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Supporting Information

For

MOF Encapsulation of Ru Olefin Metathesis Catalysts to Block Catalyst Decomposition

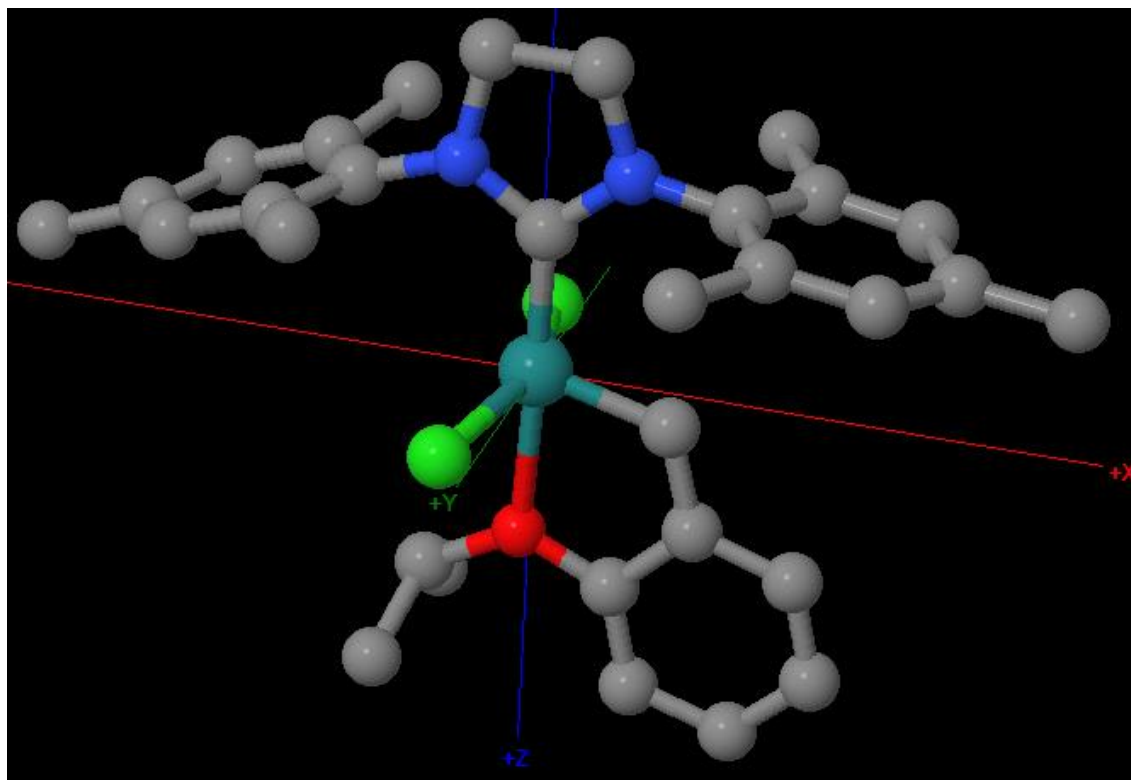
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Steric maps

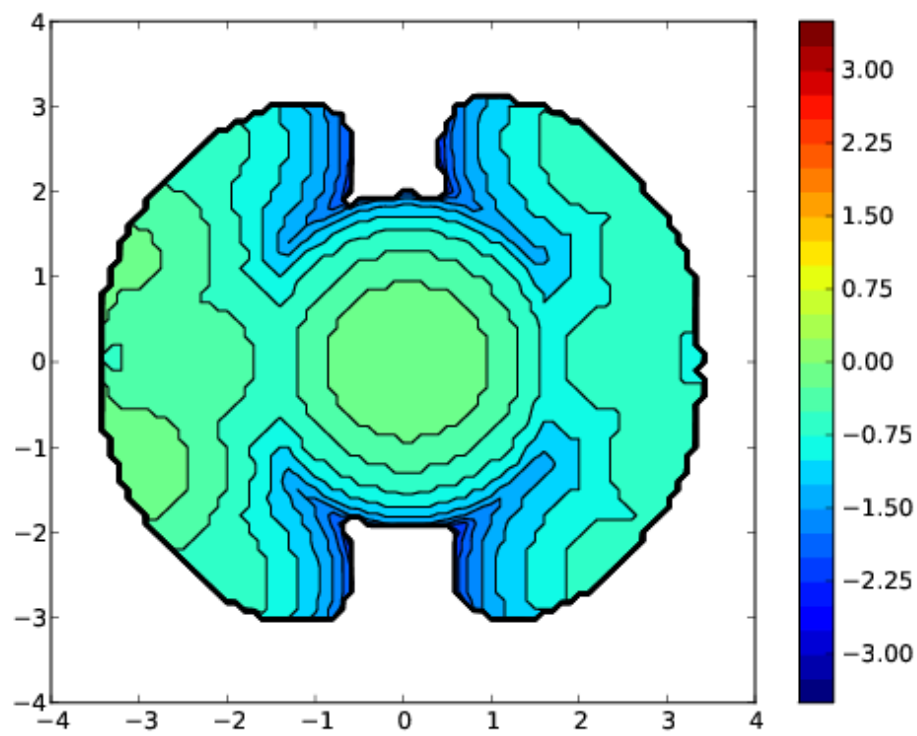
HOV



At 3.5 Å:

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

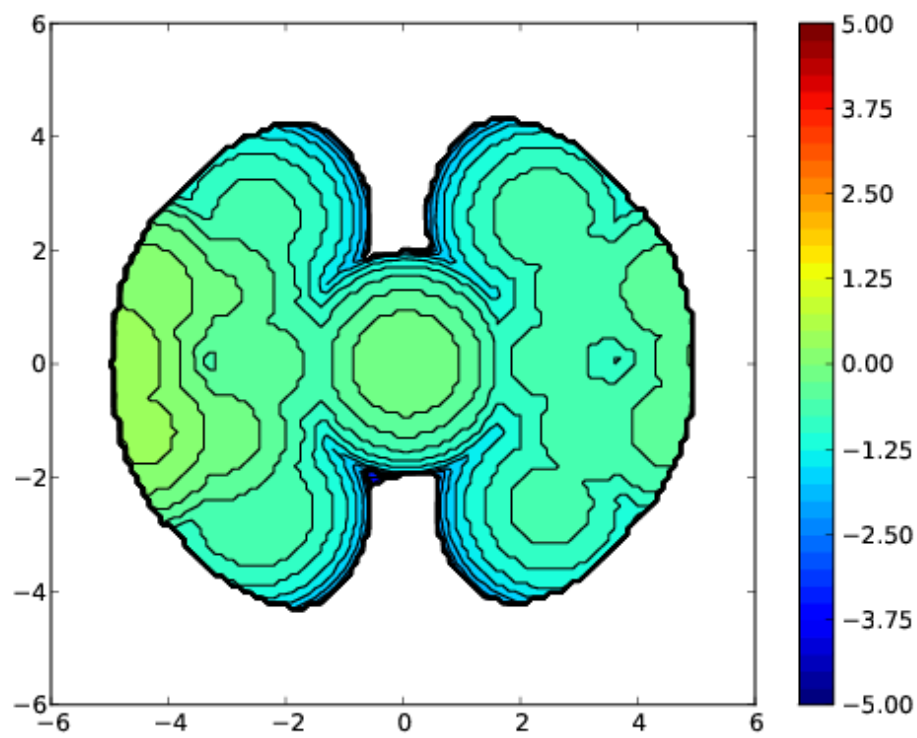
Quadrant	V f	V b	V t	%V f	%V b
SW	29.4	15.5	44.9	65.4	34.6
NW	29.7	15.2	44.9	66.2	33.8
NE	30.2	14.7	44.9	67.3	32.7
SE	30.8	14.0	44.9	68.7	31.3



At 5.0 Å:

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

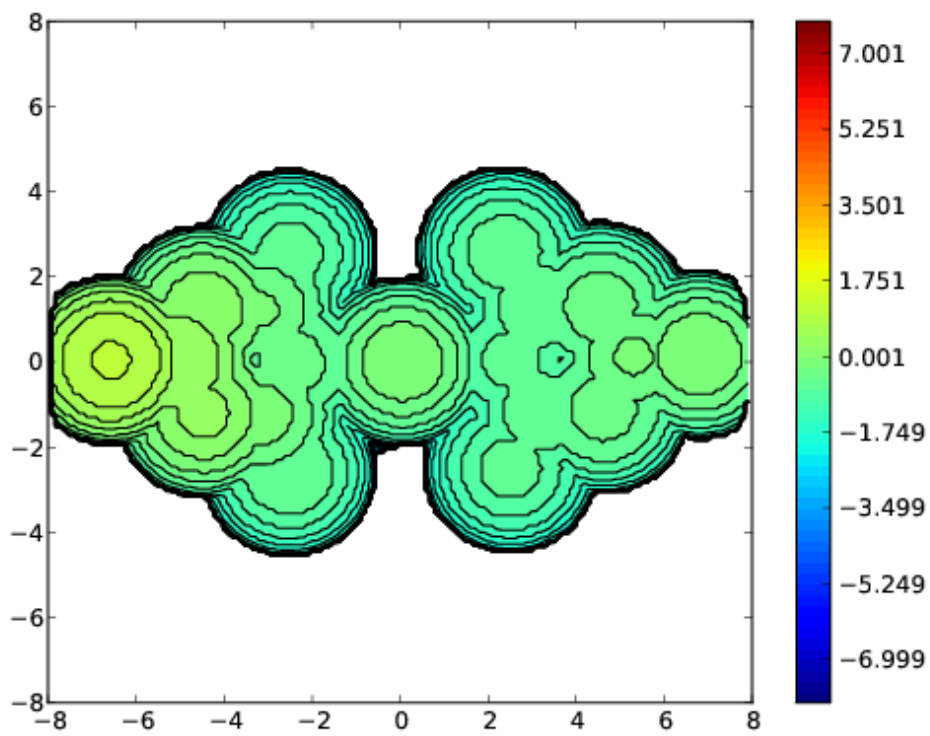
Quadrant	V f	V b	V t	%V f	%V b
SW	82.1	48.7	130.8	62.8	37.2
NW	83.6	47.2	130.8	63.9	36.1
NE	85.1	45.7	130.8	65.1	34.9
SE	87.4	43.5	130.8	66.8	33.2



At 8.0 Å:

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

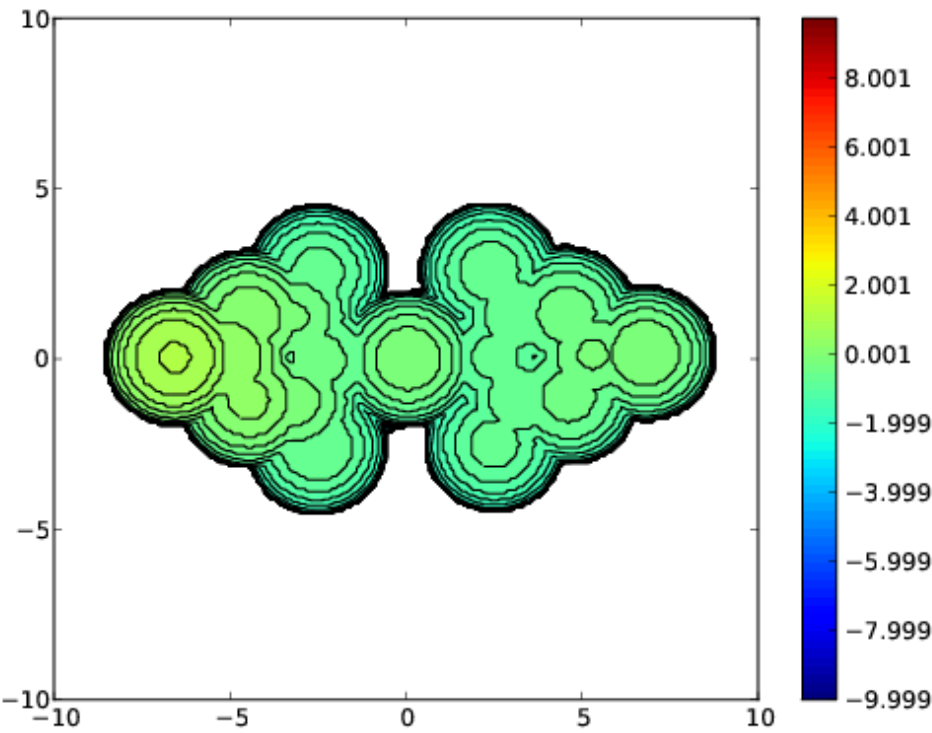
Quadrant	V f	V b	V t	%V f	%V b
SW	445.2	90.7	535.9	83.1	16.9
NW	446.4	89.5	535.9	83.3	16.7
NE	445.2	90.7	535.9	83.1	16.9
SE	451.3	84.7	535.9	84.2	15.8



At 10.0 Å:

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

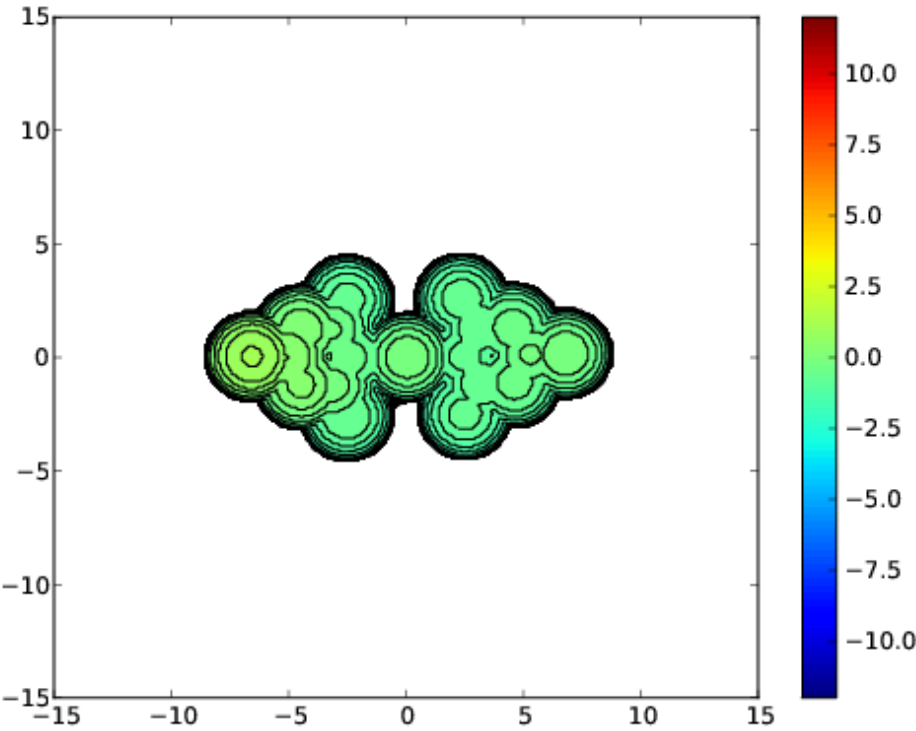
Quadrant	V f	V b	V t	%V f	%V b
SW	954.7	92.5	1047.2	91.2	8.8
NW	953.3	90.7	1044.0	91.3	8.7
NE	946.6	94.3	1040.9	90.9	9.1
SE	956.3	87.7	1044.0	91.6	8.4



At 12.0 Å:

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

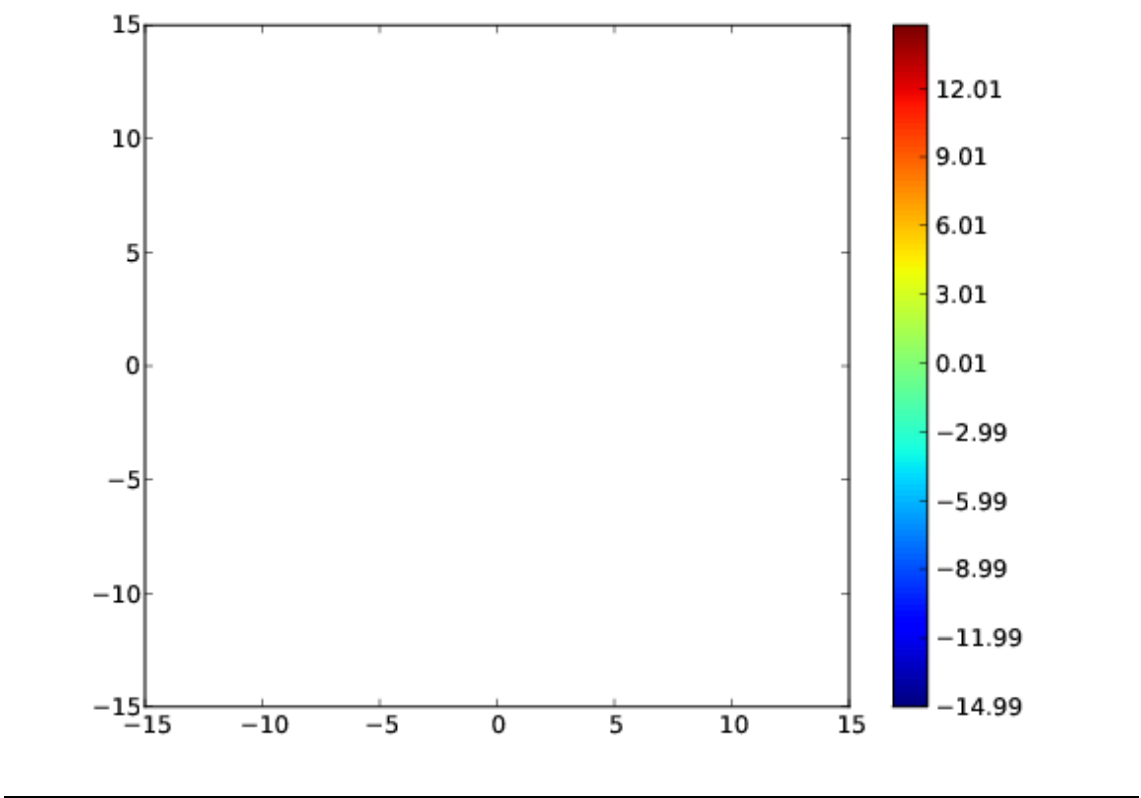
Quadrant	V f	V b	V t	%V f	%V b
SW	1717.1	92.0	1809.1	94.9	5.1
NW	1718.2	91.0	1809.1	95.0	5.0
NE	1714.4	94.7	1809.1	94.8	5.2
SE	1721.6	87.5	1809.1	95.2	4.8



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

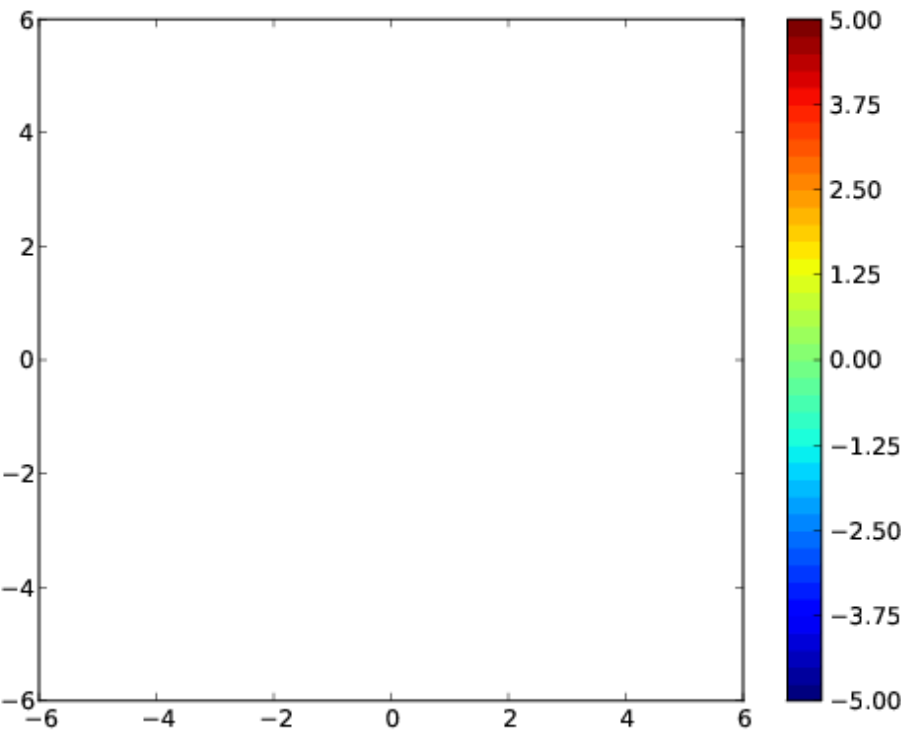


MOF without the Ru catalyst:

At 3.5 and 5.0 Å:

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

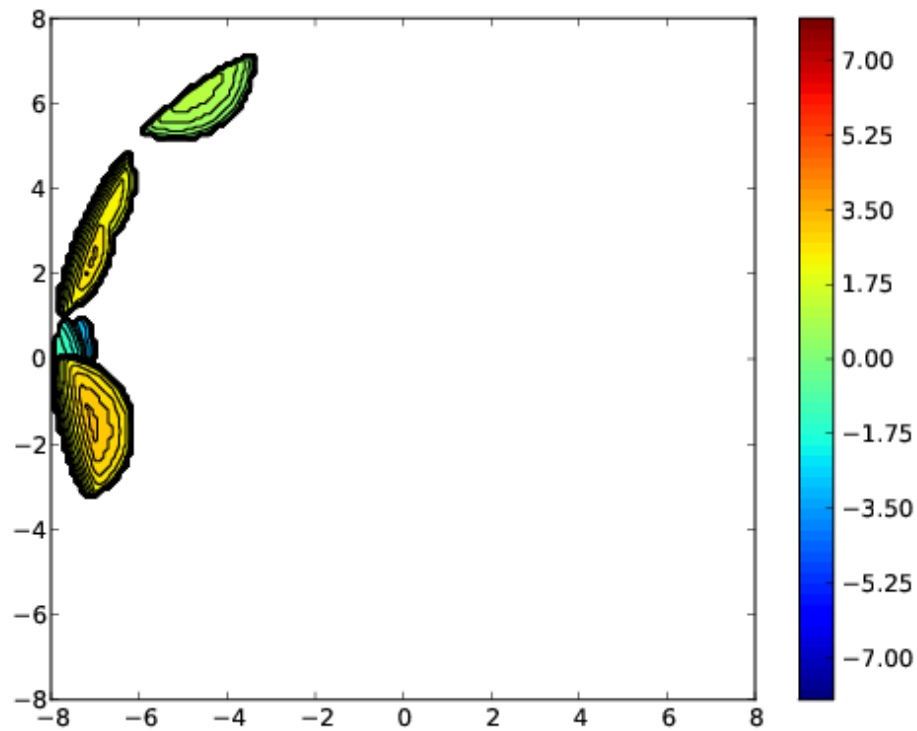
Quadrant	V f	V b	V t	%V f	%V b
SW	130.8	0.0	130.8	100.0	0.0
NW	130.8	0.0	130.8	100.0	0.0
NE	130.8	0.0	130.8	100.0	0.0
SE	130.8	0.0	130.8	100.0	0.0



At 8.0 Å:

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

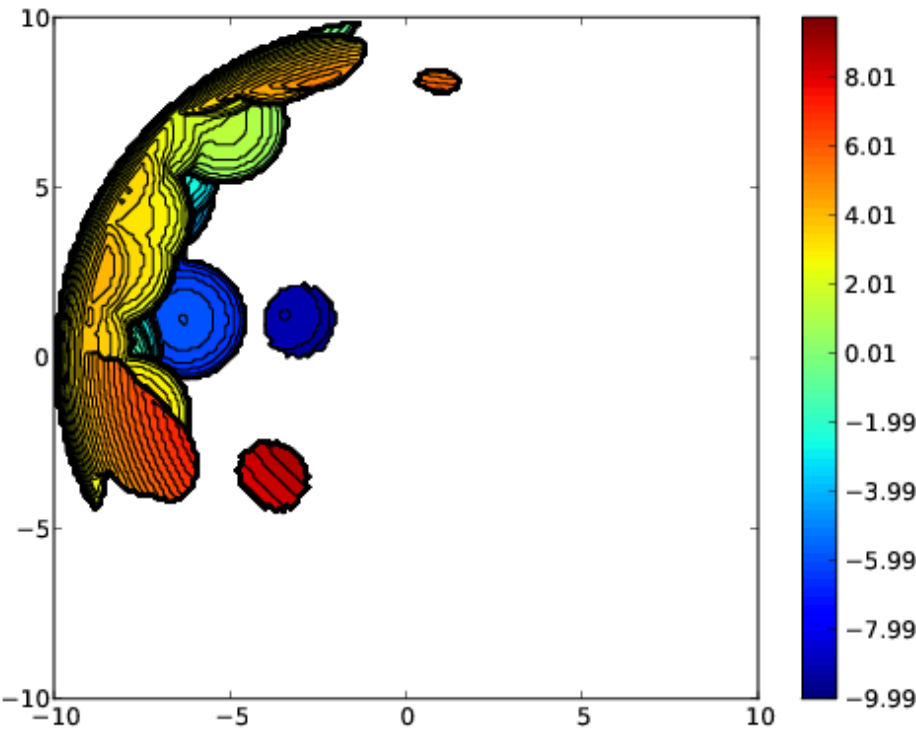
Quadrant	V f	V b	V t	%V f	%V b
SW	526.8	9.1	535.9	98.3	1.7
NW	525.2	10.7	535.9	98.0	2.0
NE	535.9	0.0	535.9	100.0	0.0
SE	535.9	0.0	535.9	100.0	0.0



At 10.0 Å:

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

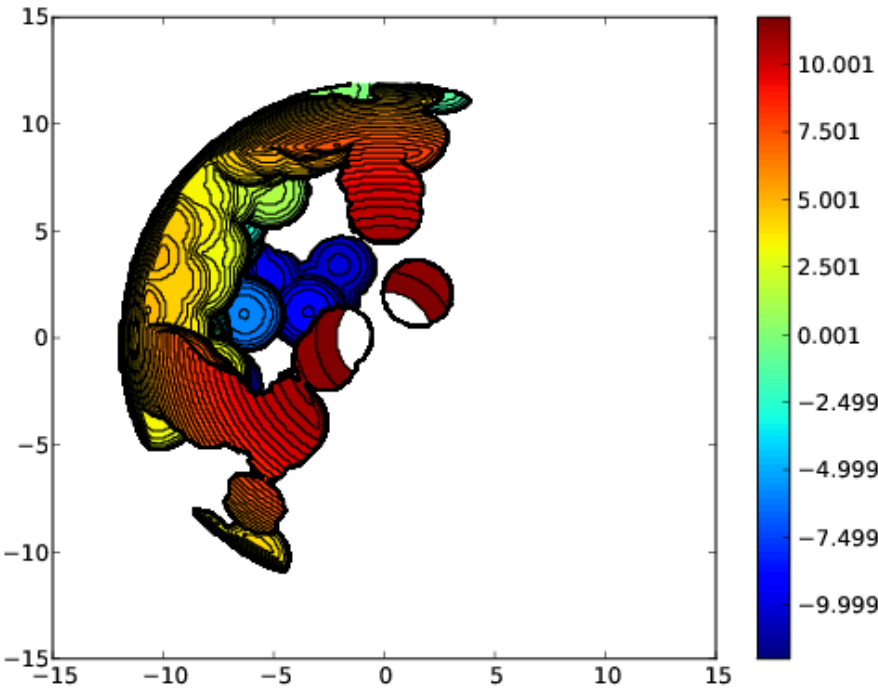
Quadrant	V f	V b	V t	%V f	%V b
SW	982.7	64.5	1047.2	93.8	6.2
NW	901.9	142.1	1044.0	86.4	13.6
NE	1040.8	0.1	1040.9	100.0	0.0
SE	1044.0	0.0	1044.0	100.0	0.0



At 12.0 Å:

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

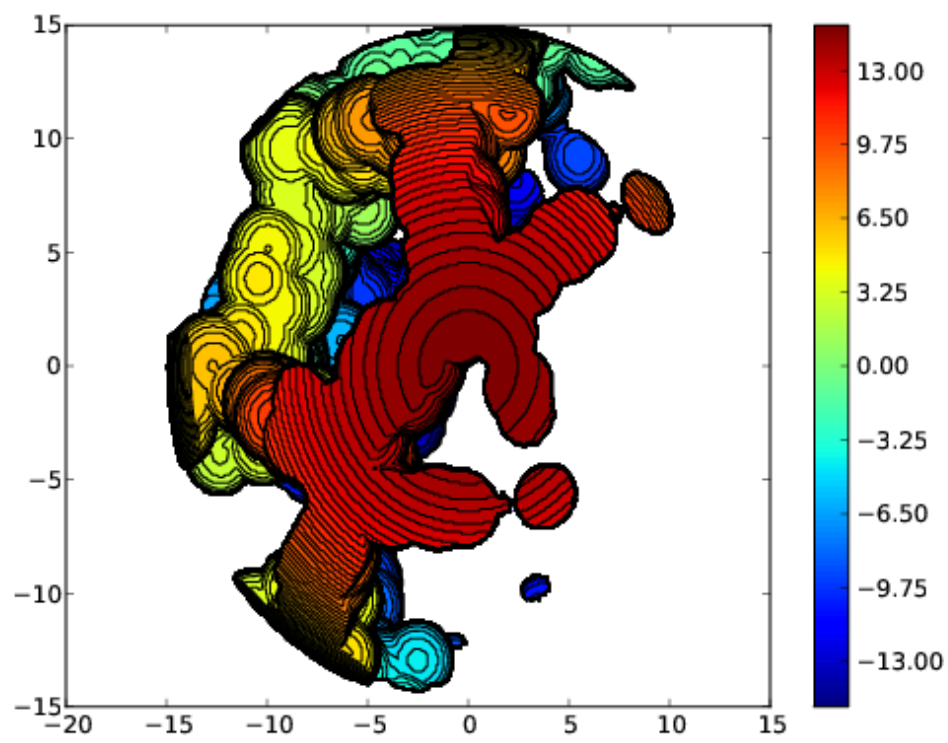
Quadrant	V f	V b	V t	%V f	%V b
SW	1578.4	230.8	1809.2	87.2	12.8
NW	1339.6	469.3	1808.9	74.1	25.9
NE	1774.2	34.4	1808.6	98.1	1.9
SE	1808.9	0.0	1808.9	100.0	0.0

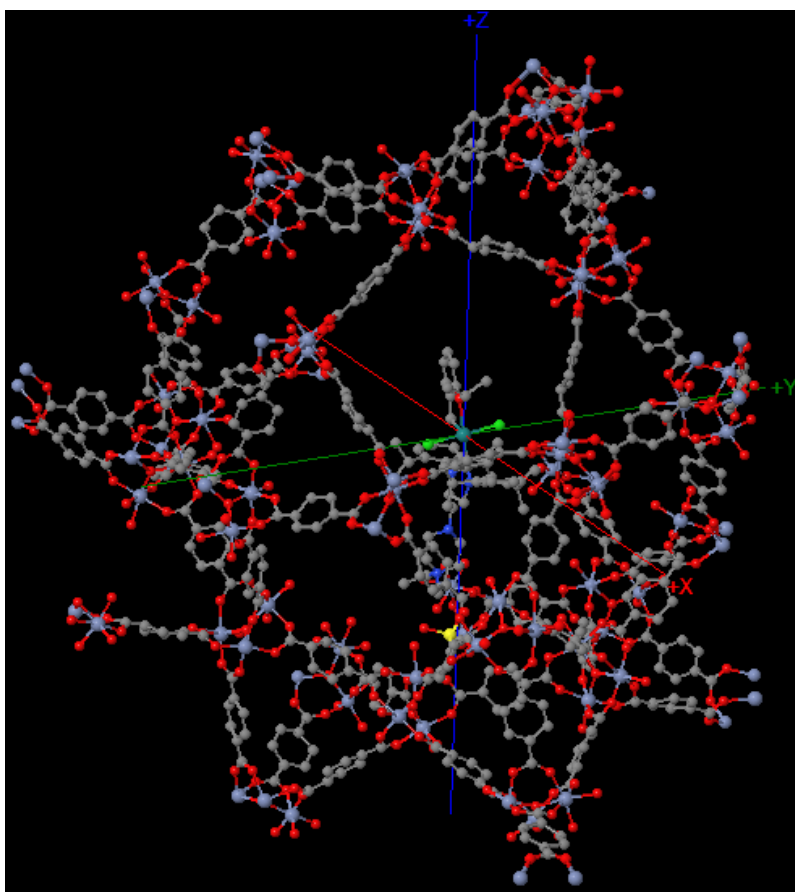


At 15.0 Å:

%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

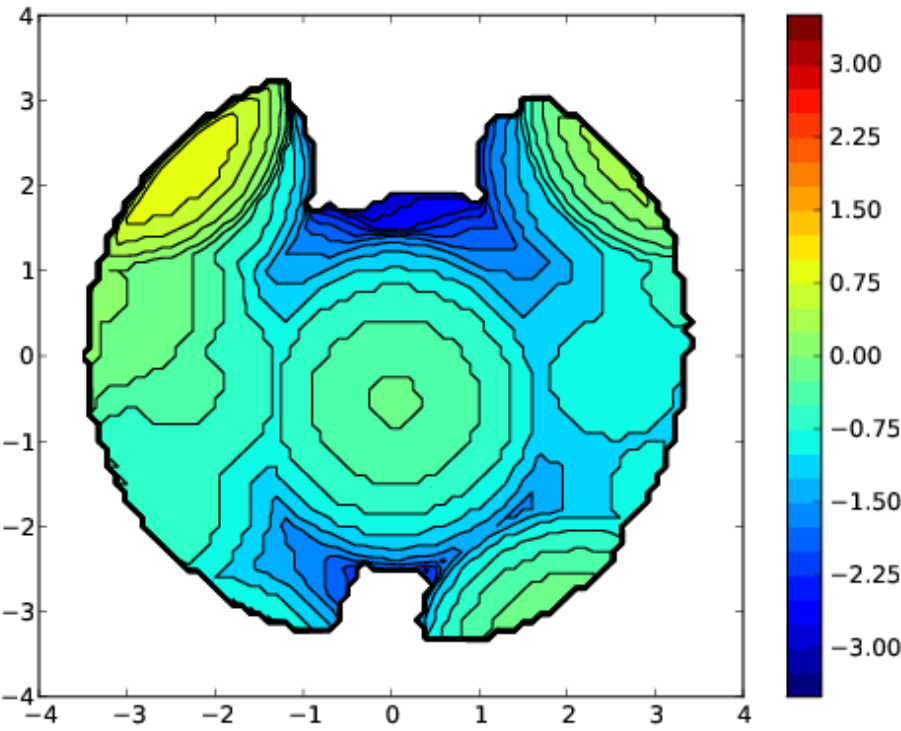




At 3.5 Å:

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

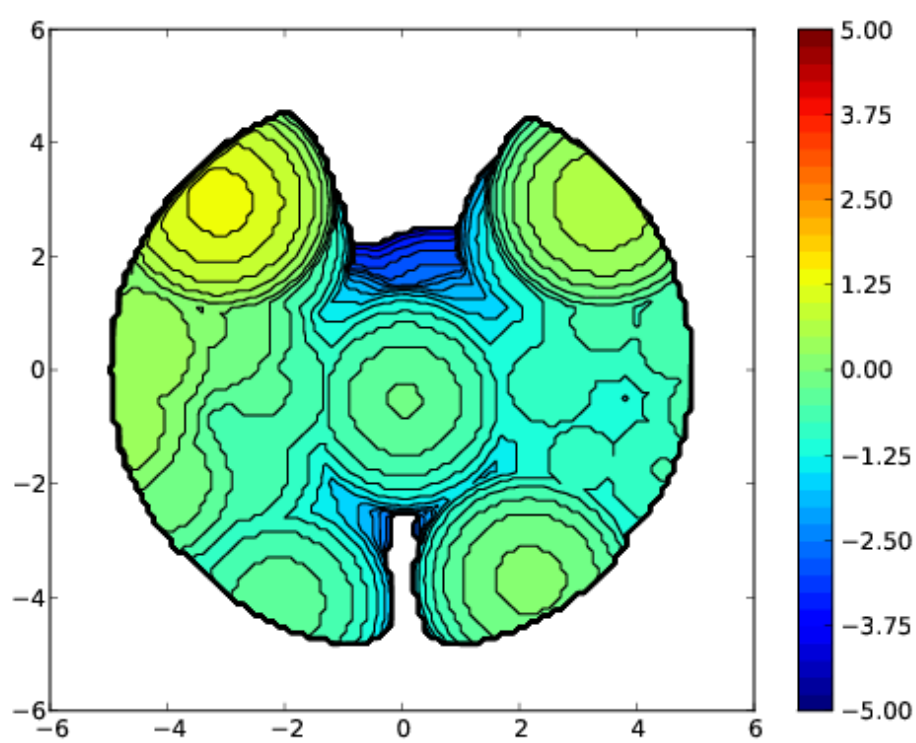
Quadrant	V f	V b	V t	%V f	%V b
SW	29.3	15.5	44.9	65.4	34.6
NW	28.3	16.6	44.9	63.1	36.9
NE	33.0	11.9	44.9	73.5	26.5
SE	29.8	15.1	44.9	66.4	33.6



At 5.0 Å:

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

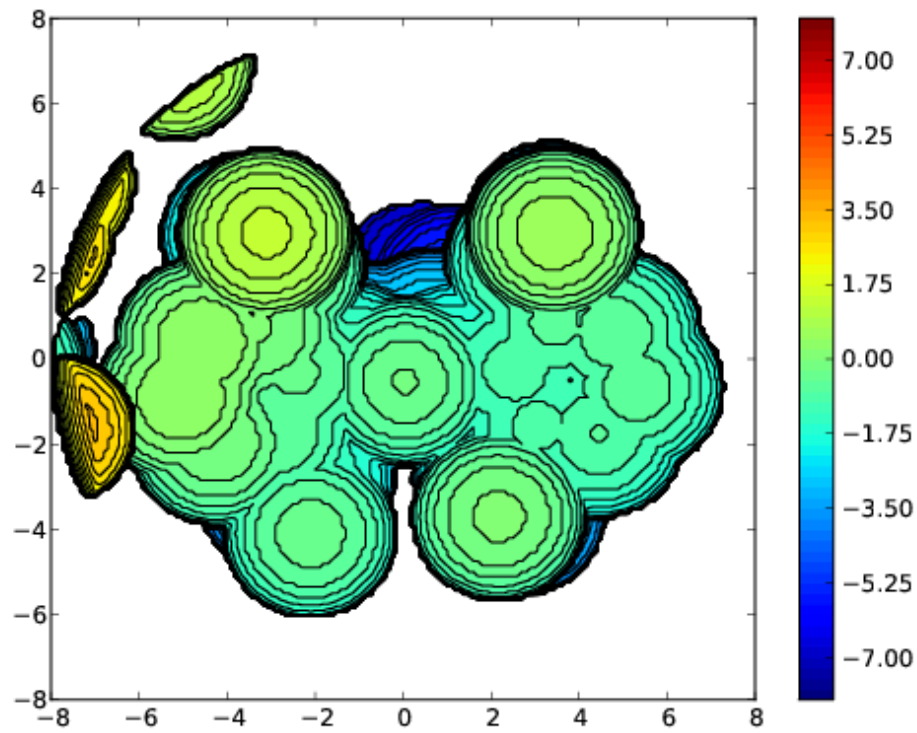
Quadrant	V f	V b	V t	%V f	%V b
SW	77.2	53.6	130.8	59.0	41.0
NW	74.6	56.2	130.8	57.0	43.0
NE	84.6	46.3	130.8	64.6	35.4
SE	79.9	50.9	130.8	61.1	38.9



At 8.0 Å:

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

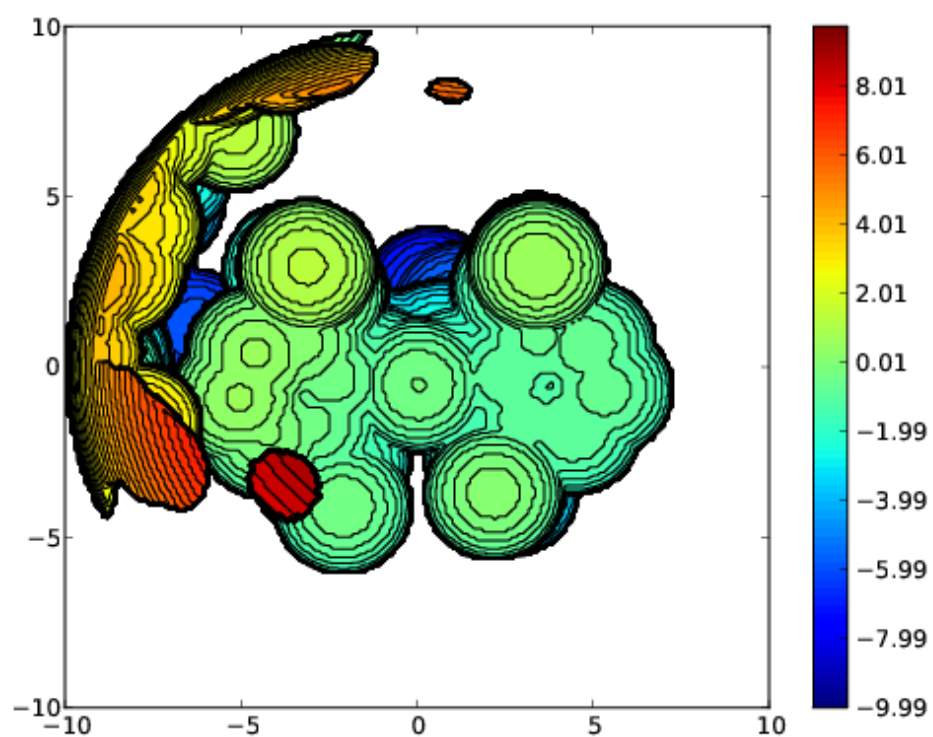
Quadrant	V f	V b	V t	%V f	%V b
SW	394.5	141.4	535.9	73.6	26.4
NW	414.1	121.8	535.9	77.3	22.7
NE	407.6	128.3	535.9	76.1	23.9
SE	395.8	140.1	535.9	73.9	26.1



At 10.0 Å:

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

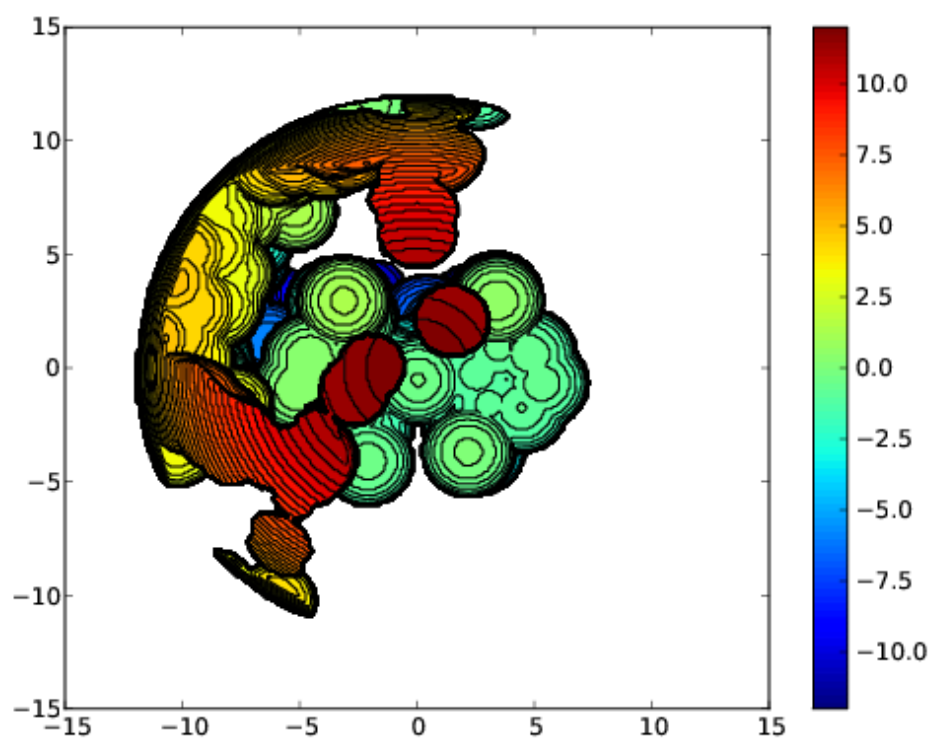
Quadrant	V f	V b	V t	%V f	%V b
SW	844.2	202.8	1046.9	80.6	19.4
NW	780.5	266.4	1046.9	74.6	25.4
NE	895.4	151.6	1046.9	85.5	14.5
SE	895.2	151.8	1046.9	85.5	14.5



At 12.0 Å:

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

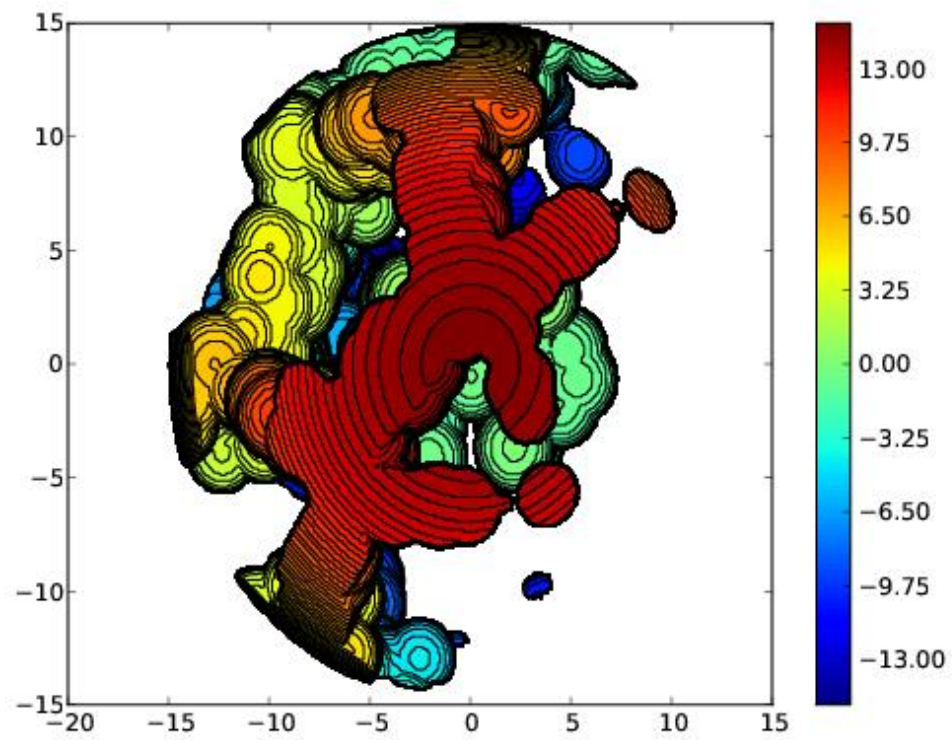
Quadrant	V f	V b	V t	%V f	%V b
SW	1439.1	370.3	1809.4	79.5	20.5
NW	1204.9	600.1	1805.0	66.8	33.2
NE	1583.8	216.7	1800.5	88.0	12.0
SE	1649.5	155.5	1805.0	91.4	8.6



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

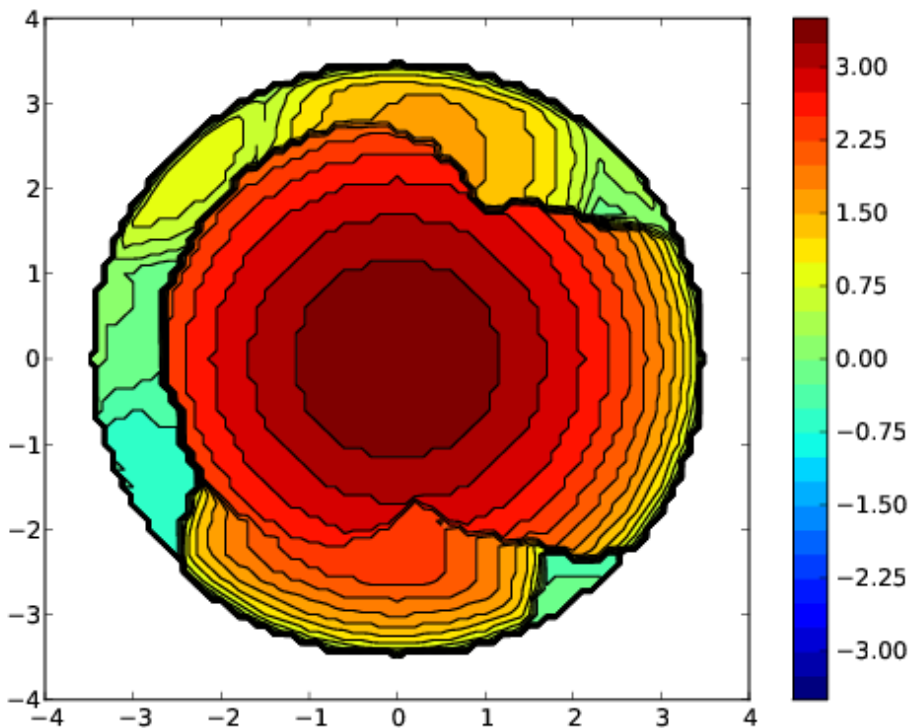


Including all the ruthenium catalyst and the MOF as well:

At 3.5 Å:

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

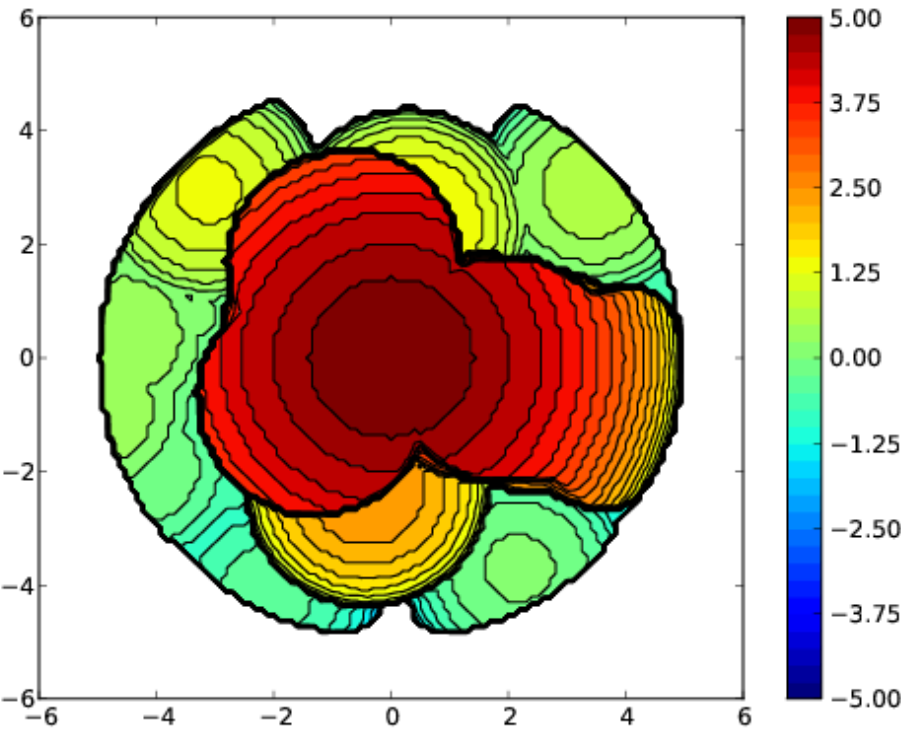
Quadrant	V f	V b	V t	%V f	%V b
SW	5.4	39.5	44.9	11.9	88.1
NW	5.7	39.2	44.9	12.7	87.3
NE	3.1	41.8	44.9	6.9	93.1
SE	1.9	43.0	44.9	4.2	95.8



At 5.0 Å:

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

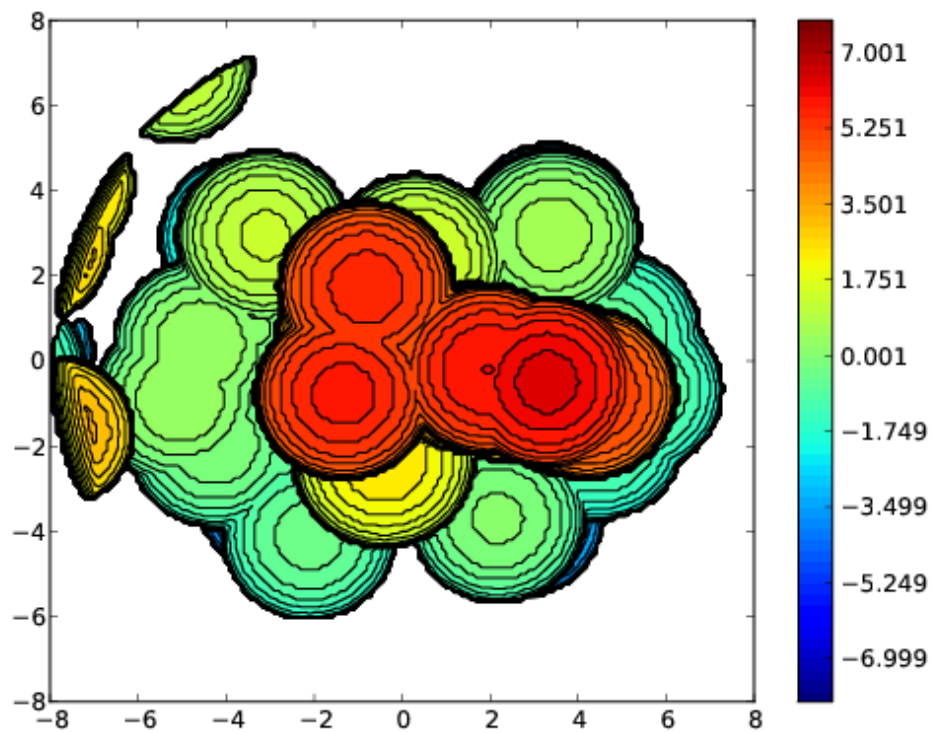
Quadrant	V f	V b	V t	%V f	%V b
SW	36.0	94.9	130.8	27.5	72.5
NW	35.1	95.7	130.8	26.8	73.2
NE	33.9	96.9	130.8	25.9	74.1
SE	28.1	102.8	130.8	21.4	78.6



At 8.0 Å:

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

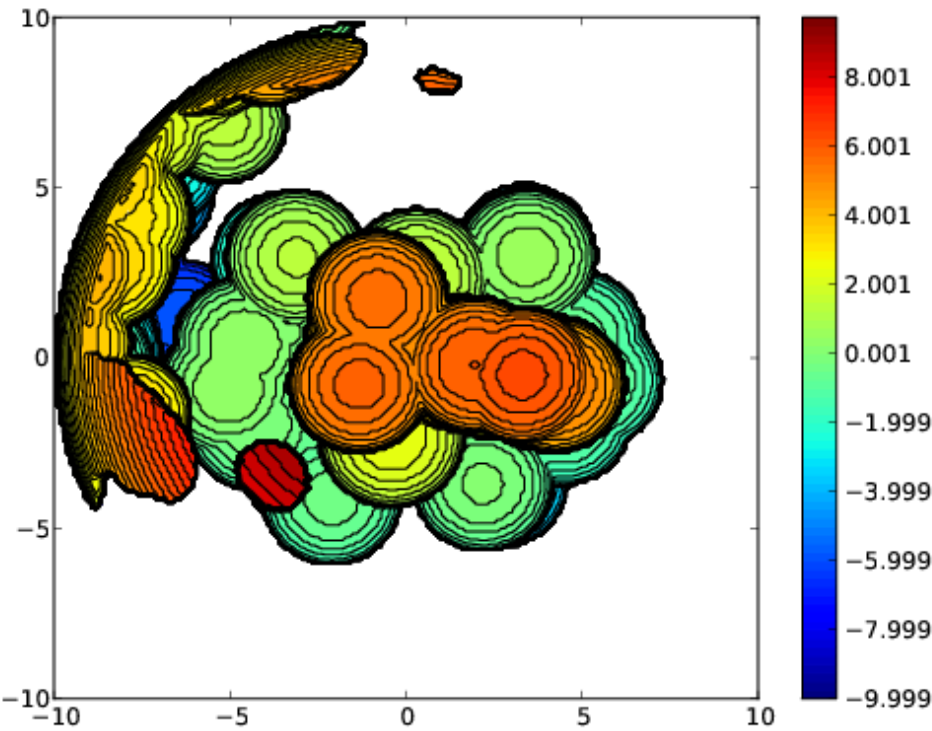
Quadrant	V f	V b	V t	%V f	%V b
SW	345.2	190.7	535.9	64.4	35.6
NW	365.3	170.5	535.8	68.2	31.8
NE	342.1	193.5	535.6	63.9	36.1
SE	312.1	223.7	535.8	58.3	41.7



At 10.0 Å:

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

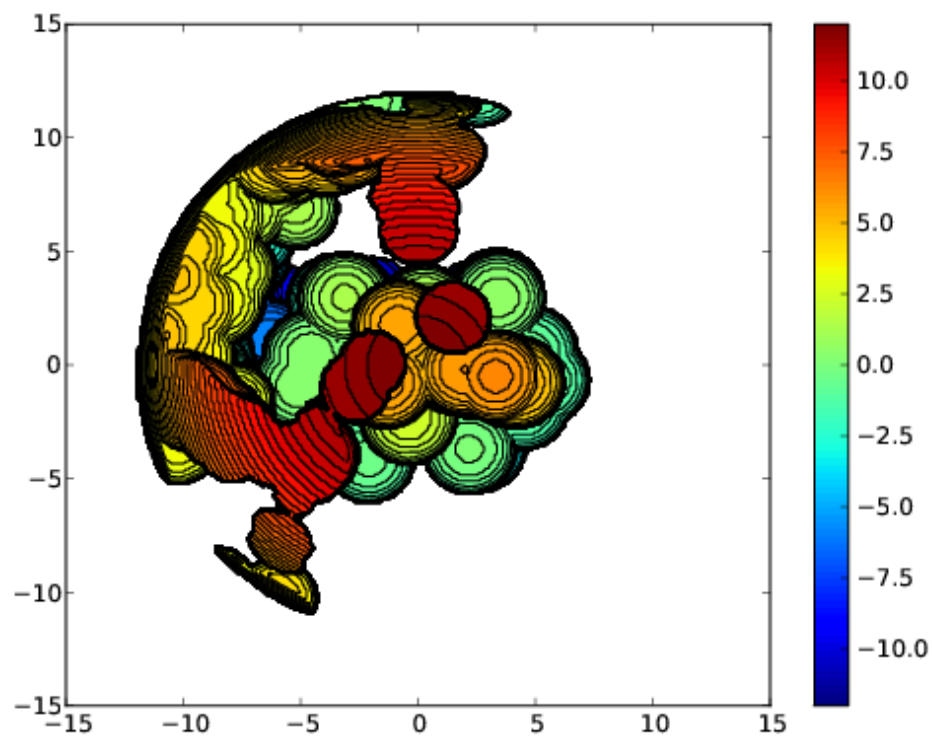
Quadrant	V f	V b	V t	%V f	%V b
SW	794.9	252.0	1046.9	75.9	24.1
NW	731.8	315.2	1046.9	69.9	30.1
NE	830.1	216.8	1046.9	79.3	20.7
SE	811.6	235.4	1046.9	77.5	22.5



At 12.0 Å:

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

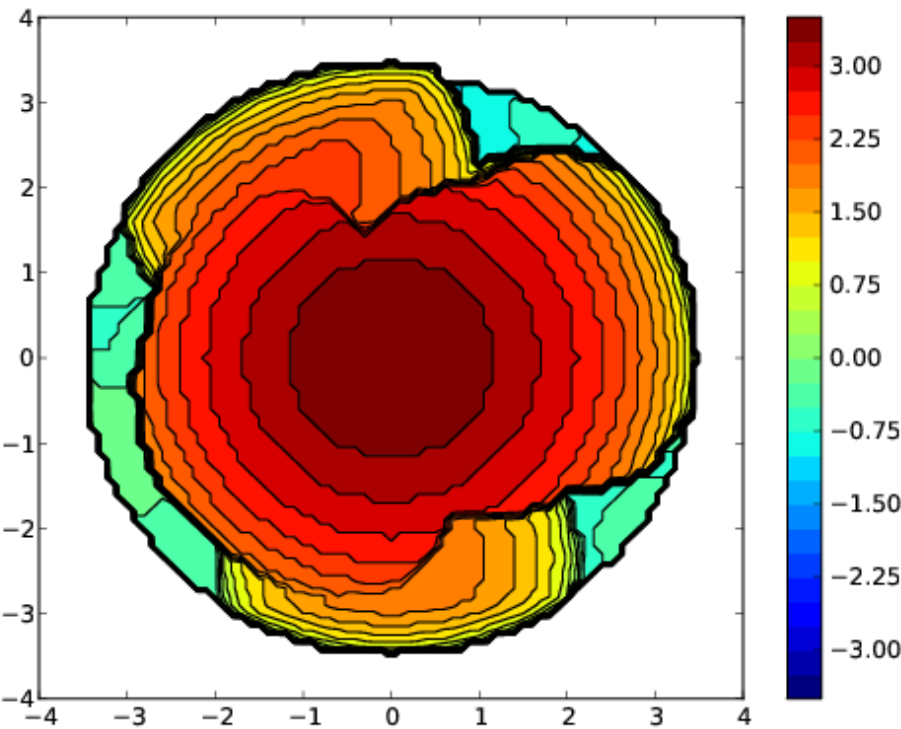
Quadrant	V f	V b	V t	%V f	%V b
SW	1389.5	419.6	1809.1	76.8	23.2
NW	1157.7	651.4	1809.1	64.0	36.0
NE	1525.7	283.5	1809.1	84.3	15.7
SE	1570.3	238.8	1809.1	86.8	13.2



AquaMet™ including all atoms:

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

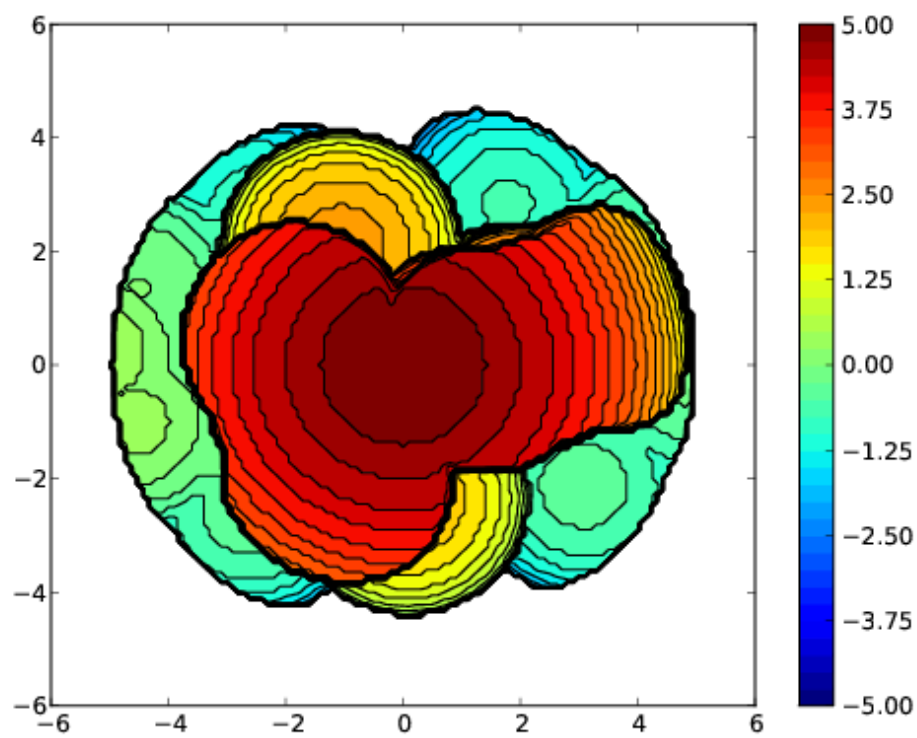
Quadrant	V f	V b	V t	%V f	%V b
SW	5.3	39.5	44.9	11.9	88.1
NW	3.6	41.3	44.9	7.9	92.1
NE	4.2	40.7	44.9	9.3	90.7
SE	4.3	40.5	44.9	9.7	90.3



At 5.0 Å:

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

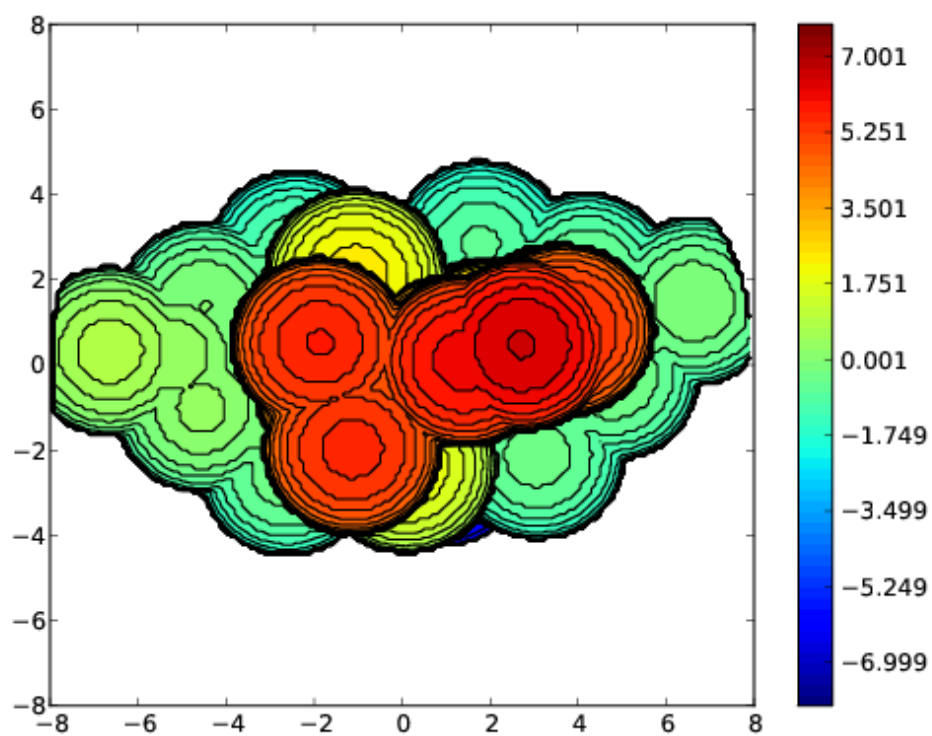
Quadrant	V f	V b	V t	%V f	%V b
SW	37.6	93.2	130.8	28.7	71.3
NW	39.1	91.8	130.8	29.9	70.1
NE	35.5	95.3	130.8	27.2	72.8
SE	44.6	86.2	130.8	34.1	65.9



At 8.0 Å:

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

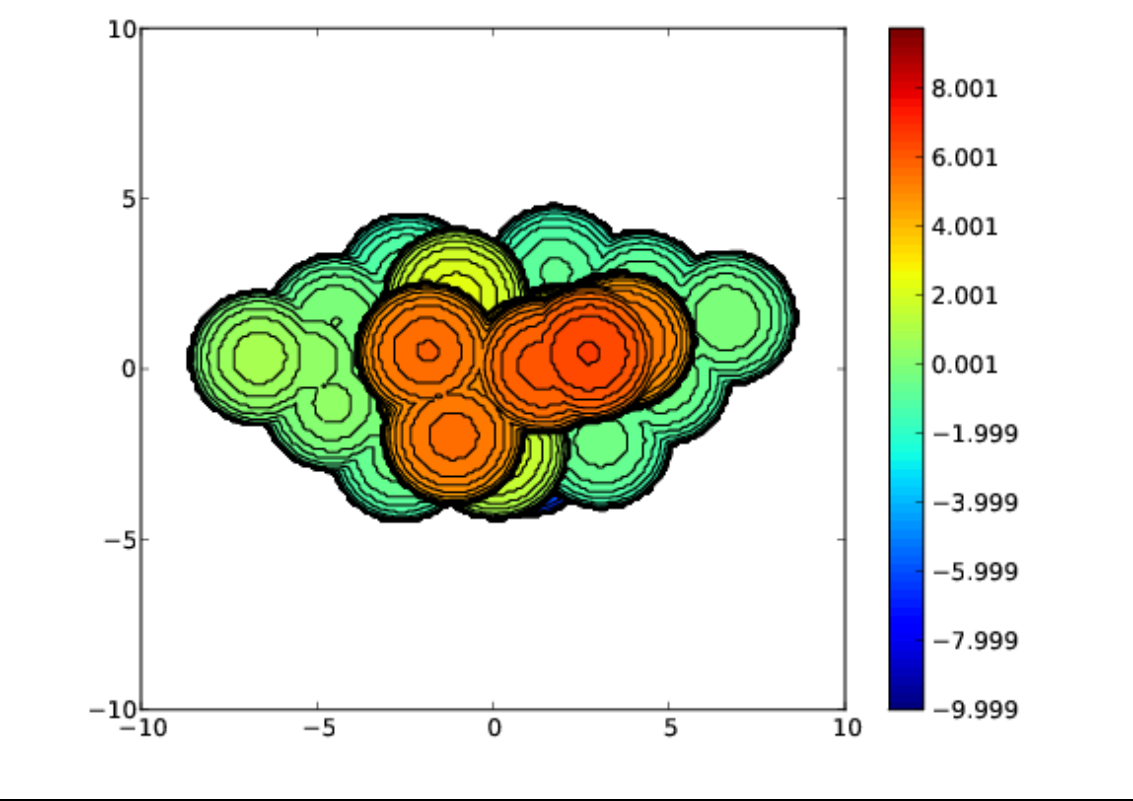
Quadrant	V f	V b	V t	%V f	%V b
SW	386.2	149.7	535.9	72.1	27.9
NW	388.6	147.2	535.8	72.5	27.5
NE	345.2	190.4	535.6	64.4	35.6
SE	381.6	154.2	535.8	71.2	28.8



At 10.0 Å:

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

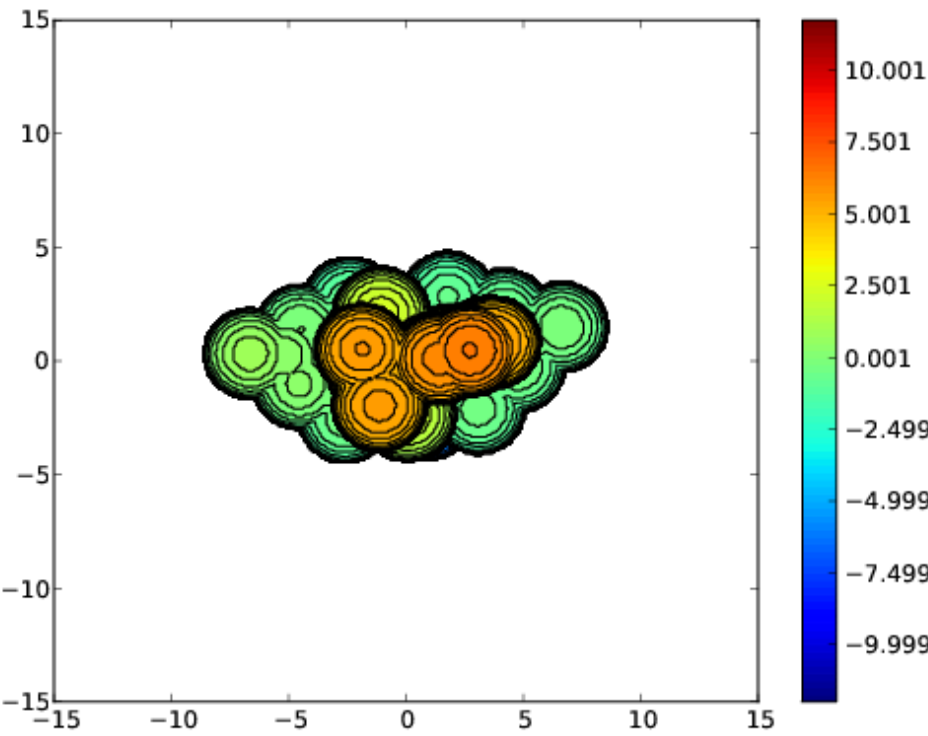
Quadrant	V f	V b	V t	%V f	%V b
SW	883.7	163.3	1047.0	84.4	15.6
NW	893.8	153.0	1046.8	85.4	14.6
NE	838.6	207.9	1046.5	80.1	19.9
SE	867.0	179.7	1046.8	82.8	17.2



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

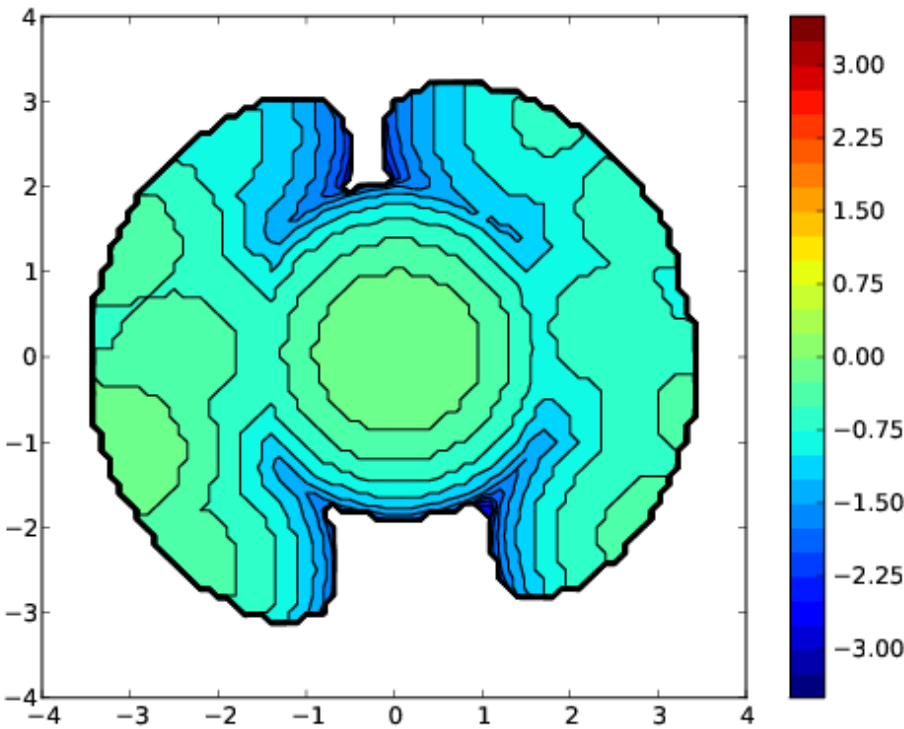


AquaMet™

At 3.5 Å:

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

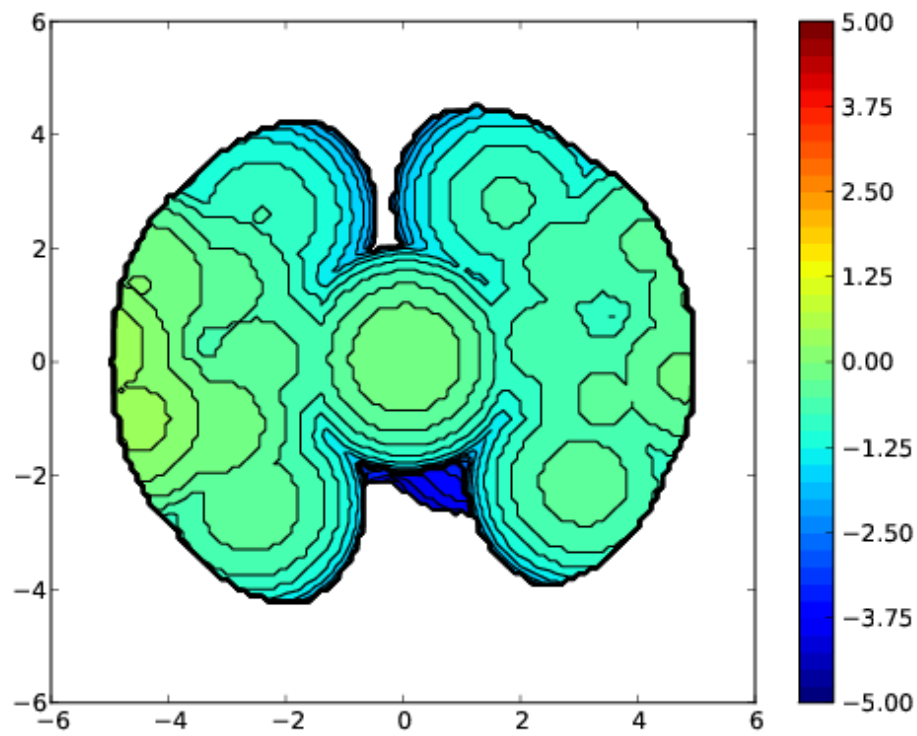
Quadrant	V f	V b	V t	%V f	%V b
SW	29.2	15.7	44.9	65.0	35.0
NW	29.9	15.0	44.9	66.6	33.4
NE	29.2	15.6	44.9	65.2	34.8
SE	31.4	13.4	44.9	70.0	30.0



At 5.0 Å:

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

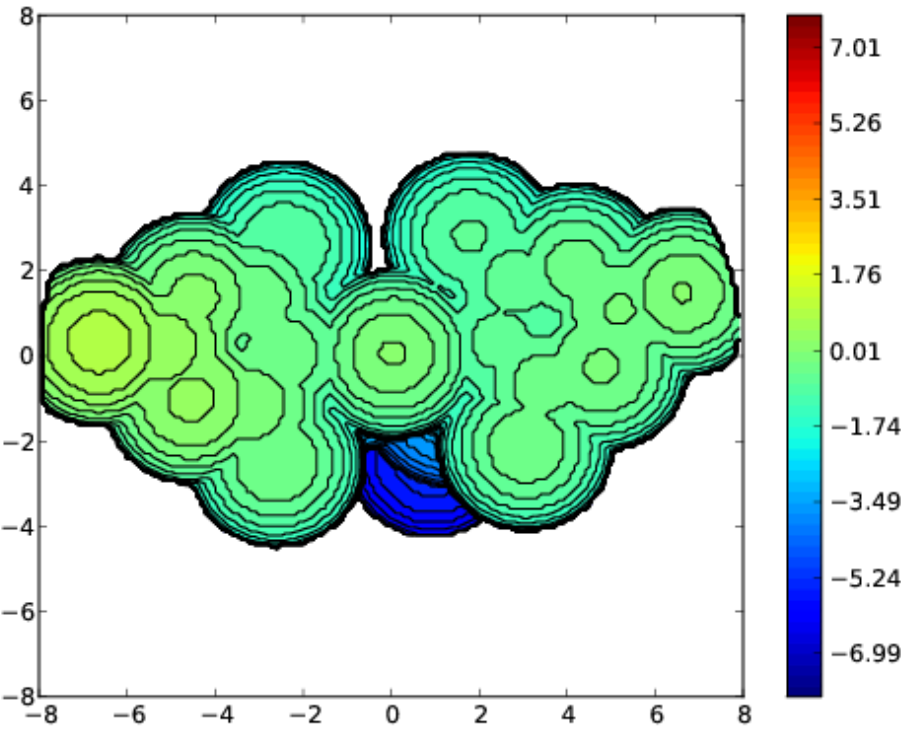
Quadrant	V f	V b	V t	%V f	%V b
SW	82.2	48.6	130.8	62.9	37.1
NW	83.9	46.9	130.8	64.2	35.8
NE	81.4	49.5	130.8	62.2	37.8
SE	89.5	41.4	130.8	68.4	31.6



At 8.0 Å:

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

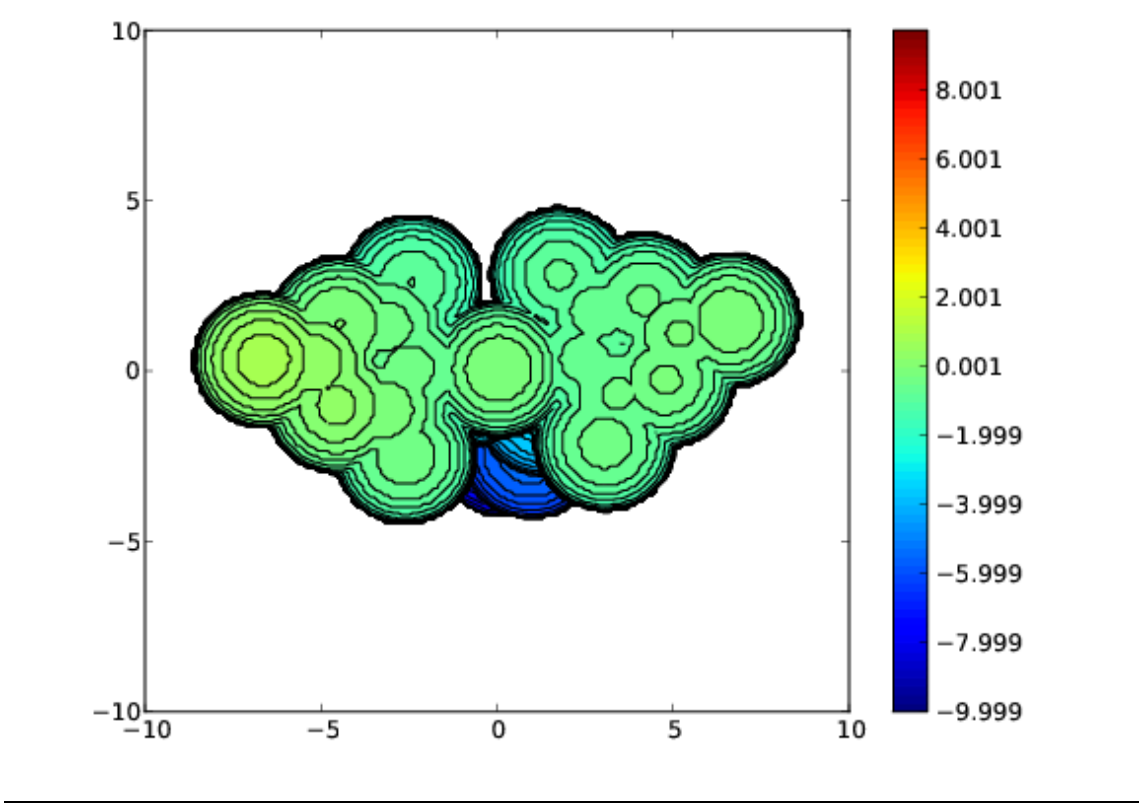
Quadrant	V f	V b	V t	%V f	%V b
SW	443.1	93.0	536.1	82.7	17.3
NW	439.9	94.2	534.1	82.4	17.6
NE	416.9	115.3	532.2	78.3	21.7
SE	437.3	96.8	534.1	81.9	18.1



At 10.0 Å:

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

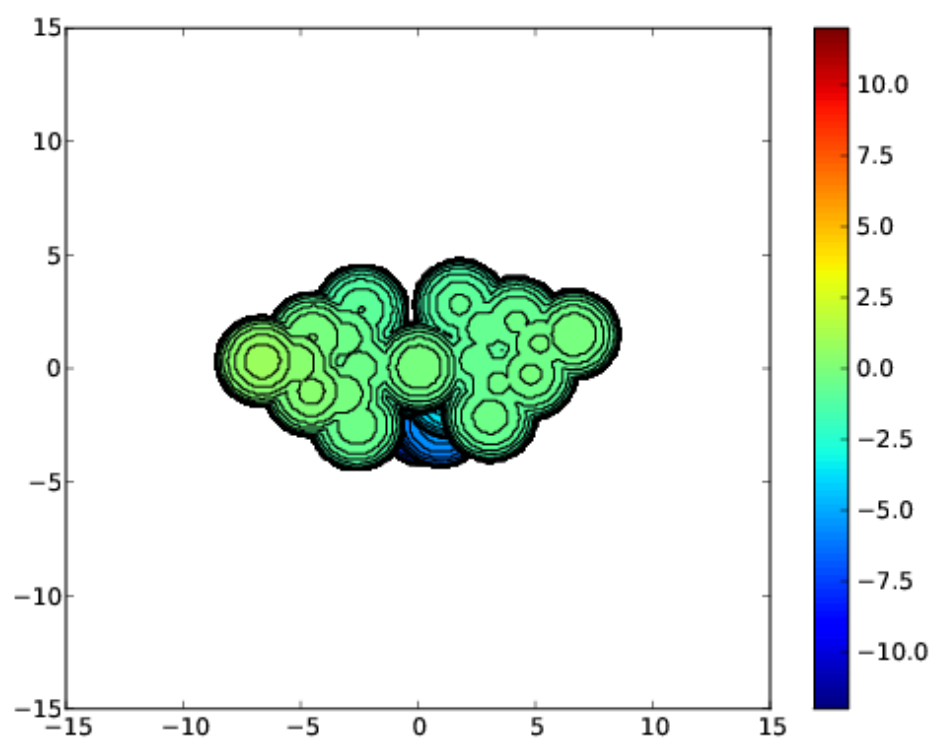
Quadrant	V f	V b	V t	%V f	%V b
SW	941.0	106.1	1047.0	89.9	10.1
NW	946.5	100.3	1046.8	90.4	9.6
NE	913.2	133.4	1046.5	87.3	12.7
SE	924.6	122.2	1046.8	88.3	11.7



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

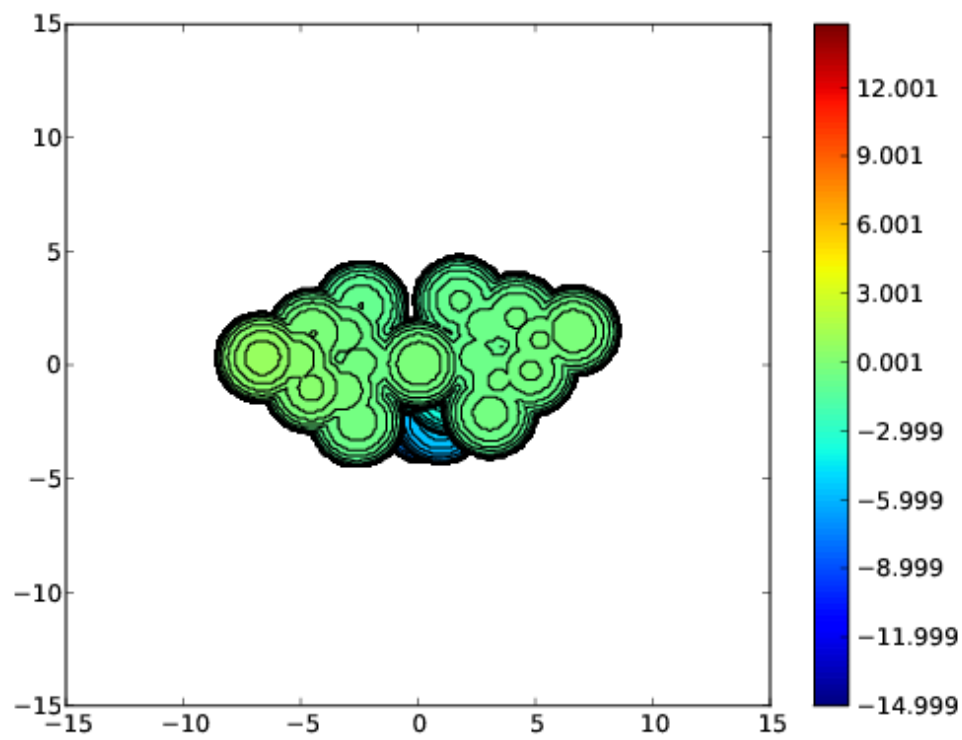
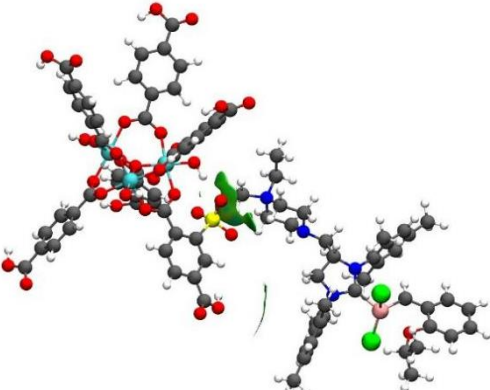
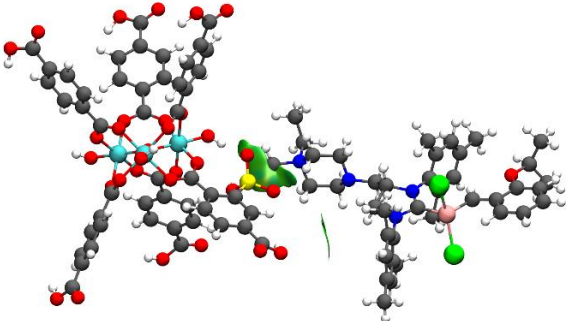
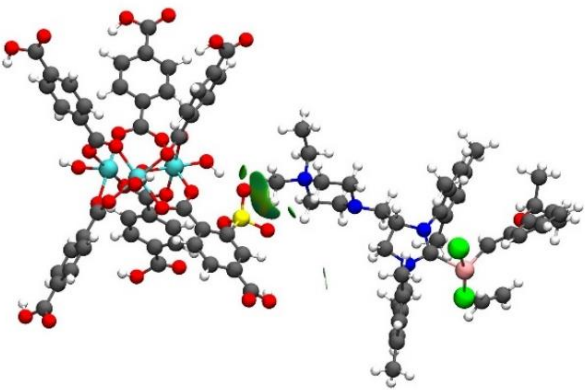
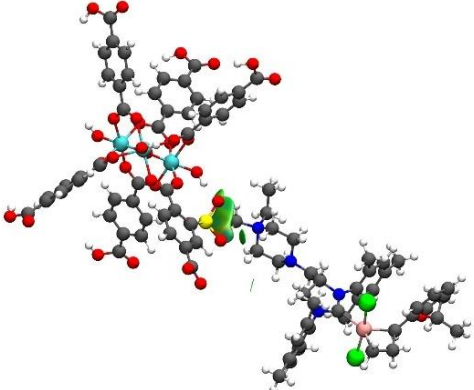
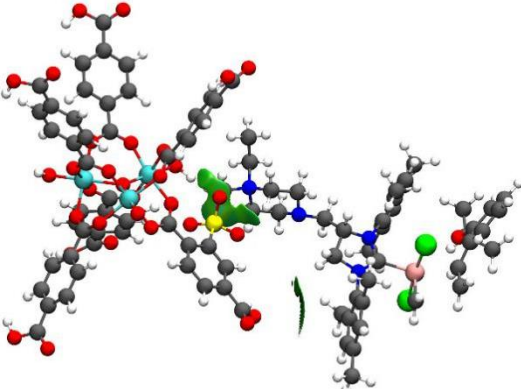
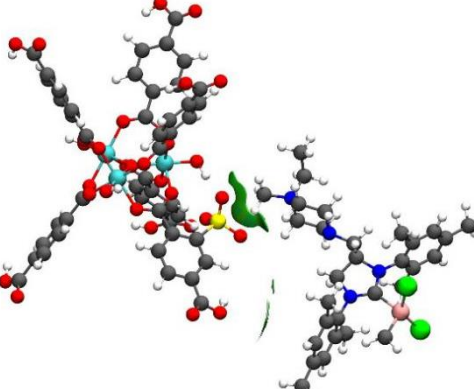


Table S1. NCI plots of the truncated MOF in combination with the Precat. Previously optimised geometries have been evaluated using the promolecular approach suitable for large structures.

Precat	Act
	
Cl1	MCy
	
Cl2	l14e
	

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	-2.438579	2.690545	-0.211031
C	-2.152519	2.151803	0.024327	C	-2.430687	1.317093	-0.585665
C	-1.621242	4.558719	0.022465	C	-3.444597	3.556687	-0.680788
C	-3.000721	4.842574	0.049817	C	-4.434004	3.048476	-1.544811
C	-3.958169	3.811132	0.063995	C	-4.426902	1.700118	-1.941573
C	-3.532661	2.476086	0.051176	C	-3.445801	0.830102	-1.435484
H	-3.325683	5.895208	0.060285	H	-5.214216	3.729312	-1.921439
H	-0.898320	5.383528	0.012163	H	-3.454473	4.618813	-0.403573
H	-4.263385	1.651288	0.062407	H	-3.463929	-0.241963	-1.685847
H	-5.032024	4.052482	0.085424	H	-5.200918	1.319460	-2.625985
H	-2.447742	-0.001196	0.022009	H	-2.052822	-0.334128	0.854102
Act				TS_Ci1			
75				81			
act SCF Done: -2403.22255201 A.U.				ts_ci1 SCF Done: -2481.74738224 A.U.			
Ru	0.627109	-0.718288	0.465266	Ru	-0.578506	-0.558024	-0.365879
C	1.196552	1.067988	0.019576	C	-1.072999	1.280672	-0.041270
N	2.532158	1.375315	-0.173760	N	-2.394236	1.648533	0.151532
N	0.507331	2.261842	-0.008875	N	-0.344410	2.449143	-0.100110
C	1.379035	3.410058	-0.331032	C	-1.170386	3.646381	0.157067
C	2.786888	2.826047	-0.151334	C	-2.599394	3.102817	0.032910
H	1.171303	4.260055	0.350923	H	-0.941912	4.442531	-0.580669
H	1.190874	3.761513	-1.372407	H	-0.955845	4.055806	1.171569
H	3.487179	3.114951	-0.961892	H	-3.278407	3.471112	0.829243
H	3.243223	3.127667	0.819015	H	-3.058074	3.353545	-0.950833
C	-0.909095	2.495595	0.014208	C	1.078152	2.633756	-0.167100
C	3.625094	0.454025	-0.350208	C	-3.523433	0.784367	0.385268
C	4.464025	0.115198	0.744794	C	-4.365608	0.392880	-0.690322
C	5.534422	-0.772718	0.508884	C	-5.468750	-0.437736	-0.400636
C	5.811115	-1.295085	-0.768152	C	-5.780172	-0.845712	0.909758
C	5.001939	-0.877716	-1.844237	C	-4.972921	-0.366107	1.960868
C	3.916421	-0.001417	-1.665828	C	-3.853575	0.454268	1.729639
C	4.276107	0.719728	2.116326	C	-4.159184	0.898839	-2.098542
H	6.178473	-1.055315	1.358724	H	-6.114603	-0.761100	-1.234443
C	6.934890	-2.284066	-0.981344	C	-6.942863	-1.772503	1.185136
H	5.222836	-1.244410	-2.860778	H	-5.224424	-0.634178	3.000873
C	3.093018	0.446407	-2.849680	C	-3.041981	0.976936	2.890549
H	3.211124	0.731507	2.423783	H	-3.092714	0.882031	-2.398793
H	4.656241	1.765560	2.146753	H	-4.532783	1.942522	-2.200654
H	4.842090	0.148385	2.878254	H	-4.724107	0.281902	-2.824953
H	7.705500	-2.208620	-0.187836	H	-7.698821	-1.735770	0.374997
H	7.431340	-2.135892	-1.962411	H	-7.447012	-1.524442	2.141781
H	6.549577	-3.327530	-0.967776	H	-6.597577	-2.826919	1.265520
H	3.578275	0.152928	-3.801196	H	-3.578968	0.822439	3.847088
H	2.949693	1.547507	-2.862293	H	-2.822108	2.060395	2.789835
H	2.086783	-0.022370	-2.819726	H	-2.069791	0.443205	2.949807
C	-1.528023	2.880621	1.231713	C	1.681831	2.906353	-1.421734
C	-1.641633	2.427813	-1.198483	C	1.833976	2.633357	1.033170
C	-2.900845	3.194721	1.206688	C	3.065447	3.169251	-1.447835
C	-3.011855	2.757609	-1.168566	C	3.213956	2.909003	0.951236
C	-3.659937	3.148408	0.019452	C	3.849708	3.180038	-0.276345
C	-5.124781	3.526910	0.026651	C	5.335988	3.453774	-0.346675
H	-3.391539	3.488078	2.150206	H	3.543928	3.376014	-2.420137
C	-0.988483	1.957642	-2.478137	C	1.190626	2.292917	2.358273
H	-3.589006	2.705892	-2.107353	H	3.808957	2.909102	1.880118
C	-0.743336	2.935607	2.520764	C	0.868540	2.902644	-2.693784
H	-0.298688	1.947066	2.765830	H	0.359815	1.926228	-2.843530
H	-1.389439	3.248556	3.364151	H	1.509386	3.104301	-3.574299
H	0.100023	3.656964	2.458701	H	0.071945	3.678034	-2.675068
H	-0.637094	0.907345	-2.382975	H	0.761932	1.267255	2.344370
H	-0.098907	2.565960	-2.746842	H	0.356936	2.982427	2.610765
H	-1.696879	2.007062	-3.327961	H	1.927889	2.346781	3.182886
H	-5.622921	3.258683	-0.926336	H	5.762099	3.667739	0.653950
H	-5.255997	4.621329	0.173859	H	5.560275	4.317473	-1.006788
H	-5.670611	3.025923	0.853444	H	5.884710	2.581132	-0.764092
C	-1.212821	-0.617475	0.352105	C	1.263300	-0.478554	-0.291435
Cl	1.011697	-0.461072	2.763305	Cl	-0.971026	-0.409153	-2.682484
Cl	1.073855	-1.976926	-1.443404	Cl	-0.969051	-1.507828	1.745710
O	-3.572466	-1.135935	-0.918593	O	3.520125	-1.060702	1.111009
C	-4.729521	-1.211794	-1.789219	C	4.524261	-1.263083	2.137919
C	-4.743984	-2.481982	-2.648773	C	4.356266	-2.596543	2.875258
H	-4.526620	-0.358681	-2.471243	H	4.251050	-0.457067	2.851900

C	-6.046560	-0.902084	-1.065780	C	5.949736	-0.966730	1.653336
H	-6.388243	-1.721757	-0.403922	H	6.365978	-1.757924	0.999258
H	-6.844225	-0.722624	-1.816282	H	6.622815	-0.870513	2.530612
H	-5.940224	0.015484	-0.453020	H	5.975175	-0.008650	1.096514
H	-3.751957	-2.639461	-3.117579	H	3.300116	-2.735419	3.181612
H	-5.492992	-2.366973	-3.459492	H	4.982330	-2.590519	3.791525
H	-5.004114	-3.394936	-2.078131	H	4.657901	-3.471937	2.267393
C	-3.302677	-1.981430	0.111325	C	3.323185	-1.863276	0.030982
C	-2.054897	-1.728412	0.789944	C	2.120228	-1.585464	-0.715483
C	-4.117030	-3.054913	0.531083	C	4.176006	-2.906676	-0.386702
C	-3.716082	-3.879148	1.597412	C	3.856419	-3.675083	-1.520681
C	-2.503220	-3.649530	2.268458	C	2.688225	-3.419358	-2.257621
C	-1.688311	-2.585616	1.862928	C	1.830474	-2.389263	-1.849598
H	-4.371010	-4.710888	1.903404	H	4.540662	-4.482887	-1.826932
H	-5.068945	-3.263477	0.027863	H	5.096952	-3.129928	0.165828
H	-0.755302	-2.365473	2.406515	H	0.923052	-2.156560	-2.428302
H	-2.198866	-4.289518	3.110608	H	2.449072	-4.016037	-3.151295
H	-1.733317	0.201606	-0.176656	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				Ci1			
81				81			
ts_con_2 SCF Done: -2481.74092917 A.U.				ci1 SCF Done: -2481.75876594 A.U.			
C	0.686060	-1.308393	0.002036	Ru	0.747112	-0.865237	0.228104
C	0.588520	-3.680114	0.106329	C	1.188578	1.111130	0.049888
H	0.090828	-4.399318	-0.574956	N	2.502051	1.507078	0.007801
H	0.595393	-4.128541	1.125602	N	0.427539	2.242758	0.121644
C	1.983377	-3.267853	-0.369432	C	1.233745	3.483143	0.046082
H	2.801310	-3.712261	0.233091	C	2.669220	2.961872	0.206820
H	2.164475	-3.529630	-1.436436	H	0.934767	4.190366	0.846481
C	-2.174424	-2.646162	1.506884	H	1.065404	3.990175	-0.931326
C	-3.559205	-2.895435	1.569989	H	3.374069	3.380702	-0.540631
H	-4.029420	-3.000617	2.562342	H	3.081736	3.168117	1.219489
C	-4.352242	-3.031733	0.411413	C	-1.002295	2.375506	0.069276
C	-3.720543	-2.910513	-0.841297	C	3.658230	0.667494	-0.194946
H	-4.317002	-3.030151	-1.761271	C	4.433360	0.229669	0.914421
C	-2.338729	-2.650195	-0.964873	C	5.555561	-0.586078	0.658241
C	-1.578270	-2.499040	0.223604	C	5.953907	-0.930626	-0.646897
C	-1.358616	-2.534178	2.772855	C	5.223200	-0.391055	-1.724352
H	-1.998926	-2.666526	3.666840	C	4.089907	0.420834	-1.529655
H	-0.847453	-1.548015	2.848037	C	4.137400	0.674839	2.326212
H	-0.561103	-3.307218	2.818519	H	6.146913	-0.947317	1.516521
C	-5.838148	-3.293648	0.519743	C	7.132299	-1.846606	-0.889448
H	-6.276367	-3.580922	-0.456787	H	5.550135	-0.598392	-2.757196
H	-6.379634	-2.390079	0.875922	C	3.379931	1.026531	-2.715340
H	-6.056444	-4.104081	1.246334	H	3.056553	0.606311	2.565868
C	-1.695732	-2.544021	-2.325331	H	4.464562	1.727284	2.482780
H	-2.438532	-2.714840	-3.128750	H	4.689140	0.053287	3.058758
H	-0.882813	-3.291512	-2.455084	H	7.831639	-1.853841	-0.029147
H	-1.232716	-1.543318	-2.476737	H	7.700319	-1.552942	-1.796116
C	3.218813	-1.106433	-0.216591	H	6.793159	-2.894465	-1.046274
C	3.927517	-0.955035	1.008095	H	3.984835	0.908649	-3.635850
C	5.201268	-0.354207	0.970383	H	3.182708	2.109744	-2.571628
H	5.750631	-0.224684	1.918112	H	2.401210	0.523621	-2.874853
C	5.790777	0.078423	-0.235157	C	-1.721638	2.579913	1.275779
C	5.084029	-0.141188	-1.432975	C	-1.644379	2.421217	-1.194897
H	5.541769	0.154901	-2.391868	C	-3.106129	2.821038	1.187779
C	3.810934	-0.749456	-1.457330	C	-3.031713	2.670061	-1.224775
C	3.335725	-1.410844	2.318587	C	-3.780242	2.875589	-0.049284
H	4.077836	-1.329708	3.136808	C	-5.269348	3.137534	-0.101021
H	2.994118	-2.467051	2.273147	H	-3.674078	2.975773	2.120724
H	2.444910	-0.798481	2.586893	C	-0.873873	2.177784	-2.471979
C	7.136991	0.766867	-0.236601	H	-3.539530	2.711457	-2.203275
H	7.650853	0.663158	-1.213461	C	-1.022990	2.540774	2.613453
H	7.804527	0.362446	0.551644	H	-0.441024	1.602048	2.739659
H	7.024719	1.855876	-0.039065	H	-1.752736	2.619938	3.442858
C	3.133371	-1.036504	-2.776015	H	-0.303066	3.381629	2.724536

H	3.697951	-0.583683	-3.614653	H	-0.455056	1.146516	-2.508634
H	2.093046	-0.645387	-2.803890	H	-0.009397	2.867718	-2.576243
C	3.080894	-2.130195	-2.972184	H	-1.522430	2.317307	-3.358870
C	-1.504054	0.487568	0.365528	H	-5.619367	3.316744	-1.137377
H	-1.891980	-0.094059	1.227338	H	-5.547943	4.021703	0.510286
C	-2.501855	1.317023	-0.323448	H	-5.842555	2.275653	0.304601
C	-3.735156	0.755547	-0.746870	C	-1.115350	-0.709325	0.111814
H	-3.937266	-0.303327	-0.524740	Cl	0.961697	-0.603380	2.626859
C	-4.660979	1.511924	-1.479008	Cl	0.960687	-1.299265	-2.133007
H	-5.597285	1.045280	-1.823646	O	-3.436094	-1.174224	-1.221488
C	-4.389575	2.859820	-1.776946	C	-4.457386	-1.485775	-2.205728
H	-5.108015	3.455948	-2.361805	C	-4.686678	-2.993712	-2.357115
C	-3.204314	3.453348	-1.312587	H	-3.957462	-1.133514	-3.132661
C	-2.271236	2.698915	-0.580119	C	-5.734606	-0.651664	-2.041420
N	-0.146917	-2.395106	0.118862	H	-6.383406	-0.992717	-1.210439
N	1.957240	-1.801326	-0.197028	H	-6.331779	-0.711195	-2.974974
Cl	0.420400	0.651491	2.482731	H	-5.478149	0.412347	-1.867113
Cl	0.021300	0.639189	-2.395484	H	-3.719592	-3.519276	-2.487626
Ru	0.313038	0.629012	0.001772	H	-5.302434	-3.181216	-3.260958
H	-2.981385	4.512423	-1.511275	H	-5.212838	-3.443029	-1.491900
O	-1.130718	3.310832	-0.096305	C	-3.483594	-1.484976	0.098400
C	-1.169119	3.864729	1.276359	C	-2.246782	-1.287724	0.820960
C	1.886420	2.326484	-0.707853	C	-4.614798	-1.988474	0.777660
C	2.307735	2.109346	0.578046	C	-4.541685	-2.299479	2.145716
H	1.124305	3.084998	-0.950840	C	-3.344645	-2.121166	2.862238
H	2.394419	1.859561	-1.564827	C	-2.213007	-1.634435	2.198481
H	3.155102	1.445708	0.802897	H	-5.438227	-2.693258	2.651715
H	1.897834	2.671675	1.429767	H	-5.559392	-2.144988	0.243004
C	-0.108724	4.961068	1.314551	H	-1.264186	-1.475032	2.735259
H	0.875796	4.584128	0.976108	H	-3.294129	-2.365944	3.934419
H	0.009493	5.339753	2.350498	C	1.578020	-2.942028	0.645789
H	-0.397346	5.810375	0.660398	C	0.245901	-3.219625	0.401750
C	-2.545374	4.382364	1.691565	H	-1.428648	-0.121229	-0.773918
H	-0.874756	3.030070	1.954487	H	-0.109970	-3.454114	-0.613345
H	-2.887846	5.217712	1.045486	H	-0.456025	-3.380061	1.233219
H	-2.477309	4.761191	2.732323	H	2.316636	-2.989535	-0.174952
H	-3.317172	3.587835	1.674903	H	1.969071	-2.907778	1.675441
TS_MCy				MCy			
81				81			
ts_mcy SCF Done: -2481.75565653 A.U.				mcy SCF Done: -2481.76698777 A.U.			
Ru	0.689004	-0.806804	0.259894	Ru	0.612952	-0.761675	-0.040240
C	1.354959	1.037650	-0.301871	C	1.386553	1.099518	-0.097620
N	2.673566	1.339157	-0.489237	N	2.708579	1.412666	-0.163184
N	0.620946	2.143698	-0.600341	N	0.658780	2.246598	-0.093933
C	1.451796	3.272284	-1.079044	C	1.517394	3.453266	-0.084152
C	2.887332	2.745033	-0.899530	C	2.925429	2.871654	-0.307601
H	1.246264	4.184938	-0.481131	H	1.418428	3.981724	0.889878
H	1.208147	3.504986	-2.138965	H	1.205425	4.157115	-0.883099
H	3.484099	2.790286	-1.834381	H	3.324622	3.097468	-1.320794
H	3.452720	3.293579	-0.114384	H	3.667617	3.228746	0.435721
C	-0.805607	2.310826	-0.522327	C	-0.770136	2.379953	0.055961
C	3.807450	0.469482	-0.281219	C	3.838391	0.512800	-0.156574
C	4.430018	0.425856	0.996911	C	4.484954	0.240819	1.079261
C	5.548126	-0.417439	1.161710	C	5.606994	-0.611454	1.067393
C	6.080719	-1.175081	0.101274	C	6.109493	-1.173681	-0.122080
C	5.489680	-1.039264	-1.170354	C	5.478969	-0.830515	-1.333860
C	4.369617	-0.214854	-1.395138	C	4.356531	0.020887	-1.384908
C	3.946828	1.271545	2.149162	C	4.002031	0.839236	2.377872
H	6.027205	-0.464975	2.154198	H	6.107728	-0.834035	2.024689
C	7.252512	-2.105922	0.318303	C	7.287734	-2.121718	-0.097549
H	5.920778	-1.582965	-2.027845	H	5.880394	-1.225243	-2.282519
C	3.816458	-0.052593	-2.789128	C	3.756383	0.403841	-2.715287
H	2.948204	0.932276	2.503405	H	3.024505	0.395620	2.669394
H	3.847236	2.340447	1.864068	H	3.854757	1.937672	2.304755
H	4.654636	1.215103	2.999274	H	4.728507	0.649728	3.192181
H	6.902041	-3.136121	0.549961	H	7.979734	-1.894108	0.738702
H	7.885875	-1.778797	1.167751	H	7.863861	-2.085290	-1.044402
H	7.892865	-2.177157	-0.584586	H	6.948449	-3.172623	0.037817
H	4.428697	-0.614229	-3.521578	H	4.333056	-0.044299	-3.548047
H	3.808201	1.012282	-3.107815	H	3.759853	1.505361	-2.865632
H	2.770736	-0.426761	-2.844077	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_l14e				l14e			
81				55			
ts_l14e SCF Done: -2481.74389163 A.U.				l14e 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	C	-0.894398	0.148635	2.690274
H	-2.085961	3.735638	1.867684	H	0.900553	1.408336	2.989011
H	-1.516697	2.528259	3.066464	H	1.156735	-0.321210	3.396604
H	-3.619821	1.396193	2.763769	H	-1.191130	-0.823316	3.146978
H	-4.025320	2.407302	1.338699	H	-1.454820	0.949584	3.215332
C	0.281539	2.708138	0.831791	C	2.398042	0.049647	0.944403
C	-3.674872	-0.308603	0.577903	C	-2.588736	0.077811	0.856269
C	-4.571666	-0.127388	-0.511136	C	-3.303592	1.284697	0.649826
C	-5.511950	-1.144808	-0.770603	C	-4.670981	1.199774	0.318281
C	-5.596775	-2.307758	0.020155	C	-5.333144	-0.038373	0.193669
C	-4.717150	-2.433940	1.114705	C	-4.586371	-1.216711	0.401806
C	-3.757143	-1.450528	1.422272	C	-3.217858	-1.188503	0.735406
C	-4.522965	1.109772	-1.374251	C	-2.602601	2.621136	0.727464
H	-6.205955	-1.014822	-1.618023	H	-5.233467	2.132883	0.146384
C	-6.591922	-3.399106	-0.305020	C	-6.808631	-0.105436	-0.132078
H	-4.782710	-3.326141	1.759963	H	-5.082806	-2.196169	0.296233
C	-2.836631	-1.615094	2.605354	C	-2.437691	-2.470656	0.907736
H	-3.541090	1.212965	-1.890222	H	-1.784871	2.685370	-0.022341
H	-4.665339	2.035830	-0.776275	H	-2.137089	2.790590	1.721966
H	-5.320273	1.084821	-2.142510	H	-3.309574	3.452927	0.541430
H	-6.136782	-4.165338	-0.971030	H	-7.166284	0.829243	-0.608449
H	-7.482941	-2.999450	-0.830168	H	-7.413458	-0.259132	0.788870
H	-6.934817	-3.926428	0.608390	H	-7.038599	-0.950141	-0.813392
H	-3.091926	-2.525304	3.182681	H	-3.098408	-3.353123	0.802844
H	-2.894331	-0.748898	3.299206	H	-1.952272	-2.533692	1.905141
H	-1.775673	-1.690354	2.274616	H	-1.627392	-2.553219	0.151105
C	0.375568	3.789576	-0.091256	C	3.120530	1.255079	0.732362
C	1.381417	2.346081	1.656163	C	3.059512	-1.210398	0.942606
C	1.619327	4.433063	-0.234215	C	4.484536	1.161005	0.391575
C	2.602912	3.027113	1.465783	C	4.425307	-1.243479	0.601594
C	2.748377	4.061894	0.524165	C	5.151275	-0.075123	0.296524
C	4.067991	4.778035	0.339420	C	6.601873	-0.147679	-0.123739
H	1.699047	5.266823	-0.952159	H	5.044853	2.092394	0.203357
C	1.265688	1.292918	2.730256	C	2.344652	-2.483669	1.326777
C	3.463492	2.743287	2.093732	H	4.940239	-2.218744	0.585772
C	-0.816283	4.258709	-0.887569	C	2.499833	2.616667	0.945660
H	-1.124287	3.481442	-1.621991	H	1.411997	2.619703	0.750311
H	-0.579178	5.190380	-1.437609	H	2.956878	3.370084	0.274843
H	-1.695012	4.462605	-0.239417	H	2.673529	2.960083	1.990708
H	0.429168	1.508371	3.428999	H	1.746326	-2.358332	2.253639
H	2.196005	1.242322	3.328951	H	3.070177	-3.303149	1.497278
H	1.072821	0.285501	2.297579	H	1.644521	-2.802627	0.525668
H	4.825370	4.439361	1.074034	H	7.110112	-1.034501	0.306320
H	3.951874	5.877103	0.451552	H	7.164522	0.757849	0.181881
H	4.481140	4.604924	-0.677914	H	6.687974	-0.226723	-1.230037
C	1.893721	-1.394586	-1.867651	Cl	0.864954	2.078650	-1.926201
Cl	-1.129813	1.293146	-2.658440	Cl	0.558716	-2.337906	-1.652329
Cl	0.357315	-1.573976	0.958961	C	-1.607842	0.029259	-2.075066
O	3.385273	-3.284189	-0.576208	H	-1.679703	-0.040820	-3.192039
C	3.618151	-4.339214	0.398446	H	-2.561940	0.158018	-1.529198
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				

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 PENJOLL-precate SCF Done: -3287.58987447 A.U.	103 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	-3.393382	2.325768	1.198685
H	-0.892328	4.642693	2.986745	H	-2.385944	3.293612	2.327711
H	-0.958282	7.978754	-0.423446	H	-2.066792	7.277753	-0.428222
H	-1.171022	7.536984	-2.152622	H	-1.521272	7.178402	-2.137100
H	0.461816	7.577178	-1.432355	H	-0.321689	7.260980	-0.816911
H	-1.007763	2.923672	-3.591121	H	-0.300334	2.979814	-4.124430
H	-1.818933	1.766424	-2.488067	H	-1.027485	1.495316	-3.433054
H	-0.031573	1.799586	-2.597964	H	0.679546	1.915031	-3.066336
C	0.525095	-2.335217	1.834127	C	0.787250	-3.010198	0.509249
C	0.215239	-2.381259	-0.623490	C	1.004338	-2.472047	-1.893403
C	1.020869	-3.652846	1.765820	C	1.557054	-4.170688	0.278397
C	0.712850	-3.702171	-0.628076	C	1.760938	-3.645736	-2.067670
C	1.109194	-4.361275	0.550888	C	2.038441	-4.519258	-0.996770
C	1.613051	-5.788068	0.524982	C	2.818673	-5.797355	-1.212181
H	1.350975	-4.138673	2.699885	H	1.795524	-4.819506	1.138534
C	-0.113172	-1.690634	-1.927190	C	0.792561	-1.520389	-3.048034
H	0.803205	-4.224772	-1.595598	H	2.154932	-3.877288	-3.071889
C	0.491077	-1.610235	3.158085	C	0.337812	-2.690520	1.916975
H	1.190337	-0.746818	3.161502	H	0.205414	-1.602555	2.079170
H	0.769634	-2.290356	3.987186	H	1.086946	-3.053724	2.649001
H	-0.509780	-1.187152	3.379988	H	-0.620832	-3.197322	2.163583
H	0.436338	-0.729090	-2.010068	H	1.255324	-0.533334	-2.833253
H	-1.193093	-1.448073	-2.052085	H	-0.282729	-1.327714	-3.249183
H	0.181687	-2.324285	-2.786737	H	1.243566	-1.917311	-3.978444
H	1.796938	-6.140213	-0.509847	H	2.135682	-6.660385	-1.376552
H	0.878508	-6.483828	0.987170	H	3.447137	-6.046421	-0.332667
H	2.557756	-5.896806	1.098195	H	3.478312	-5.731488	-2.101079
C	2.833654	-0.238362	0.294405	C	2.774602	-0.303442	0.398833
Cl	1.966540	1.757725	2.796195	Cl	0.628017	0.992773	2.556190
Cl	2.385084	2.303537	-1.593941	Cl	2.536671	2.299300	-1.389962
O	4.277394	-2.005350	-1.201598	O	5.044219	-1.415364	-0.632327
C	4.791470	-2.921148	-2.199651	C	6.128243	-1.807200	-1.512289
C	5.620738	-2.215000	-3.279354	C	7.101652	-0.658163	-1.797262
H	3.845305	-3.252911	-2.677903	H	5.568725	-2.005565	-2.451288
C	5.445516	-4.169902	-1.592887	C	6.791683	-3.128863	-1.100425
H	6.449346	-3.978678	-1.165337	H	7.468466	-3.029656	-0.228874
H	5.559386	-4.944128	-2.380019	H	7.394300	-3.517349	-1.947769
H	4.802178	-4.587373	-0.792547	H	6.019708	-3.885384	-0.854579
H	5.077106	-1.327259	-3.659990	H	6.543998	0.252498	-2.094288
H	5.784787	-2.909092	-4.129614	H	7.770138	-0.942590	-2.636142
H	6.613810	-1.882645	-2.918390	H	7.739761	-0.404615	-0.927955
C	5.030730	-1.260079	-0.349199	C	5.193022	-0.921610	0.626586
C	4.284928	-0.320446	0.451583	C	4.007985	-0.318745	1.185417
C	6.433126	-1.334417	-0.210181	C	6.379658	-0.961348	1.388806
C	7.104343	-0.498226	0.699691	C	6.411098	-0.417884	2.685844
C	6.394154	0.421446	1.489491	C	5.264930	0.169584	3.246961
C	5.001832	0.503805	1.359772	C	4.082397	0.221160	2.496792
H	8.200106	-0.576338	0.787481	H	7.350593	-0.463083	3.260290
H	7.015717	-2.042457	-0.812158	H	7.288831	-1.418514	0.979352
H	4.424717	1.193794	1.996746	H	3.165271	0.657654	2.923112
H	6.921390	1.066216	2.209212	H	5.290714	0.582711	4.267160
H	2.340401	-1.142612	-0.105863	C	2.524108	4.007914	1.890664
C	-2.742982	-1.083695	1.665406	C	3.828517	3.715828	1.735545
H	-2.187445	-2.013705	1.910558	H	2.683489	-1.121734	-0.340414
H	-2.707962	-0.450007	2.582416	H	4.287352	3.670968	0.734141
C	-4.460128	-2.742200	0.822089	H	4.479886	3.492201	2.597087
C	-5.211722	-0.516219	1.435935	H	1.880700	4.235456	1.024432
C	-5.157475	-2.621268	-0.540687	H	2.045995	4.032888	2.883588
H	-5.082807	-3.355602	1.529284	C	-2.567469	-1.844774	0.387871
H	-3.536547	-3.331626	0.649409	H	-2.256477	-2.921115	0.456712
C	-5.893074	-0.345952	0.071227	H	-2.231917	-1.349852	1.322042
H	-5.971439	-0.800701	2.214785	C	-4.708190	-2.272239	-0.811246
H	-4.835005	0.482014	1.737429	C	-4.748774	-1.801236	1.542089
H	-5.525850	-3.600819	-0.909662	C	-6.063961	-1.591032	-0.998265
H	-4.477119	-2.143740	-1.292082	H	-4.801038	-3.393877	-0.717164
H	-6.771390	0.327546	0.116160	H	-4.149198	-2.096162	-1.753873
H	-5.165118	0.018305	-0.697834	C	-6.097133	-1.099399	1.418282
N	-4.121440	-1.461033	1.393832	H	-4.858929	-2.874271	1.876741
N	-6.374405	-1.684103	-0.496660	H	-4.197958	-1.280651	2.353433
C	-6.819129	-1.450601	-1.919964	H	-6.654557	-2.051093	-1.816150
H	-7.150375	-2.416746	-2.346704	H	-5.903129	-0.491923	-1.168268

H -7.650936 -0.722864 -1.925186	H -6.706084 -1.182709 2.338569
H -5.934522 -1.044369 -2.472167	H -5.926854 -0.022359 1.138698
C -7.491016 -2.323499 0.318098	N -4.006614 -1.670819 0.303502
H -7.737487 -3.262702 -0.218180	N -6.936042 -1.643526 0.260802
H -7.053546 -2.611581 1.292795	C -8.086816 -0.688762 0.047048
C -8.740037 -1.474769 0.528373	H -8.688986 -1.047341 -0.809894
H -9.217996 -1.164415 -0.421670	H -8.704027 -0.655727 0.963114
H -9.481059 -2.087899 1.080486	H -7.627688 0.313264 -0.159004
H -8.546453 -0.571401 1.139586	C -7.433670 -3.063588 0.485427
Cl -3.716423 -0.343550 -2.534280	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	Cl1
109	109
PENJOLL-TSconc SCF Done: -3366.08812308 A.U.	PENJOLL-Cl1 SCF Done: -3366.10527741 A.U.
C 0.181844 0.249948 0.183002	Ru 1.874612 1.534905 0.238952
C -1.981981 -0.689529 -0.044232	C 0.023227 0.693813 0.262365
H -2.244434 -0.629092 -1.127142	N -1.073239 1.507479 0.211509
C -2.108962 0.703385 0.571237	N -0.432213 -0.597323 0.383732
H -2.863787 1.334130 0.048931	C -1.913274 -0.677383 0.212502
H -2.372818 0.652827 1.656974	C -2.337284 0.779382 0.429676
C -0.090201 -3.030616 -1.170534	H -2.139485 -0.971571 -0.840769
C 0.263994 -4.395044 -1.143603	H -3.140838 1.096840 -0.271937
H 0.226139 -4.965807 -2.087107	H -2.688559 0.947101 1.476891
C 0.659772 -5.045843 0.041334	C 0.339396 -1.809724 0.320524
C 0.693528 -4.288064 1.228439	C -1.079220 2.936218 -0.000251
H 0.982264 -4.779132 2.173256	C -1.041501 3.822597 1.111053
C 0.355328 -2.918550 1.262015	C -1.037878 5.209921 0.852910
C -0.028994 -2.290462 0.044281	C -1.128956 5.729971 -0.451308
C -0.519064 -2.388864 -2.468812	C -1.279623 4.820063 -1.516731
H -0.252684 -3.031871 -3.330886	C -1.282737 3.425561 -1.322740
H -0.037424 -1.396208 -2.607473	C -1.110515 3.327813 2.536462
H -1.620330 -2.232920 -2.509453	H -0.987563 5.903041 1.709812
C 1.060668 -6.504557 0.032897	C -1.081366 7.220224 -0.706329
H 0.902748 -6.979141 1.022725	H -1.413992 5.204976 -2.541566
H 2.138619 -6.621695 -0.216776	C -1.573724 2.499728 -2.477043
H 0.490582 -7.082544 -0.723024	H -0.367110 2.531792 2.745283
C 0.398954 -2.163292 2.566107	H -2.123674 2.925485 2.760697
H 0.528587 -2.856733 3.420141	H -0.925174 4.157316 3.247286
H -0.527337 -1.574198 2.732309	H -1.297862 7.801388 0.212763
H 1.234427 -1.426101 2.583032	H -1.808943 7.524275 -1.487316
C -0.547194 2.658175 0.548424	H -0.075357 7.531370 -1.065138
C -0.759570 3.486182 -0.589160	H -1.542291 3.054141 -3.435626
C -0.638845 4.880670 -0.420270	H -2.590138 2.051241 -2.381618
H -0.790228 5.528633 -1.300001	H -0.827485 1.683751 -2.535651
C -0.357652 5.467196 0.829245	C 0.781078 -2.418552 1.526926
C -0.229322 4.618106 1.945189	C 0.565871 -2.426348 -0.939572
H -0.055486 5.057553 2.942053	C 1.427092 -3.667662 1.444181
C -0.338573 3.216068 1.838871	C 1.210760 -3.680801 -0.961190
C -1.155992 2.912418 -1.927054	C 1.641019 -4.323453 0.215155
H -1.081861 3.685457 -2.717787	C 2.333310 -5.668183 0.171701
H -2.217830 2.570154 -1.903340	H 1.771406 -4.143503 2.378031
H -0.515664 2.054010 -2.220702	C 0.188433 -1.740722 -2.233102
C -0.199742 6.965302 0.964534	H 1.386064 -4.165452 -1.936795
H -0.902305 7.511506 0.301918	C 0.578457 -1.750742 2.864966
H 0.827605 7.284771 0.681080	H 1.028680 -0.733889 2.882914
H -0.372539 7.303799 2.006208	H 1.030810 -2.352424 3.677689
C -0.259413 2.357590 3.078293	H -0.498750 -1.619066 3.102078
H -0.208711 2.988533 3.987539	H 0.641784 -0.725797 -2.303114
H 0.639197 1.701876 3.058051	H -0.908806 -1.601592 -2.340008
H -1.146990 1.696755 3.177479	H 0.532525 -2.330683 -3.105204
C 2.686924 -1.063082 -0.378598	H 2.305233 -6.112818 -0.843409
H 2.219986 -1.706978 -1.153828	H 1.862851 -6.390486 0.872234
C 3.937200 -1.579024 0.195816	H 3.399760 -5.581362 0.473006
C 4.018258 -2.897995 0.712525	C 2.867427 -0.041006 0.064354
H 3.123127 -3.537126 0.667708	Cl 1.871940 1.646681 2.661549
C 5.195638 -3.370809 1.309839	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	-1.334091	2.983033	0.113440
C	-1.269426	3.753193	1.347587	C	-1.218250	3.807656	1.263810
C	-1.396049	5.153444	1.224364	C	-1.322611	5.203321	1.091007
C	-1.645763	5.774902	-0.012000	C	-1.570197	5.784940	-0.166645
C	-1.817383	4.953134	-1.144951	C	-1.757925	4.926861	-1.268090
C	-1.704518	3.551116	-1.085239	C	-1.665734	3.525210	-1.158740
C	-1.088327	3.131341	2.711581	C	-1.030549	3.230198	2.646825
H	-1.314281	5.771516	2.134443	H	-1.225908	5.851785	1.978296
C	-1.762832	7.278667	-0.130416	C	-1.638534	7.286947	-0.334774
H	-2.066713	5.414950	-2.115319	H	-2.000044	5.357876	-2.254195
C	-2.016198	2.710789	-2.297706	C	-1.968807	2.647640	-2.347179
H	-0.042510	2.783779	2.861328	H	-1.181577	4.011310	3.417983
H	-1.748954	2.250329	2.851691	H	-0.012355	2.803362	2.783797
H	-1.325208	3.864253	3.508127	H	-1.753474	2.411880	2.850274
H	-1.606509	7.781778	0.844602	H	-0.680227	7.688162	-0.733033
H	-2.762097	7.578827	-0.513002	H	-1.833887	7.799692	0.628814
H	-1.014305	7.684252	-0.844911	H	-2.433198	7.582303	-1.050848
H	-2.063862	3.343582	-3.206095	H	-2.024774	3.254999	-3.272269
H	-3.006499	2.209516	-2.189856	H	-2.951646	2.134477	-2.228093
H	-1.241146	1.935212	-2.460894	H	-1.181222	1.879874	-2.488474
C	0.985475	-1.922774	1.901333	C	0.902395	-1.990498	1.903717
C	0.867929	-2.397434	-0.525932	C	0.821830	-2.379534	-0.542389
C	1.816134	-3.049546	2.053190	C	1.764440	-3.098425	2.020739
C	1.702400	-3.515061	-0.313242	C	1.676784	-3.485350	-0.359371
C	2.188061	-3.859949	0.961966	C	2.169690	-3.856214	0.905621
C	3.109738	-5.043063	1.157469	C	3.127820	-5.014637	1.064670
H	2.183535	-3.301102	3.062298	H	2.123379	-3.380682	3.024709
C	0.383155	-2.064848	-1.917819	C	0.328868	-2.031655	-1.926634
H	1.980044	-4.135671	-1.182423	H	1.967613	-4.073731	-1.245869
C	0.624804	-1.073826	3.096135	C	0.485642	-1.231725	3.139029
H	1.114096	-0.074486	3.039160	H	1.041374	-0.269662	3.214008
H	0.940917	-1.561795	4.039140	H	0.689675	-1.824407	4.052629
H	-0.466467	-0.879716	3.153605	H	-0.591780	-0.969454	3.123761
H	-0.693757	-2.310099	-2.055031	H	-0.759754	-2.228484	-2.045518
H	0.943677	-2.646244	-2.676378	H	0.853189	-2.639563	-2.689884
H	0.507739	-0.983513	-2.148156	H	0.501786	-0.958208	-2.163744
H	2.874169	-5.594697	2.091199	H	2.943853	-5.574230	2.005053
H	4.167721	-4.708778	1.237016	H	4.176533	-4.646332	1.104855
H	3.048922	-5.756456	0.310731	H	3.057777	-5.727307	0.217940
C	3.131613	0.354749	-0.384204	C	3.610056	0.771242	-0.428512
Cl	2.199441	2.150337	2.330804	Cl	2.165873	1.787490	2.484288
Cl	1.255762	1.504693	-2.368048	Cl	1.333165	1.383185	-2.259359
O	4.781805	-1.366128	-1.704520	O	4.578907	-1.463020	-1.700946
C	5.599568	-2.077187	-2.668280	C	5.394936	-1.997134	-2.777146
C	7.043209	-1.561668	-2.719200	C	6.799978	-1.389164	-2.819095
H	5.108866	-1.767389	-3.615306	H	4.839839	-1.628459	-3.666585
C	5.455683	-3.602023	-2.573794	C	5.370618	-3.530752	-2.838854
H	6.009970	-4.048067	-1.725153	H	6.015206	-4.008521	-2.073569
H	5.841697	-4.063604	-3.506151	H	5.730128	-3.868340	-3.833372
H	4.386974	-3.876962	-2.471995	H	4.335285	-3.902520	-2.704606
H	7.052542	-0.455791	-2.795854	H	6.746179	-0.281844	-2.808418
H	7.548113	-1.968954	-3.619542	H	7.309344	-1.698726	-3.754964
H	7.644157	-1.851046	-1.834914	H	7.429273	-1.712789	-1.966154
C	4.975415	-1.327618	-0.361202	C	5.005475	-1.308641	-0.412205
C	4.109951	-0.428758	0.374830	C	4.473432	-0.185370	0.309237
C	5.944478	-2.087143	0.333761	C	5.893263	-2.202138	0.229402
C	6.078978	-1.970276	1.726740	C	6.264713	-2.001964	1.568185
C	5.250721	-1.100594	2.456269	C	5.742544	-0.915010	2.290663
C	4.281394	-0.350949	1.780773	C	4.855878	-0.030343	1.663441
H	6.847863	-2.570557	2.240463	H	6.958470	-2.711080	2.048522
H	6.608727	-2.771263	-0.207796	H	6.287517	-3.067156	-0.319440
H	3.626532	0.345197	2.327709	H	4.406786	0.796902	2.234205
H	5.359886	-1.007139	3.547752	H	6.018183	-0.761265	3.345632
C	2.828279	3.441330	-0.511116	C	2.566505	3.252391	-0.178473
C	3.892283	2.507685	-0.509018	C	3.848177	2.340977	-0.247872
H	3.167419	0.118899	-1.466851	H	3.564877	0.508484	-1.499056
H	4.319549	2.181021	-1.471006	H	4.354186	2.619355	-1.194623
H	4.532768	2.406714	0.381110	H	4.482813	2.514666	0.640066
H	2.419974	3.802602	-1.469645	H	2.300600	3.741193	-1.134074
H	2.690005	4.081863	0.377201	H	2.553582	3.914441	0.707775
N	-3.876034	-2.048657	0.545876	N	-3.963340	-1.987342	0.594765

H -2.520105 -1.570835 2.076889	H -2.615084 -1.493391 2.126410
H -1.898622 -2.780789 0.923218	H -1.997974 -2.735633 1.005929
C -4.990072 -1.969748 1.459927	C -5.085885 -1.860827 1.493042
C -4.112000 -2.923582 -0.578648	C -4.204825 -2.887732 -0.508175
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
N -6.593320 -2.357428 -0.474676	N -6.672578 -2.255940 -0.453350
H -5.597625 -3.151330 -2.190001	H -5.676503 -3.125188 -2.131000
H -5.181309 -1.413447 -1.725860	H -5.219043 -1.385914 -1.711308
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
H	1.109090	0.184518	-3.455683	H	-0.479932	-0.979360	1.944995
H	2.770521	-5.716292	-2.795597	H	-0.313738	-6.655413	-0.523694
H	3.955095	-5.304822	-1.520660	H	-1.591330	-6.262629	-1.712020
H	4.112375	-4.603224	-3.167086	H	-1.922614	-6.144145	0.050091
C	3.831647	1.377819	0.969533	C	-4.204211	0.182349	-1.015547
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
C	4.974556	-0.833149	1.211539	C	-5.417944	-1.140052	0.730358
C	4.115396	0.169495	1.778094	C	-4.510467	-1.112949	-0.378098
C	5.341777	-1.958834	1.984668	C	-5.769625	-2.376901	1.315814
C	4.879486	-2.099432	3.302918	C	-5.231579	-3.577260	0.824989
C	4.040652	-1.123968	3.870076	C	-4.340903	-3.564087	-0.261659
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
C	3.309654	2.598903	1.453146	C	-3.686064	0.353136	-2.304797
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
H	1.758995	3.927562	-0.436480	H	-2.365969	3.037770	0.188344
H	0.839429	3.693479	1.203948	H	-1.891051	3.334631	-1.633878
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
H	-4.098473	-3.262107	1.736734	H	6.435846	-0.592897	-1.585848
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
N	-6.517518	-2.413428	0.365251	N	6.574683	-1.257682	1.215251
C	-7.840386	-1.688207	0.293568	C	6.827424	-0.894547	2.658559
H	-8.442840	-2.134154	-0.520965	H	7.157805	-1.803998	3.196144
H	-8.363409	-1.795810	1.261119	H	7.610568	-0.116165	2.703028
H	-7.598134	-0.613302	0.088397	H	5.860144	-0.508448	3.068620
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
H	-8.349342	-3.863115	2.070295	H	9.369868	-0.537643	1.431106
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
Cl	-5.973619	1.055996	-0.239873	Cl	3.603429	0.035207	2.804848
TS_114e				114e			
109				83			
PENJOLL-TS3FFfprovarCII SCF Done: -3366.09257217 A.U.				PENJOLL-14e2 SCF Done: -2863.66506662 A.U.			

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	C	-5.955330	-1.572725	1.453111
H	-6.229093	-1.219805	4.438172	H	-6.696771	-0.955612	1.995958
C	-2.349846	0.894733	-0.274313	H	-6.382571	-2.563313	1.213146
C	-3.695194	-2.787454	0.263022	H	-5.009938	-1.681755	2.040847
H	-4.757530	-1.427438	-0.964217	C	-6.835617	-0.599114	-0.668779
H	-3.258487	-3.302533	-0.607486	H	-7.497958	0.006599	-0.016922
H	-3.436859	-3.169343	1.263175	H	-6.524971	0.051017	-1.508522
H	-2.531892	1.465683	0.663980	C	-7.569194	-1.827769	-1.194668
H	-2.708499	1.357615	-1.220673	H	-7.903754	-2.510741	-0.388972
C	3.758552	-1.117783	-0.822663	H	-8.478640	-1.481344	-1.726353
H	3.761582	-2.219260	-0.638975	H	-6.967996	-2.406591	-1.923145
H	3.693619	-0.988161	-1.924180	Cl	-2.691200	-1.360419	2.264132
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				

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

Precat	TS_Open
102	102
precatnocl_2 SCF Done: -2827.27562574 A.U.	PENJOLL-TSopen+ SCF Done: -2827.24323473 A.U.
Ru -2.060265 0.144218 -0.093212	Ru -1.992635 0.608443 -0.145316
C -0.130029 0.287434 0.165466	C -0.070178 0.545674 -0.148280
N 0.517680 1.505660 0.264766	N 0.702837 1.682489 0.027551
N 0.870381 -0.678845 0.111124	N 0.813004 -0.528879 -0.163593
C 2.225674 -0.112459 0.286404	C 2.169955 -0.124673 0.271797
C 1.975508 1.399977 0.170586	C 2.138598 1.388891 0.026369
H 2.467494 1.989911 0.972210	H 2.266426 -0.328062 1.367479
H 2.340886 1.798061 -0.805573	H 2.663349 1.969840 0.811522
C 0.707005 -2.092842 0.336437	H 2.599296 1.652545 -0.956943
C -0.064410 2.821792 0.385524	C 0.498938 -1.922069 -0.321048
C -0.295220 3.612365 -0.772506	C 0.278120 3.057834 -0.094992
C -0.846094 4.899462 -0.597565	C 0.206064 3.654828 -1.382164
C -1.120648 5.434749 0.674999	C -0.194729 5.001703 -1.468896
C -0.789678 4.656924 1.802890	C -0.492599 5.771187 -0.327835
C -0.253583 3.360957 1.688580	C -0.332513 5.168506 0.935705
C 0.104986 3.153702 -2.155864	C 0.064802 3.825033 1.083168
H -1.047230 5.510093 -1.493896	C 0.612545 2.916565 -2.638019
C -1.749927 6.800324 0.831872	H -0.277051 5.463300 -2.467074
H -0.952581 5.072377 2.811516	C -0.981180 7.195747 -0.454757
C 0.105473 2.580356 2.930059	H -0.516628 5.765152 1.844774
H -0.177406 2.099707 -2.352001	C 0.292347 3.249150 2.460443
H 1.205090 3.254017 -2.300477	H 0.392525 1.834243 -2.581517
H -0.375805 3.780992 -2.932108	H 1.701718 3.046648 -2.833889
H -1.598384 7.429712 -0.067804	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	9.041651	-1.486238	0.257735
H	8.820384	-0.494088	-1.675220
H	7.424156	-1.494942	-1.196056
H	9.839502	-0.838857	0.672041
H	9.549393	-2.347593	-0.221933
H	8.439346	-1.897806	1.091415
Act			
102			
PENJOLL-Act+ SCF Done: -2827.25391155 A.U.			
Ru	-1.774054	1.201615	-0.576155
C	-0.002532	0.776953	0.018710
N	0.920441	1.753686	0.340005
N	0.674020	-0.440331	0.049646
C	2.090980	-0.293777	0.446618
C	2.269563	1.232880	0.568552
H	2.241177	-0.790695	1.435577
H	2.651114	1.549835	1.563372
H	2.982699	1.623300	-0.193805
C	0.097720	-1.759522	0.133209
C	0.695594	3.174370	0.468817
C	0.942957	4.033146	-0.636593
C	0.747197	5.417336	-0.456855
C	0.353459	5.967116	0.778675
C	0.191163	5.091189	1.869904
C	0.364226	3.699655	1.746874
C	1.436536	3.509458	-1.965418
H	0.921835	6.088377	-1.314497
C	0.103806	7.450222	0.927265
H	-0.081172	5.503185	2.855944
C	0.180346	2.809998	2.953069
H	0.714019	2.804460	-2.428914
H	2.401837	2.966221	-1.859180
H	1.605210	4.343006	-2.674733
H	0.703819	8.043146	0.207867
H	0.335820	7.805780	1.951585
H	-0.965496	7.688483	0.735039
H	0.255331	3.395313	3.890528
H	0.928227	1.991521	2.996704
H	-0.824597	2.336840	2.922828
C	-0.024921	-2.568718	-1.027208
C	-0.303530	-2.242759	1.409792
C	-0.513789	-3.882884	-0.868774
C	-0.773759	-3.566260	1.510407
C	-0.874991	-4.410421	0.385795
C	-1.351739	-5.839155	0.519973
H	-0.626677	-4.511753	-1.768023
C	-0.304657	-1.339037	2.622525
H	-1.088969	-3.942055	2.498409
C	0.314340	-2.058710	-2.409398
H	0.045598	-0.990474	-2.534357
H	-0.231544	-2.639496	-3.178814
H	1.397494	-2.167992	-2.639332
H	-0.955907	-0.454718	2.454827
H	0.705094	-0.945511	2.870623
H	-0.678482	-1.874865	3.516340
H	-1.978849	-5.981019	1.422771
H	-0.492011	-6.539994	0.606576
H	-1.939663	-6.158960	-0.364136
C	-2.677204	-0.406872	-0.423619
Cl	-1.186555	1.282653	-2.846964
Cl	-2.752423	2.318642	1.214238
O	-4.461963	-2.054647	0.824420
C	-5.236821	-2.837416	1.774435
C	-6.288472	-1.999985	2.510244
H	-4.447116	-3.096369	2.511489
C	-5.752865	-4.157719	1.188433
H	-6.620428	-4.032072	0.511431
H	-6.072965	-4.823791	2.016249
H	-4.947710	-4.673232	0.627366
H	-5.837204	-1.063048	2.893851
C	8.001785	-1.778538	0.705841
H	8.354553	-1.941287	1.744430
H	7.120260	-2.428465	0.553449
C	9.092954	-2.108997	-0.303865
H	10.009766	-1.499362	-0.180839
H	9.388964	-3.164421	-0.135803
H	8.750150	-2.039913	-1.355100
TS_Ci1			
108			
PENJOLL-TS1+ SCF Done: -2905.77972796 A.U.			
Ru	-1.513141	1.093843	-0.434447
C	0.123678	0.529143	0.389743
N	1.091971	1.431855	0.796629
N	0.690092	-0.738141	0.508032
C	2.129439	-0.671052	0.842584
C	2.306571	0.783188	1.304987
H	2.347311	-1.392263	1.660921
H	2.377005	0.877366	2.413083
H	3.221596	1.242283	0.874081
C	0.031114	-2.017040	0.600967
C	0.974907	2.869022	0.883931
C	1.446254	3.674138	-0.188718
C	1.341941	5.074809	-0.067604
C	0.827302	5.691405	1.089004
C	0.449687	4.863445	2.164895
C	0.522002	3.459217	2.096001
C	2.090956	3.072097	-1.415153
H	1.690999	5.703302	-0.904069
C	0.680702	7.192996	1.176425
H	0.084232	5.325083	3.097359
C	0.115882	2.627115	3.288904
H	1.389716	2.414244	-1.972234
H	2.976425	2.454443	-1.141929
H	2.441346	3.866529	-2.102962
H	1.360179	7.715488	0.473633
H	0.884618	7.565970	2.200805
H	-0.356897	7.501224	0.920914
H	0.016692	3.258942	4.192958
H	0.847453	1.824224	3.515460
H	-0.866726	2.144917	3.098367
C	-0.114641	-2.860276	-0.529456
C	-0.411193	-2.439542	1.889140
C	-0.672169	-4.144275	-0.333145
C	-0.957873	-3.726813	2.026248
C	-1.085973	-4.605184	0.927991
C	-1.650712	-5.995470	1.113550
H	-0.796625	-4.800699	-1.211105
C	-0.339103	-1.509275	3.078956
H	-1.303354	-4.051937	3.022201
C	0.255812	-2.432246	-1.931203
H	0.450673	-1.346301	-2.007279
H	-0.576657	-2.658347	-2.628549
H	1.140515	-2.991892	-2.308660
H	-0.919873	-0.580307	2.897352
H	0.701538	-1.194489	3.310865
H	-0.746867	-1.994756	3.986712
H	-0.927042	-6.654474	1.641407
H	-1.891000	-6.474493	0.143874
H	-2.574363	-5.981635	1.728635
C	-2.493919	-0.475455	-0.392375
Cl	-0.541378	1.053160	-2.587865
Cl	-2.625161	2.184912	1.311484
O	-4.547667	-1.940784	0.644273
C	-5.515773	-2.625232	1.488141
C	-6.680936	-1.719297	1.899747
H	-4.900055	-2.802974	2.395237
C	-5.922746	-4.000720	0.944761
H	-6.629481	-3.948815	0.093497
H	-6.417635	-4.579542	1.751843
H	-5.027547	-4.566979	0.617738
H	-6.300684	-0.750599	2.281214

H -6.673023 -2.575864 3.377121	H -7.252713 -2.208219 2.715215
H -7.155470 -1.730607 1.875919	H -7.387919 -1.512061 1.072632
C -4.965512 -1.409985 -0.258943	C -4.799896 -1.428452 -0.586117
C -4.033780 -0.540145 -0.938231	C -3.728210 -0.639769 -1.149106
C -6.287906 -1.519043 -0.739953	C -5.993857 -1.597637 -1.319474
C -6.699468 -0.786198 -1.866087	C -6.140636 -1.007826 -2.586629
C -5.806218 0.064251 -2.541317	C -5.106677 -0.240345 -3.151333
C -4.492028 0.180532 -2.076783	C -3.920265 -0.057400 -2.432536
H -7.738056 -0.890395 -2.218657	H -7.082944 -1.158065 -3.137564
H -7.010031 -2.174662 -0.238723	H -6.820765 -2.188926 -0.908708
H -3.769724 0.812301 -2.618644	H -3.088895 0.518548 -2.867647
H -6.131339 0.625122 -3.430462	H -5.224395 0.206910 -4.150028
H -2.313189 -1.241175 0.203423	C -2.688900 3.900597 -1.988593
C 3.049806 -0.934199 -0.575705	C -3.975060 3.526774 -1.860335
H 2.770512 -2.004572 -0.736957	H -2.280590 -1.272043 0.344657
H 2.918304 -0.412380 -1.545711	H -4.453079 3.450977 -0.869904
C 4.866963 -1.752307 0.855341	H -4.595812 3.275880 -2.736759
C 5.405480 -0.802423 -1.273919	H -2.078965 4.164144 -1.107991
C 6.247380 -1.401259 1.406020	H -2.196183 3.966028 -2.972520
H 4.833529 -2.816143 0.493438	C 2.990389 -1.008747 -0.398410
H 4.167308 -1.709570 1.715795	H 2.707033 -2.015809 -0.787292
C 6.793425 -0.396899 -0.785978	H 2.737511 -0.273970 -1.190514
H 5.446255 -1.783949 -1.821242	C 4.978603 -2.077271 0.565836
H 5.098635 -0.046532 -2.026704	C 5.243279 -0.596214 -1.296837
H 6.598158 -2.143105 2.150488	C 6.408584 -1.809662 1.030526
H 6.216881 -0.400130 1.879163	H 4.919964 -3.018756 -0.045492
H 7.539923 -0.388214 -1.602269	H 4.387645 -2.282501 1.482771
H 6.746527 0.613891 -0.334821	C 6.670227 -0.255760 -0.876521
N 4.459291 -0.799511 -0.167156	H 5.239156 -1.404829 -2.077725
N 7.322171 -1.315689 0.316450	H 4.831349 0.307676 -1.792405
C 8.560265 -0.702147 0.913660	H 6.860453 -2.697699 1.515201
H 8.928715 -1.353756 1.727873	H 6.416743 -0.964383 1.746026
H 9.334245 -0.598852 0.132857	H 7.314394 -0.003975 -1.739885
H 8.307981 0.295345 1.317642	H 6.656144 0.605397 -0.179550
C 7.643194 -2.729995 -0.194742	N 4.435575 -0.920037 -0.129489
H 8.026700 -3.271435 0.693725	N 7.344827 -1.395705 -0.110850
H 6.674989 -3.190344 -0.466231	C 8.631140 -0.890534 0.486656
C 8.623545 -2.815412 -1.357090	H 9.114972 -1.710835 1.049270
H 9.615061 -2.374281 -1.133458	H 9.300389 -0.538470 -0.318191
H 8.794544 -3.890932 -1.566378	H 8.403765 -0.051967 1.170068
H 8.230816 -2.369329 -2.291798	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	Ci1
108	108
PENJOLL-TScon+ SCF Done: -2905.77136054 A.U.	PENJOLL-Ci1+ SCF Done: -2905.79069465 A.U.
C -0.071550 0.459862 0.006261	Ru -1.813609 1.408301 -0.312015
C 2.212074 -0.055549 0.382874	C 0.080675 0.857063 0.094935
H 2.393523 0.013017 1.483307	N 1.045974 1.819424 0.248030
C 2.111143 1.350763 -0.216099	N 0.717490 -0.364539 0.117143
H 2.660823 2.116059 0.366763	C 2.168602 -0.241574 0.408494
H 2.492654 1.382382 -1.265739	C 2.408021 1.273178 0.279304
C 0.752642 -2.752826 1.338986	H 2.346413 -0.580930 1.458578
C 0.676867 -4.158231 1.251675	H 2.983591 1.702405 1.125354
H 0.761259 -4.747530 2.180231	H 2.956334 1.520888 -0.659372
C 0.494326 -4.827040 0.025078	C 0.107201 -1.664457 0.257291
C 0.387094 -4.044110 -1.142518	C 0.848344 3.249404 0.329785
H 0.254087 -4.544695 -2.116308	C 0.989494 4.060705 -0.830826
C 0.447780 -2.635217 -1.117134	C 0.788190 5.449728 -0.695031
C 0.624148 -1.995744 0.141558	C 0.510320 6.053470 0.546527
C 0.965660 -2.088091 2.679530	C 0.489900 5.230157 1.689919
H 0.743336 -2.791441 3.505922	C 0.673769 3.836174 1.615076
H 0.312985 -1.195279 2.796323	C 1.428663 3.496794 -2.161535
H 2.022365 -1.761661 2.817161	H 0.871867 6.081224 -1.595328
C 0.383296 -6.333635 -0.034436	C 0.248784 7.538264 0.651624
H -0.676925 -6.656132 0.061019	H 0.333968 5.686759 2.681509
H 0.944259 -6.820823 0.788353	C 0.704792 3.010238 2.877142

H	0.757652	-6.735571	-0.997663	H	0.882793	2.567952	-2.425965
C	0.318620	-1.851267	-2.398963	H	2.520835	3.277141	-2.152603
H	0.354279	-2.521808	-3.279349	H	1.257011	4.229924	-2.973900
H	1.121942	-1.091619	-2.509882	H	0.753878	8.103852	-0.157118
H	-0.637088	-1.279563	-2.434434	H	0.585200	7.946736	1.626042
C	0.201884	2.967391	-0.321248	H	-0.839614	7.752318	0.568935
C	0.104690	3.788093	0.836707	H	0.792535	3.660358	3.769468
C	-0.289790	5.129987	0.667529	H	1.557066	2.297872	2.887161
H	-0.381776	5.768826	1.561933	H	-0.230430	2.415320	2.967974
C	-0.552993	5.680584	-0.603514	C	-0.094830	-2.481499	-0.888282
C	-0.372423	4.856071	-1.731520	C	-0.218064	-2.128759	1.561181
H	-0.530454	5.277593	-2.738244	C	-0.586939	-3.787275	-0.689746
C	0.018412	3.505243	-1.623984	C	-0.696631	-3.447583	1.698936
C	0.438686	3.256576	2.210202	C	-0.877591	-4.298197	0.590983
H	0.286163	4.036121	2.982014	C	-1.395434	-5.709430	0.757078
H	1.502504	2.935347	2.273639	H	-0.757075	-4.423433	-1.574673
H	-0.179915	2.369691	2.476173	C	-0.140705	-1.220215	2.767138
C	-1.017177	7.111567	-0.749302	H	-0.949806	-3.814306	2.707843
H	-0.747017	7.532668	-1.738363	C	0.175360	-1.985782	-2.290832
H	-0.588079	7.764968	0.037228	H	-0.138631	-0.929797	-2.429052
H	-2.123637	7.177708	-0.657271	H	-0.370380	-2.605618	-3.029001
C	0.234672	2.678883	-2.867785	H	1.253706	-2.053365	-2.555923
H	0.160347	3.308240	-3.775804	H	-0.885541	-0.394056	2.693915
H	-0.527641	1.870717	-2.938960	H	0.850345	-0.731736	2.882520
H	1.233609	2.192270	-2.877156	H	-0.346208	-1.781853	3.699132
C	-2.335515	-1.277435	0.342109	H	-1.543953	-5.970985	1.823446
H	-1.788252	-1.858646	1.114658	H	-0.696135	-6.453168	0.318951
C	-3.407836	-2.006230	-0.344540	H	-2.367188	-5.843311	0.235673
C	-3.157484	-3.301488	-0.872278	C	-2.602339	-0.291389	-0.203499
H	-2.160208	-3.744591	-0.730577	Cl	-1.225770	1.402386	-2.657738
C	-4.135779	-3.990167	-1.601595	Cl	-2.364890	1.863429	1.992389
H	-3.906893	-4.979641	-2.027446	O	-4.290412	-2.037327	1.022233
C	-5.404864	-3.413098	-1.791907	C	-5.236566	-2.641771	1.950976
H	-6.174811	-3.942389	-2.375120	C	-6.631293	-2.016409	1.857223
C	-5.697038	-2.163854	-1.222226	H	-4.795240	-2.326185	2.919725
C	-4.719714	-1.466842	-0.489026	C	-5.212622	-4.174761	1.921787
N	0.833107	-0.572745	0.175368	H	-5.737814	-4.608266	1.047873
N	0.666797	1.609090	-0.169377	H	-5.710618	-4.564716	2.833463
Cl	-1.651829	0.396943	2.589508	H	-4.167749	-4.544171	1.919630
Cl	-2.390034	0.489938	-2.249112	H	-6.563946	-0.911148	1.904747
Ru	-2.032351	0.545393	0.136205	H	-7.242391	-2.357287	2.718109
H	-6.689752	-1.704533	-1.340696	H	-7.171985	-2.293493	0.930828
O	-5.037038	-0.263236	0.099644	C	-4.439221	-1.968886	-0.323070
C	-5.623454	-0.262363	1.459121	C	-3.577413	-1.020638	-0.995718
C	-3.411312	2.482031	-0.229278	C	-5.358015	-2.730079	-1.079561
C	-3.166007	2.528145	1.120520	C	-5.441081	-2.565698	-2.471542
H	-4.303129	1.985466	-0.642135	C	-4.617087	-1.641470	-3.140727
H	-2.801370	3.062417	-0.939671	C	-3.710061	-0.873364	-2.404119
H	-2.360390	3.146851	1.540724	H	-6.169457	-3.169305	-3.036844
H	-3.846712	2.068958	1.852706	H	-6.017648	-3.454526	-0.586443
C	-6.560634	0.941105	1.515270	H	-3.048374	-0.145110	-2.899510
H	-6.047530	1.869444	1.196305	H	-4.689748	-1.517594	-4.232067
H	-6.929627	1.091560	2.550519	C	-3.194081	3.131891	-0.921877
H	-7.435750	0.786199	0.850592	C	-4.097497	2.099684	-0.769576
C	-6.328399	-1.562938	1.839870	H	-2.352020	-0.810971	0.743511
H	-4.766067	-0.110787	2.156013	H	-4.585596	1.909865	0.198854
H	-7.207190	-1.766449	1.194038	H	-4.473186	1.546965	-1.643510
H	-6.689149	-1.470071	2.884903	H	-2.976443	3.812861	-0.079420
H	-5.650851	-2.438317	1.795424	H	-2.853363	3.439462	-1.923646
C	3.299692	-0.929194	-0.260638	C	3.044563	-1.081913	-0.535118
N	4.632160	-0.310236	-0.141426	H	2.715779	-2.150484	-0.510682
H	3.071650	-1.036183	-1.341206	H	2.890756	-0.715568	-1.570677
H	3.278998	-1.958505	0.174407	C	4.900273	-1.730502	0.938306
C	5.587277	-0.764516	-1.142560	C	5.368652	-1.172096	-1.340265
C	5.211743	-0.401932	1.191436	C	6.313952	-1.343644	1.366478
C	6.831993	0.117247	-1.121937	H	4.817282	-2.837560	0.761549
H	5.141541	-0.663816	-2.154207	H	4.242199	-1.518677	1.806850
H	5.863698	-1.848826	-1.033300	C	6.787710	-0.736868	-0.984723
C	6.460504	0.470877	1.298293	H	5.357539	-2.233654	-1.710871
H	5.428388	-1.461584	1.497424	H	5.048807	-0.545301	-2.198773
H	4.495552	-0.014497	1.945557	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
C	3.025549	0.123396	-0.040572	H	1.876530	-5.963301	0.155148
Cl	1.508995	2.072015	2.289931	C	3.524646	0.407444	-0.280110
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
H	2.689377	3.901525	0.524593	H	2.701465	3.479398	-1.235397
C	-2.987789	-0.980729	0.385732	H	2.771666	3.723073	0.613651
N	-4.409483	-1.097471	0.019116	N	-4.503784	-1.120647	0.154480
H	-2.913686	-0.307617	1.264712	H	-3.069509	-0.729558	1.637972
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
C	-4.704583	-2.248934	-0.822062	C	-4.765287	-2.002609	-0.974174
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
H	-4.524563	-3.226322	-0.296738	H	-4.615946	-3.087286	-0.720052
H	-4.031064	-2.258992	-1.704160	H	-4.050920	-1.788719	-1.796234
N	-7.186755	-2.045427	-0.267436	N	-7.269701	-1.903723	-0.493930
H	-6.390034	-3.063871	-1.971294	H	-6.400127	-2.453179	-2.370286
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
C	-7.307124	-3.384791	0.477128	C	-7.437643	-3.390333	-0.139362
C	-8.249487	-3.404992	1.673155	C	-8.437401	-3.709344	0.964011
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 PENJOLL-TS2+ SCF Done: -2905.78053899 A.U.				108 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
C	3.634235	-1.606676	3.751624	C	-6.685897	-1.821647	1.063455
C	3.389909	-0.411737	3.064675	C	-5.460079	-1.987894	0.410196
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

C	-4.584418	-2.414528	-0.863889	C	5.854973	-0.412173	0.390368
C	-4.828372	-1.355048	1.271191	C	5.397796	1.041056	-1.453888
C	-6.084499	-2.304671	-1.130966	C	7.029525	0.456580	0.836655
H	-4.319563	-3.428379	-0.456381	H	6.205070	-1.274683	-0.239814
H	-4.085901	-2.353706	-1.853945	H	5.437765	-0.868039	1.312368
C	-6.330063	-1.187919	1.061973	C	6.534316	1.977093	-1.053574
H	-4.610298	-2.277520	1.875204	H	5.737743	0.313041	-2.240384
H	-4.493666	-0.498071	1.892413	H	4.618559	1.668965	-1.934102
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
N	-4.130660	-1.328600	-0.007766	N	4.841510	0.393744	-0.273772
N	-6.920661	-2.267240	0.153541	N	7.659085	1.252670	-0.312297
C	-8.331966	-1.887217	-0.204507	C	8.596352	2.275478	0.272329
H	-8.758237	-2.662070	-0.868879	H	9.396107	1.755431	0.831965
H	-8.936300	-1.804638	0.715978	H	9.036798	2.880660	-0.539685
H	-8.319951	-0.912548	-0.725720	H	8.028792	2.933066	0.955911
C	-6.909442	-3.658486	0.807472	C	8.446184	0.292488	-1.220714
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
TS_I14e				I14e			
108 PENJOLL-TS3+ SCF Done: -2905.76875751 A.U.				82 PENJOLL-14e2+ SCF Done: -2403.34511303 A.U.			
Ru	1.854666	-0.044646	-0.192670	Ru	2.856638	0.390341	-0.916519
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
H	-1.036116	-2.520074	-2.585212	H	-0.756185	-2.749574	-1.442631
H	0.026085	-3.734188	-3.367048	H	0.206073	-3.854617	-2.471353
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	0.358442	1.304941	3.013001
H	-0.870036	3.062472	2.865060	H	1.403572	2.594746	3.680060
H	-0.177575	1.506092	2.291779	H	2.085710	1.392935	2.541559
H	-1.495211	6.744443	-0.173524	H	0.548110	7.250753	0.005083
H	-1.514605	6.492968	-1.954036	H	2.105530	6.905345	0.814089
H	0.036215	6.576174	-1.075893	H	0.618349	7.041320	1.788701
C	3.427942	2.459548	-0.365182	Cl	1.883585	0.195256	-3.029845
Cl	2.180902	-0.048464	-2.571900	Cl	3.947694	1.821972	0.541511
Cl	1.937854	0.173432	2.188770	C	3.841939	-1.121494	-0.790828
O	4.619063	0.059838	-0.165790	H	4.808093	-1.068570	-1.356195
C	5.424255	-0.758186	-1.084973	H	3.642410	-2.060309	-0.239578
C	6.479039	0.074066	-1.811690	C	-2.077392	0.343491	-0.379520
H	4.651355	-1.066261	-1.820353	H	-2.220042	1.380445	-0.766230
C	5.983722	-2.009649	-0.401862	H	-1.686184	-0.262785	-1.222551
H	6.849161	-1.787588	0.255264	C	-4.171530	0.662785	0.850429
H	6.330721	-2.726940	-1.174765	C	-4.137913	-0.839444	-1.012355
H	5.203443	-2.511609	0.204681	C	-5.360748	-0.067022	1.470622
H	6.017515	0.943882	-2.320168	H	-4.510654	1.556769	0.259534
H	6.968613	-0.551641	-2.585939	H	-3.581062	1.072420	1.696285
H	7.268298	0.444603	-1.126233	C	-5.304808	-1.638133	-0.438245
C	5.177607	1.026023	0.645977	H	-4.501302	-0.084414	-1.761626
C	4.513476	2.278539	0.618718	H	-3.508936	-1.555486	-1.581616
C	6.246652	0.799733	1.531869	H	-6.024457	0.624220	2.026633
C	6.660730	1.831059	2.393184	H	-5.001503	-0.854651	2.161547
C	6.000126	3.072387	2.392196	H	-5.925685	-2.103091	-1.226626
C	4.927363	3.288657	1.513068	H	-4.916543	-2.434201	0.227382
H	7.499486	1.651961	3.084392	N	-3.351904	-0.247878	0.062963
H	6.733928	-0.183538	1.572603	N	-6.228601	-0.786284	0.432891
H	4.418298	4.265226	1.486422	C	-7.190626	-1.691661	1.155509
H	6.325893	3.873622	3.073338	H	-7.842701	-1.080035	1.806711
C	2.343301	-1.801655	-0.075993	H	-7.802723	-2.242791	0.419633
C	2.235460	3.053126	-0.111655	H	-6.616799	-2.409725	1.769554
H	3.615992	2.076119	-1.384173	C	-7.017711	0.254791	-0.380962
H	1.502617	3.214521	-0.916281	H	-7.674873	0.753121	0.360186
H	1.977548	3.412633	0.897387	H	-6.282481	1.006182	-0.724316
H	2.542380	-2.284473	0.906538	C	-7.821652	-0.286259	-1.555761
H	2.644461	-2.384570	-0.976075	H	-8.571159	-1.048544	-1.264910
C	-3.571845	0.405583	-0.605496	H	-8.385426	0.563897	-1.990639
H	-3.554709	1.523396	-0.619027	H	-7.186082	-0.693810	-2.366405
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				

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
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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
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C	28.6147666020	12.7581374811	23.0899712123	C	28.8719316900	12.6966374296	23.0901179375
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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
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C	20.0535279478	14.4038812938	22.8651771816	C	20.3498139207	14.3031682085	22.8707799808
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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
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C	24.9603981896	15.2615243231	12.6962198700	C	25.1984441835	15.1780626665	12.6888629472
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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
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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
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H	27.8769625752	20.0922864781	18.6435139043	H	28.1132999600	20.0432258365	18.6498635196
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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
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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
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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
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H	20.7988430049	9.5698483044	17.9050243653	H	21.0641795421	9.4796102231	17.9648272513
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C	22.3798950912	7.5262872810	18.4074854745	C	22.6568442197	7.4481909168	18.4096688851
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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
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H	21.2167241172	14.9708972459	26.3673623600	H	21.5272657083	14.8782914581	26.3664765871
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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
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O	19.3733844201	24.1153002642	16.0368158946	O	19.6050672164	24.0374232495	16.0341690159
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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	7.7099612270	26.5000230427	17.2511388736	H	16.0587867328	16.8105120562	16.2857794612
C	13.1290468631	23.9941022283	16.9101130056	H	15.4663268190	14.6877981005	16.0965039771
C	9.6059760204	19.5957710053	16.3246614675	H	17.1171956319	14.1970995463	15.6361083398
H	6.6192217684	26.5765854244	17.3199610850	C	16.0937770068	14.3365613337	15.2686964947
H	15.7263440252	16.9156910875	16.3009975913	H	14.1410657555	18.3503816299	15.9313247188
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C	15.8347088442	14.4654523643	15.2535300675	H	16.5781427625	18.3191421797	15.5100981688
H	13.7977865683	18.4386484762	15.9217831135	H	14.3976036797	26.3850047531	16.3812499422
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	15.4961458186	13.4692486642	14.9327126184	C	13.6414551519	24.5392422443	15.5852400113
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C	8.2174450328	26.3929688393	15.8171506398	C	14.1627082171	25.8375331276	15.4696949566
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C	9.2603131780	19.4447942725	14.8606417633	C	8.4338995470	18.5133997843	14.5393473733
H	13.5789360700	16.9435765890	15.0052219496	N	16.6087976753	16.6403643071	14.2383709715
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C	13.8122912119	25.9170255450	15.4498180193	C	12.6437023602	20.1808709051	14.4890823038
H	5.4058711515	26.1501720790	15.6245126096	C	13.6274042258	21.3502901738	14.3631988772
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C	15.7723410281	15.3882304030	14.0439150240	C	10.1768105883	20.0490561561	13.8700756253
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C	12.3736197245	20.3115821455	14.4819233364	C	13.0073870993	19.0005197204	13.5805398434
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H	3.3373103472	24.9816607948	14.9713609650	H	16.5755767634	14.8187759170	13.2058288858
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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H	8.2212610688	28.4546131228	15.2302561427	C	14.9528550457	27.8386906155	14.1406170473
C	6.7815412129	23.2649335041	14.3464302858	H	16.9875697979	18.3784071920	13.1232314978
C	11.0831027212	22.3019449439	14.2793710213	C	14.9420541922	17.8060967534	12.7174812385
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C	4.3444170893	23.2289176419	14.2095167742	C	13.6016885991	24.3997239732	13.1306619416
C	12.9569463196	23.9633134357	14.3470655420	C	9.7666587725	19.9292094380	12.5217396226
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
C	9.9399244842	20.1281151409	13.8357161118	Cl	10.2710173510	24.9541527184	12.9025031849
H	14.7399184312	15.5011660523	13.6987560344	C	8.6931884158	19.0799769340	12.223184305
C	5.5775586137	22.6187349897	13.9886479806	H	12.9740467446	19.3450864006	12.5379550020
H	6.7085199883	27.6366893441	14.8066423161	H	16.8383037288	16.8913203968	12.1418201021
C	12.7432203001	19.1456779042	13.5644893524	H	14.9207545691	18.4556902145	11.8291766833
C	14.0854260920	26.5162919425	14.2164200080	C	13.3628534888	23.6361781846	11.8523300462
H	16.3597488624	14.9834990195	13.2103407130	C	10.4368242851	20.7023044530	11.4134945250
H	11.9884815908	18.3408230883	13.6328452508	H	14.3524889665	26.1239521260	12.0997218959
H	3.4232182495	22.7246283536	13.9279948306	H	8.3784768032	18.9821888556	11.1844634235
C	7.7924155422	18.4665999844	13.1615346333	H	4.4123839477	20.1937981352	15.7634787869
C	16.1489834650	17.6245150631	13.0070652279	H	6.3002578182	26.6466629179	15.8669373652
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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H	16.6069525058	17.0697741145	12.1791996651	H	3.4634212210	22.4900561603	12.7956585457
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C	13.1276111804	23.7293231799	11.7923936419	H	4.7382154038	21.8094646026	11.7621105812
C	10.2525363115	20.7699369814	11.3636711837	C	8.4351189062	22.7826103774	14.3994909808
H	14.0790224945	26.2153700905	12.0822539613	H	8.2975004301	21.7788090451	13.9937458205
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H	12.5057784200	24.6062687596	17.5767690990	H	12.8723404352	24.5330912695	17.6045936853
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H	10.4153813545	20.3092839408	16.5089766254	H	6.6799582605	17.4263820015	11.7811409098
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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	27.3628862921	16.9677417642	16.7197033781	O	27.6848097078	17.0286097984	16.7172032658
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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	22.5957811863	11.4338266106	17.7761012076	C	22.9559295799	11.4451334265	17.7826673142
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C	27.1274411264	15.3725864429	20.1232503969	C	27.4884412797	15.4241615273	20.1246100909
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H	28.8943342356	17.9376787161	15.0857374628	H	29.2461302885	17.9895502034	15.1053015482
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H	25.0618070789	19.0019724062	21.3103364360	H	25.3243973110	19.0317207627	21.3281709363
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H	31.0647480890	11.5983586643	22.8949494874	H	31.4079080536	11.6105795073	22.9147342567
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O	31.1805206766	23.1743767595	15.8627669165	O	31.4995358468	23.2502063185	15.8670748365
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H	21.6809654834	15.2131104221	26.3838012871	H	22.0063301496	15.1692050355	26.3740924405
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
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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	15.7941558860	13.6530238651	17.0991281320	H	13.8860514743	21.0074099998	13.8835140164
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H	18.2220673061	17.7754872629	15.5060635887	C	9.6838912226	18.6867891331	13.6207428474
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H	14.6017288420	17.8178538805	12.8011632428	H	17.0909688386	14.8074299370	14.3220385387
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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	16.4443829263	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	12.729378674	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	CI	7.7160355229	23.6874031668	12.3586250040
CI	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	15.566092291	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-SO₃⁻.

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	18.403538137900
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
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C	12.317860155000	11.984982777800	7.730623479400	C	17.348997243400	17.011527481000	12.693649247100
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C	11.063716043700	12.597466934500	5.748429821400	C	16.085564710000	17.659611318500	10.723756310700
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C	10.204177829300	15.579529083100	13.036388222600	C	15.137095138000	20.538848619500	17.947313349900
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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
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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	21.32309816800
H	12.015742991800	15.428890107500	16.427297033200	H	20.453247982900	15.895817055700	17.010502657900
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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
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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
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O	10.707128946300	3.346520390600	13.202356367200	H	16.565772380800	8.733175122400	17.827207705800

H	11.512493268900	3.727299957400	12.807035153200	H	14.137341668200	18.164413323300	25.072525024700
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H	6.698522628600	10.379775754600	17.855632145400	O	12.682391794400	16.489279205400	26.527708936300
O	7.723926308400	11.404080404100	21.495801928400	H	13.601005106300	16.781059300700	26.382182374900
H	8.652801311100	11.654583094300	21.339546354800	O	10.963707145600	15.787307294400	25.277131831200
O	5.935722302200	10.857785960400	20.242367287200	C	12.714075903800	25.769137854000	17.061727170400
C	7.698295250500	20.683292479800	12.046311047700	H	11.639017239000	23.274199565000	16.398733530900
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H	6.781432653200	19.956271083200	10.506601684200	O	12.995062547500	26.747260492400	17.731820202300
O	7.964871925800	21.650195786000	12.731580874400	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