	18.4882803157	16.7829661632				
H	8.9413337299	19.7394265137	16.9725667911				
H	13.4937852181	24.2871694809	10.9963956067				
H	12.1675678436	23.3779929798	11.7527350564				
H	13.8368100830	22.7572135228	11.8137806203				
H	15.0305410679	28.1408562892	13.1479677680				
H	15.8626539482	27.8750118698	14.6946363465				
H	14.2314543734	28.5572763447	14.6770292574				
H	9.9181555472	20.2440546740	10.4402254505				
H	11.4291601881	20.3933185998	11.3586477603				
H	10.2023167559	21.6609227292	11.4751281867				
H	6.7988157419	17.0796980924	11.8759426962				
H	6.0036882185	17.4206218585	13.4281074781				
H	7.2572449701	16.1795361737	13.3327167980				

Table S6. Coordinates data set, absolute energies (a.u.) for DFT optimized cluster (Cr)Mil-101 and (Cr)Mil-101-SO_3^-.

Cluster Mil-101				Cluster Mil-101-SO_3^-			
112				115			
E = -1002.2448612961				E = -1060.0288698801			
Cr	13.294580566200	11.840878504300	12.233590096600	Cr	18.323338812000	16.878326438700	17.232930761300
Cr	10.018140883000	12.602137834100	12.579580672900	Cr	15.033753755100	17.563226109100	17.544046393200
Cr	12.331837884600	14.189934393000	14.465127952200	Cr	17.299960111900	19.223559243500	19.416295780200
O	12.033161594100	12.893742129000	13.129382907100	O	17.031112951400	17.895332026600	18.117330255000
O	12.488413965800	10.160136294600	12.735243530400	O	17.503629616700	15.161741738000	17.738326436300
O	12.440680202600	11.861618107800	10.480679812200	O	17.491823235600	16.880877935300	15.469873687400
O	14.218974514500	13.526216258600	11.714521599300	O	19.287301555600	18.574152354500	16.715138989400
O	14.376895703300	11.645410791700	13.903110477700	O	19.441678119000	16.723201197000	18.900333163100
O	10.470314069100	12.975804003200	10.696490252700	O	15.487192095200	17.959231301700	15.654494534600
O	9.539372644600	12.189033692500	14.453155090300	O	14.623862957500	17.124319567300	19.457085115600
O	10.302292864300	10.641838535300	12.337812407800	O	15.317309269000	15.616229137400	17.333579549200
O	13.284170149300	12.803777738600	15.539938106200	O	18.276731782500	17.819254944600	20.530059262800
O	13.989220349000	14.772130832100	13.605514738200	O	18.982947260800	19.836876851000	18.586769953000
O	10.762543769600	13.756333677200	15.556872567400	O	15.709553245900	18.815545626100	20.534191029300
C	11.244170836500	9.839014716800	12.594948987500	C	16.267721739800	14.831974426200	17.612293057800
C	10.903150188600	8.407509552800	12.766016802600	C	15.920265422500	13.390809370100	17.812803599800
C	9.560414117800	8.009354585600	12.653848148200	C	14.571431186000	12.995449806900	17.771762741800
C	11.903550800600	7.472144705400	13.066253916600	C	16.920615240900	12.438487164300	18.055462851400
C	11.559903006600	6.136802347200	13.256903130800	C	16.575244087500	11.101731222400	18.246298498800
C	10.218617544400	5.735532030100	13.153136379200	C	15.228770007900	10.698890388500	18.203207178800
C	9.221082367700	6.678320924200	12.854967004300	C	14.229449168500	11.661274723500	17.974195416200
H	12.933299564000	7.807189847000	13.158118227400	H	17.957786796000	12.761876124400	18.094575251300
H	8.807462297800	8.759057103100	12.419256666400	H	13.812649840800	13.753182282200	17.582063267800
C	14.755488987400	11.071894619600	16.162650268600	C	19.797606221100	16.125909336200	21.158373034300
C	15.508859196100	9.954072048400	15.775655491900	C	20.554063365800	15.012670128400	20.765043282700
C	14.604370713700	11.383282474600	17.524231311500	C	19.648804583200	16.421976955300	22.523468988900
C	16.122423788500	9.163008525300	16.742777113400	C	21.158821618800	14.205151179000	21.725087495800
C	15.980951198600	9.477079280900	18.104251030000	C	21.007481019500	14.494261999000	23.092004198100
C	15.206083445100	10.583133877000	18.489227963700	C	20.242301256800	15.606535629000	23.483384948000

C	16.609907957300	8.658917208300	19.184376370900	C	21.600074121300	13.632096573800	24.156382362000
H	14.012738100500	12.251846568500	17.803444792200	H	19.058553474800	17.289986094400	22.808464414400
C	14.088065648000	11.904461678300	15.124549293800	C	19.116906947400	16.959883099900	20.116809098700
C	9.878202505900	12.821163605200	15.498959862900	C	14.892695760100	17.818111399200	20.481753498100
C	9.174086494300	12.459087955800	16.754670977000	C	14.183360880500	17.450454651600	21.746784409600
C	9.498019447600	13.081802516000	17.968019395300	C	14.535751557700	18.037459661000	22.970913135600
C	8.828594200400	12.714069165100	19.132796953500	C	13.867607425200	17.670818345500	24.138884470300
C	7.828755672100	11.729077086100	19.087023059200	C	12.831858538900	16.720493379300	24.098185770800
C	7.490641226100	11.125455137400	17.865742710700	C	12.468498162100	16.151737301400	22.865349077600
C	8.165435522100	11.481059332100	16.706209689200	C	13.142432057100	16.506412946600	21.701190523600
H	10.267728530100	13.848559383200	17.985529850000	H	15.330458178200	18.778654247800	22.992381264600
H	7.928309676800	11.018075577500	15.751366297800	H	12.874963109400	16.073086804800	20.739631535900
C	7.068207971300	11.294274684100	20.293972930900	C	12.069553935300	16.291758065400	25.310038483100
O	9.531506700400	14.524891750600	12.810473115600	O	14.531855324200	19.453521911400	17.731965176900
O	11.401278308400	15.615471266700	13.506095284600	O	16.333964512100	20.615491070900	18.430538137900
H	15.592825733400	9.712159771900	14.719599829300	H	20.638605087500	14.784460609800	19.705815948900
C	11.407125618800	12.463927134200	10.009822429700	C	16.452485701300	17.476853782500	14.991906415400
C	11.301283085300	12.529949802300	8.529215664500	C	16.354896248300	17.574917670900	13.506784764400
C	12.317860155000	11.984982777800	7.730623479400	C	17.348997243400	17.011527481000	12.693649247100
C	12.198801959800	12.022990009800	6.343789175900	C	17.215062323700	17.057879950700	11.307674525900
C	11.063716043700	12.597466934500	5.748429821400	C	16.085564710000	17.659611318500	10.723756310700
C	10.041482529200	13.126072343000	6.553730720000	C	15.094365967000	18.222480528800	11.546333552600
C	10.161419840500	13.100109669500	7.938096322800	C	15.228483606500	18.190279553300	12.931358013200
H	9.380566950000	13.500709120900	8.580408426000	H	14.469963830100	18.623180657600	13.584852074100
H	13.179107220200	11.526591165400	8.210647550400	H	18.201721100800	16.528119329800	13.165476446100
C	10.204177829300	15.579529083100	13.036388222600	C	15.137095138000	20.538848619500	17.947313349900
C	9.558832752000	16.887853915100	12.755122738700	C	14.436876955700	21.838451745500	17.661968298900
C	8.279291548800	16.919483159600	12.179859773900	C	13.164735981300	21.958744881500	17.036904931600
C	7.663242042600	18.142738873500	11.929100515800	C	12.626724657800	23.240859995800	16.858260893900
C	8.316464337200	19.340986515500	12.260917359800	C	13.292359209000	24.402324009500	17.270783810700
C	9.589187596300	19.304458483700	12.853608220000	C	14.540509237700	24.278182172600	17.898779927800
C	10.214071450900	18.085348099800	13.089430652900	C	15.096113949000	23.015666304000	18.077601926800
H	11.203725282100	18.040387972800	13.537876226400	S	12.114657082700	20.618523051300	16.356833027200
H	7.782471627300	15.982409283300	11.941581359400	C	19.498587306500	19.595249026200	17.445520078400
C	14.471815519600	14.539977182700	12.445310609700	C	20.459752817200	20.615926691300	16.920294526800
C	15.433533514600	15.538465856100	11.908895709000	C	20.733005320800	21.770686777100	17.671182906900
C	15.774224645500	16.660776049700	12.681941521900	C	21.602667753500	22.735772954100	17.172473659700
C	16.664859930200	17.599743819900	12.177131454800	C	22.221118545800	22.560877113500	15.922375572200
C	17.230955619900	17.421958221500	10.904021644500	C	21.945458051600	21.399441326500	15.176257098100
C	16.884073650200	16.300972066800	10.132874313200	C	21.069848226700	20.432633808400	15.670434900800
C	15.987058750500	15.359922822800	10.632303492700	H	20.835194726900	19.536658504200	15.099470934500
H	15.698579847800	14.490011778400	10.047211984300	H	20.246215083000	21.891974151200	18.636682410100
H	15.330185908700	16.777496971200	13.668072405200	O	13.286082219200	17.188028291000	17.112440503400
O	8.256169219600	12.324266715900	12.105088719700	O	19.686635878600	15.951513038000	16.411714510200
O	14.687372597100	11.018015217800	11.406653555900	O	17.733437149200	20.452271301200	20.706307448900
O	12.742727089400	15.383963534600	15.777615361900	H	16.985443174200	20.547673369600	21.323903816800
H	12.015742991800	15.428890107500	16.427297033200	H	20.453247982900	15.895817055700	17.010502657900
H	15.443778590000	10.915682019700	12.014881607000	H	12.735803126200	18.002001655800	17.128495348700
H	7.691957325700	13.043409324000	12.434535652800	H	20.125986053300	15.809322730000	24.545939693100
H	15.094737415800	10.794149035100	19.550759872600	H	21.705285909800	13.320005075800	21.400519187000
H	16.675264663000	8.277943031900	16.428999419900	O	21.155405778200	13.535059245400	25.283317881000
O	16.173241646300	8.592119474400	20.315869485600	O	22.716604564000	12.908174607100	23.801830084900
O	17.740614940800	7.962919731900	18.835640180500	H	23.011130809500	13.186040939000	22.915267486500
H	18.022415446700	8.220033508500	17.938825086700	H	21.818430628000	23.643144231800	17.731995144600
H	16.938867363000	18.485633159700	12.746005636700	H	22.373008307100	21.252200657500	14.184011933300
H	17.277062266300	16.172612330700	9.124470229200	C	23.125617068400	23.653623305800	15.443510567900
C	18.159633465000	18.486606314000	10.422663809800	O	23.100609189400	24.795289557500	15.865609672500
O	18.134982603200	19.621856988200	10.853944831400	O	24.035246690900	23.318016018100	14.464348098400
O	19.064885956200	18.130808301400	9.452248521600	H	23.995416454600	22.355380574400	14.308945608300
H	19.022774085400	17.168979772700	9.300738179700	C	15.877128596900	17.690289853800	9.246699011200
C	10.868639948900	12.639260472600	4.269340980200	H	14.222371364100	18.676778571800	11.080640377800
H	9.162713131100	13.545277328500	6.068425251800	H	17.970244955800	16.574165476900	10.688715877900
H	12.973594368800	11.560289745400	5.732931569500	O	14.786607726700	17.735528099200	8.708991847700
O	9.773344190800	12.658415878500	3.742672682200	O	17.024113470900	17.657002968900	8.474030890500
O	12.014374246500	12.656169015200	3.506346760600	H	17.797239350800	17.747054424900	9.060644438200
H	12.789925839500	12.749207803300	4.089251581500	H	13.190451622900	11.338454738000	17.956907060000
H	8.188818446000	6.340168081700	12.795143921400	H	17.365059364900	10.384447122300	18.468986411100
H	12.337121562000	5.423894361500	13.530740567700	C	14.805305097600	9.281086406300	18.409987240000
C	9.774894213300	4.333460191800	13.396210999900	O	13.686059333200	8.943654898200	18.744641844000
O	8.650021703400	4.050984233300	13.754559338400	O	15.769201453100	8.315864762600	18.200720128600
O	10.707128946300	3.346520390600	13.202356367200	H	16.565772380800	8.733175122400	17.827207705800

H	11.512493268900	3.727299957400	12.807035153200
H	9.063718983800	13.225601808700	20.065774629800
H	6.698522628600	10.379775754600	17.855632145400
O	7.723926308400	11.404080404100	21.495801928400
H	8.652801311100	11.654583094300	21.339546354800
O	5.935722302200	10.857785960400	20.242367287200
C	7.698295250500	20.683292479800	12.046311047700
H	6.655889887800	18.154377706700	11.513481480100
H	10.064554469600	20.245953760800	13.120571022900
O	6.794690685200	20.786908336000	11.016699145000
H	6.781432653200	19.956271083200	10.506601684200
O	7.964871925800	21.650195786000	12.731580874400

H	14.137341668200	18.164413323300	25.072525024700
H	11.653048474200	15.432028073000	22.846798819000
O	12.682391794400	16.489279205400	26.527708936300
H	13.601005106300	16.781059300700	26.382182374900
O	10.963707145600	15.787307294400	25.277131831200
C	12.714075903800	25.769137854000	17.061727170400
H	11.639017239000	23.274199565000	16.398733530900
H	15.059412807600	25.175411309600	18.229765882300
O	11.819844031700	25.899621056100	16.023982772300
H	11.722712138200	25.040486890400	15.569673117200
O	12.995062547500	26.747260492400	17.731820202300
O	11.746352045900	19.753547048700	17.496013620400
O	12.935723353900	19.979303669100	15.315642213900
O	10.948609486300	21.324569909700	15.789096666400
H	16.067975208300	22.907669052000	18.551651778000