

Supporting Information

For

MOF Encapsulation of Ru Olefin Metathesis Catalysts to Block Catalyst Decomposition

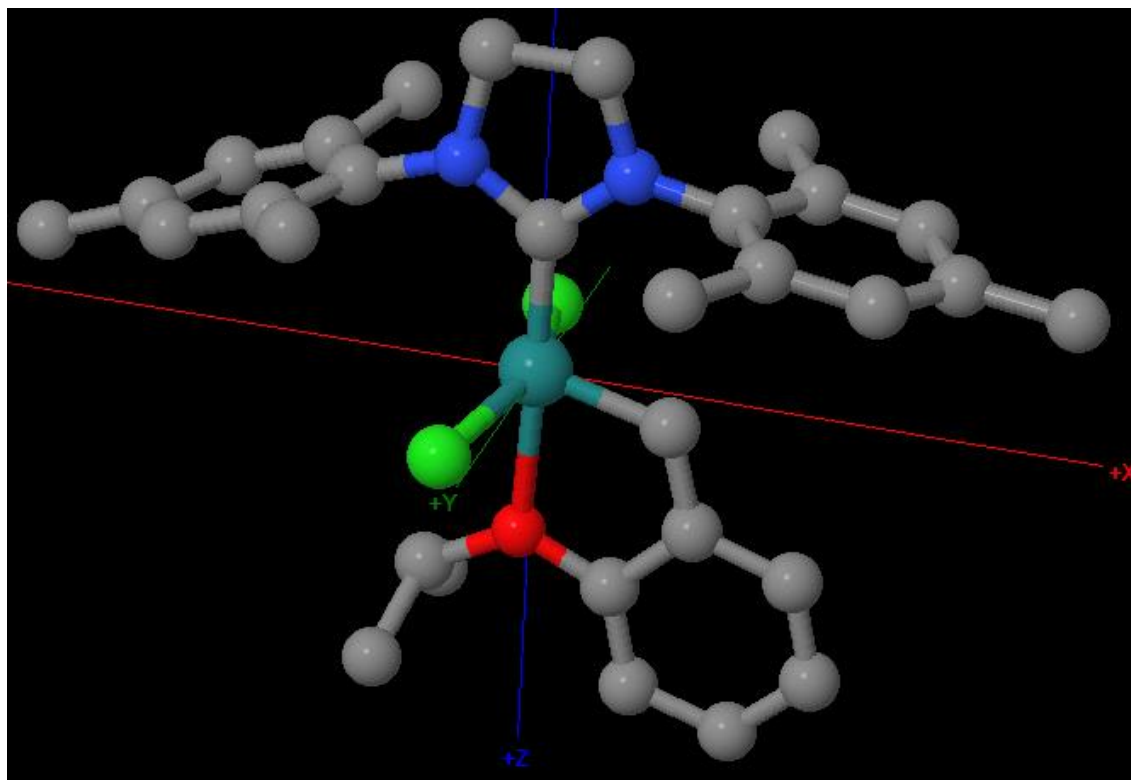
Gerard Pareras,¹ Davide Tiana,¹ and Albert Poater^{1,2,*}

¹ School of Chemistry, University College Cork, College Road, Cork, Ireland

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

Steric maps

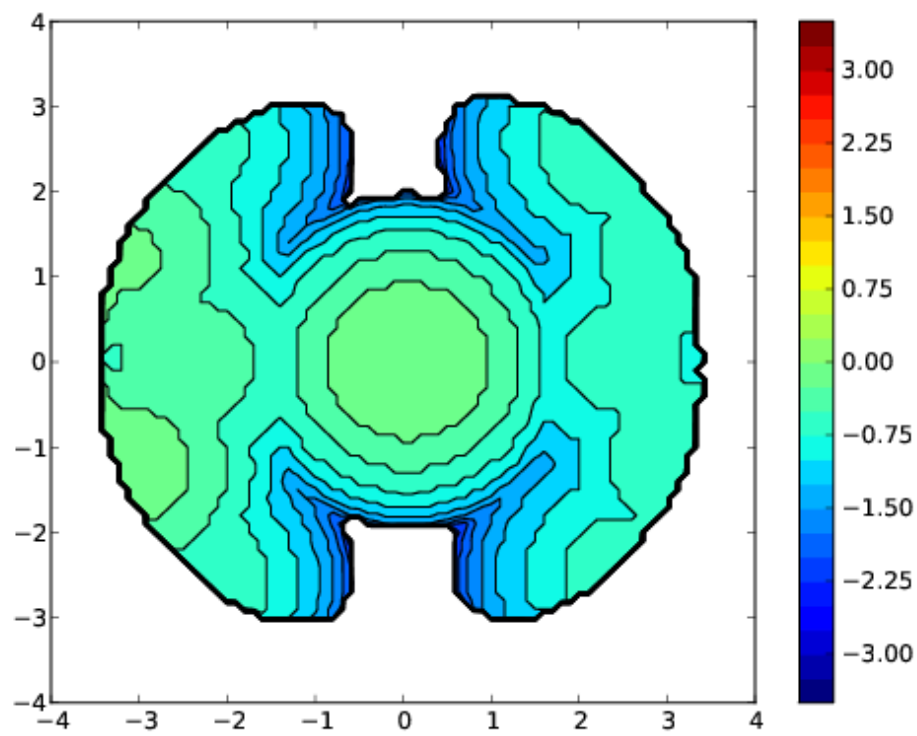
HOV



At 3.5 Å:

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

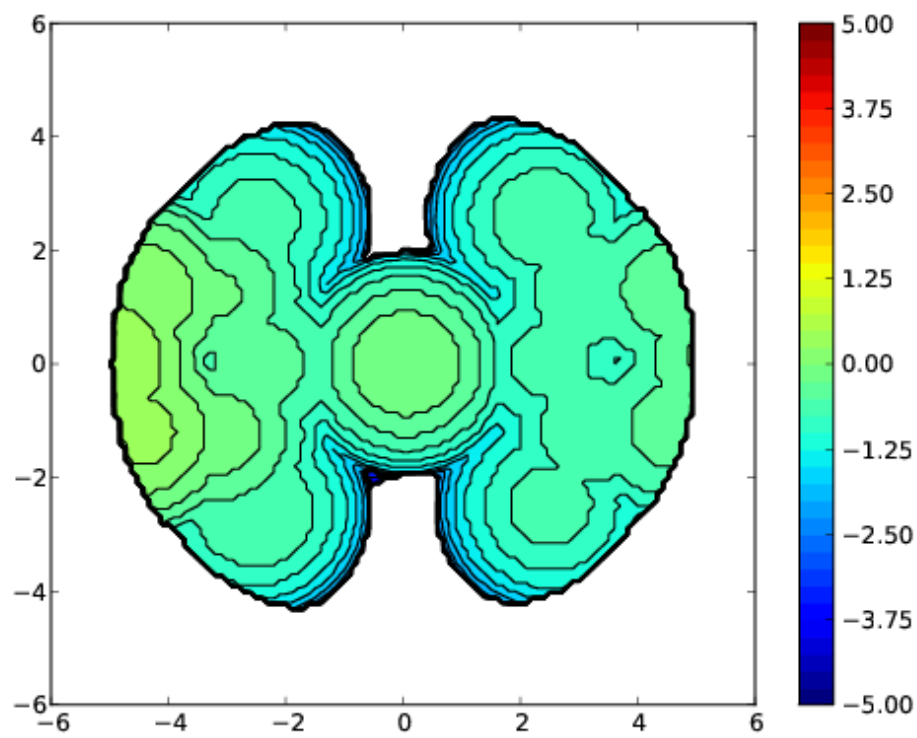
Quadrant	V f	V b	V t	%V f	%V b
SW	29.4	15.5	44.9	65.4	34.6
NW	29.7	15.2	44.9	66.2	33.8
NE	30.2	14.7	44.9	67.3	32.7
SE	30.8	14.0	44.9	68.7	31.3



At 5.0 Å:

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

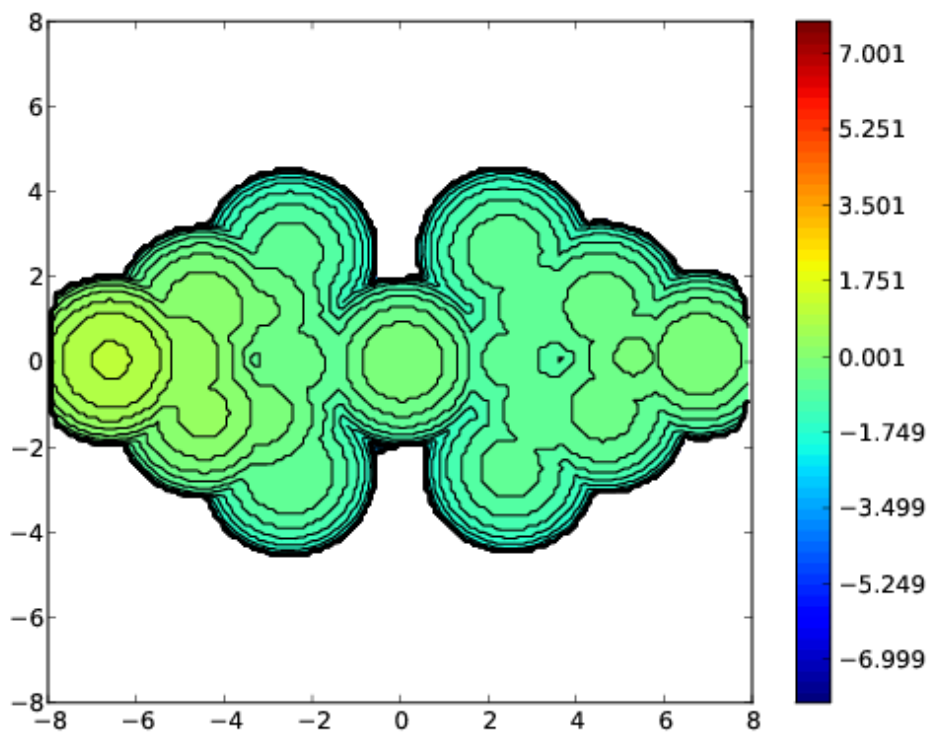
Quadrant	V f	V b	V t	%V f	%V b
SW	82.1	48.7	130.8	62.8	37.2
NW	83.6	47.2	130.8	63.9	36.1
NE	85.1	45.7	130.8	65.1	34.9
SE	87.4	43.5	130.8	66.8	33.2



At 8.0 Å:

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

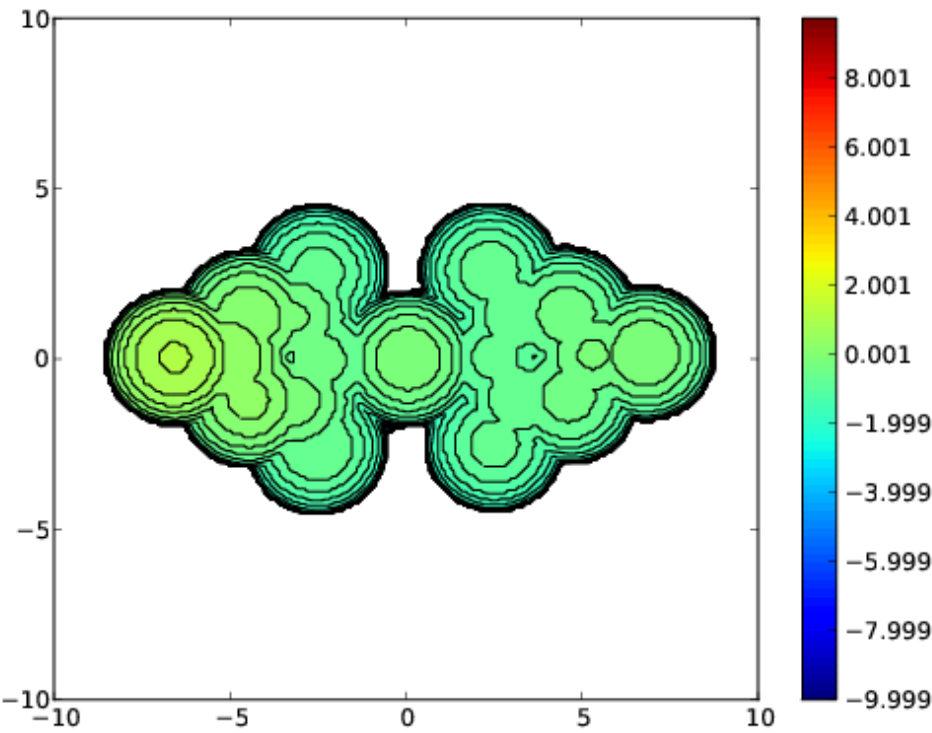
Quadrant	V f	V b	V t	%V f	%V b
SW	445.2	90.7	535.9	83.1	16.9
NW	446.4	89.5	535.9	83.3	16.7
NE	445.2	90.7	535.9	83.1	16.9
SE	451.3	84.7	535.9	84.2	15.8



At 10.0 Å:

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

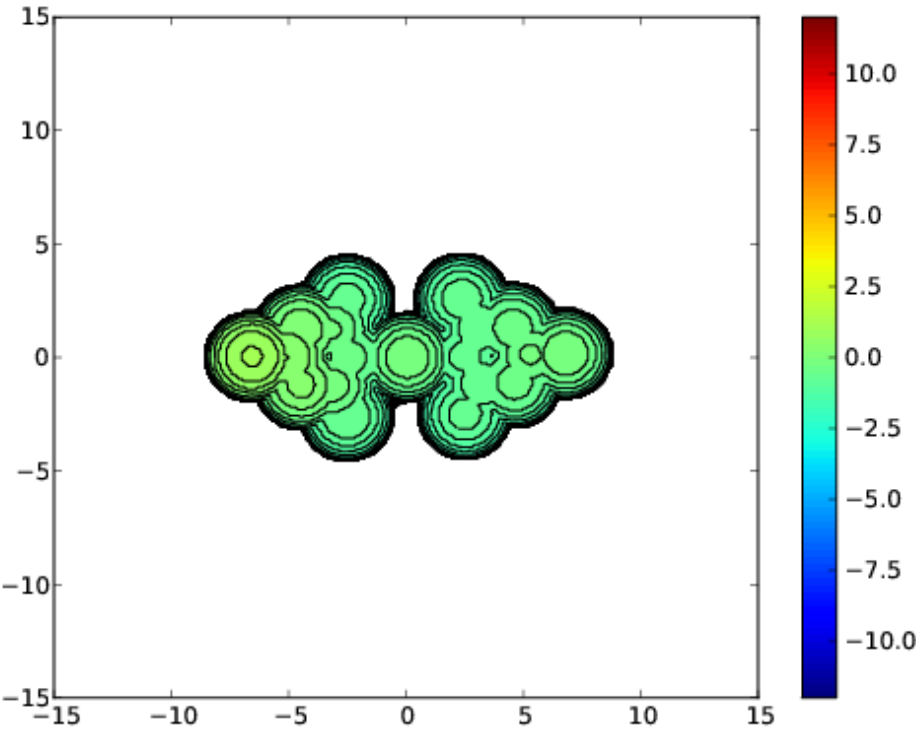
Quadrant	V f	V b	V t	%V f	%V b
SW	954.7	92.5	1047.2	91.2	8.8
NW	953.3	90.7	1044.0	91.3	8.7
NE	946.6	94.3	1040.9	90.9	9.1
SE	956.3	87.7	1044.0	91.6	8.4



At 12.0 Å:

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

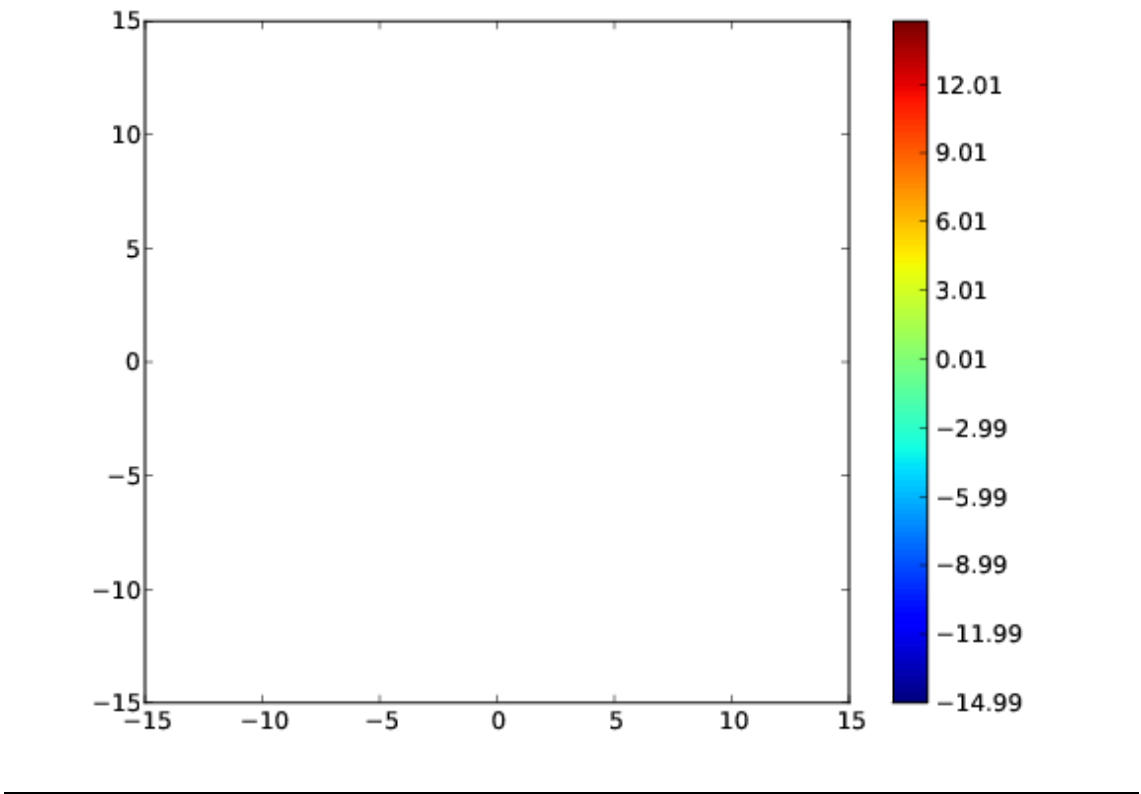
Quadrant	V f	V b	V t	%V f	%V b
SW	1717.1	92.0	1809.1	94.9	5.1
NW	1718.2	91.0	1809.1	95.0	5.0
NE	1714.4	94.7	1809.1	94.8	5.2
SE	1721.6	87.5	1809.1	95.2	4.8



At 15.0 Å:

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

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

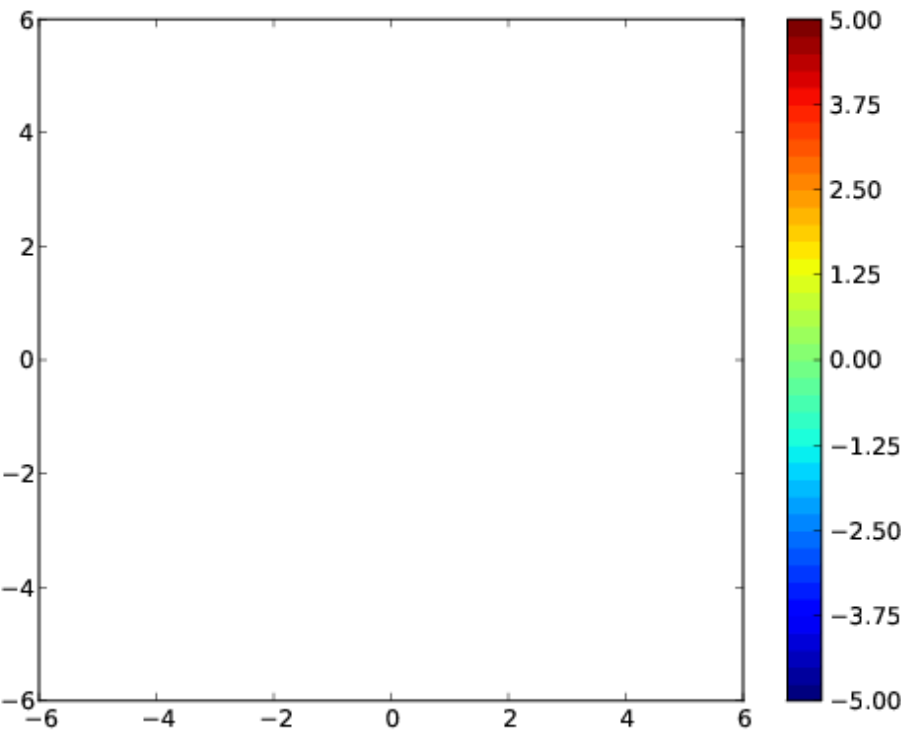


MOF without the Ru catalyst:

At 3.5 and 5.0 Å:

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

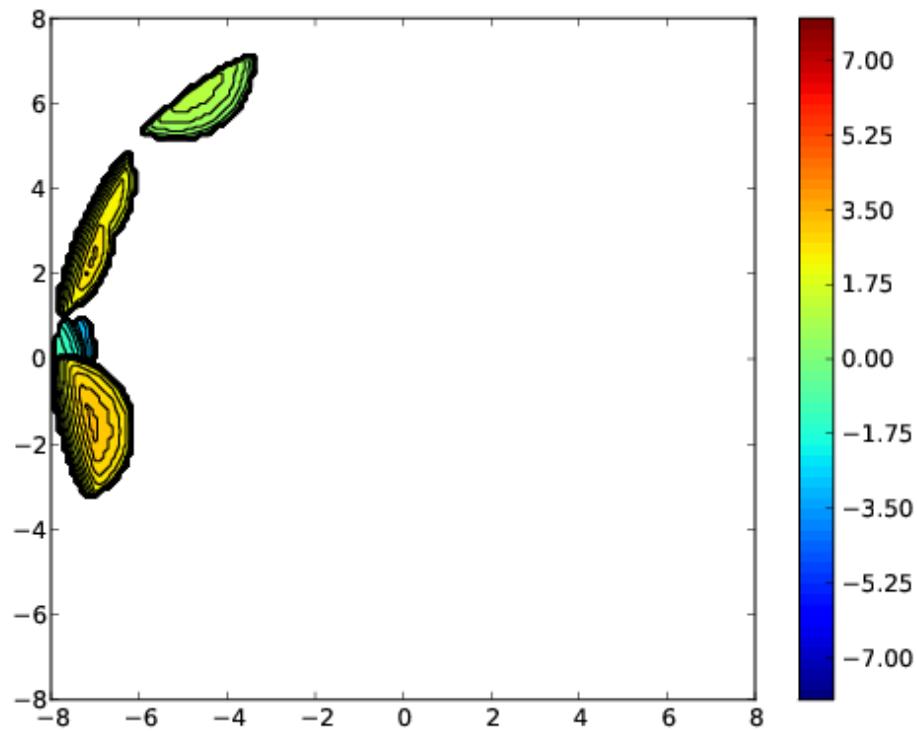
Quadrant	V f	V b	V t	%V f	%V b
SW	130.8	0.0	130.8	100.0	0.0
NW	130.8	0.0	130.8	100.0	0.0
NE	130.8	0.0	130.8	100.0	0.0
SE	130.8	0.0	130.8	100.0	0.0



At 8.0 Å:

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

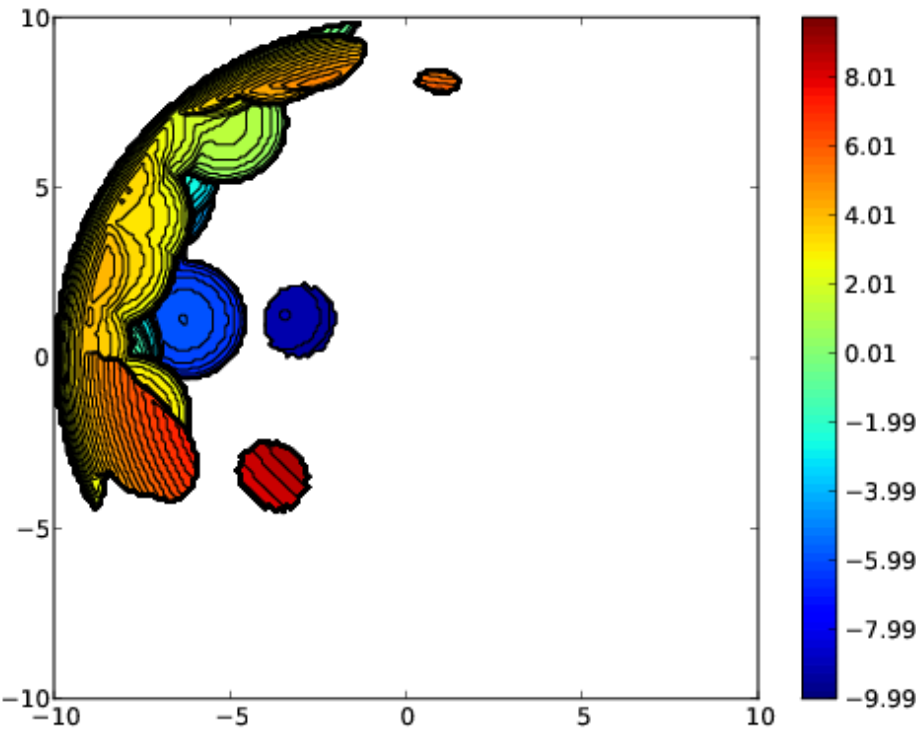
Quadrant	V f	V b	V t	%V f	%V b
SW	526.8	9.1	535.9	98.3	1.7
NW	525.2	10.7	535.9	98.0	2.0
NE	535.9	0.0	535.9	100.0	0.0
SE	535.9	0.0	535.9	100.0	0.0



At 10.0 Å:

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

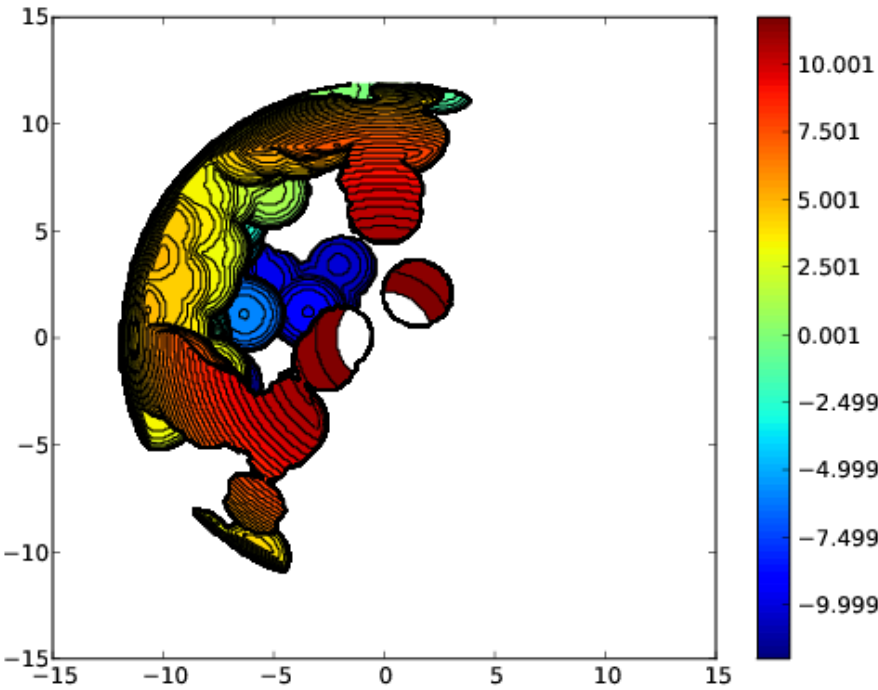
Quadrant	V f	V b	V t	%V f	%V b
SW	982.7	64.5	1047.2	93.8	6.2
NW	901.9	142.1	1044.0	86.4	13.6
NE	1040.8	0.1	1040.9	100.0	0.0
SE	1044.0	0.0	1044.0	100.0	0.0



At 12.0 Å:

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

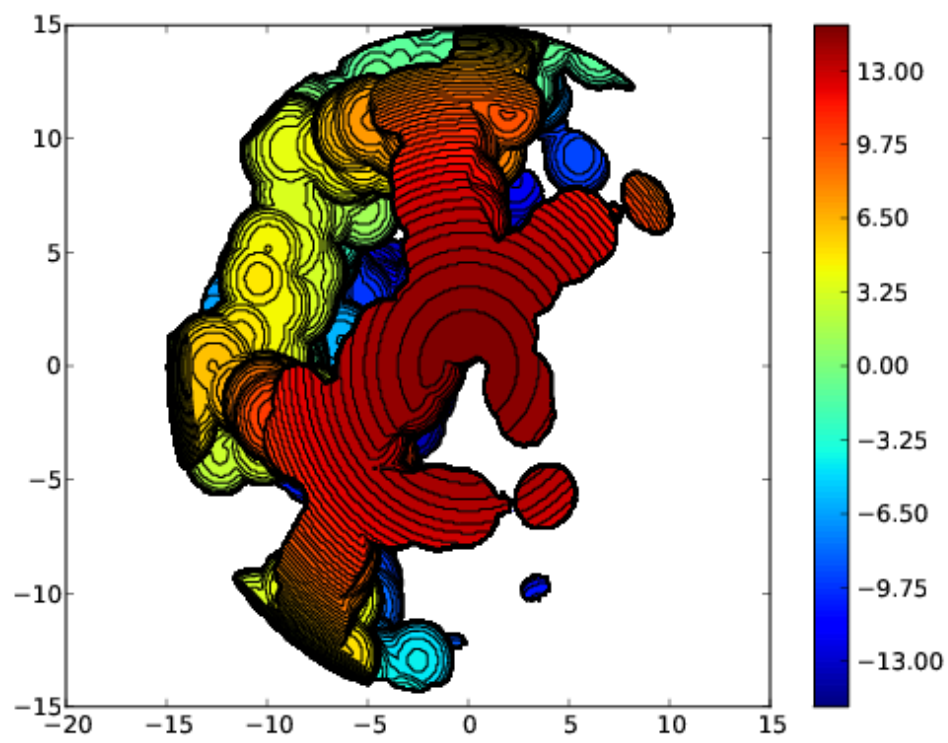
Quadrant	V f	V b	V t	%V f	%V b
SW	1578.4	230.8	1809.2	87.2	12.8
NW	1339.6	469.3	1808.9	74.1	25.9
NE	1774.2	34.4	1808.6	98.1	1.9
SE	1808.9	0.0	1808.9	100.0	0.0

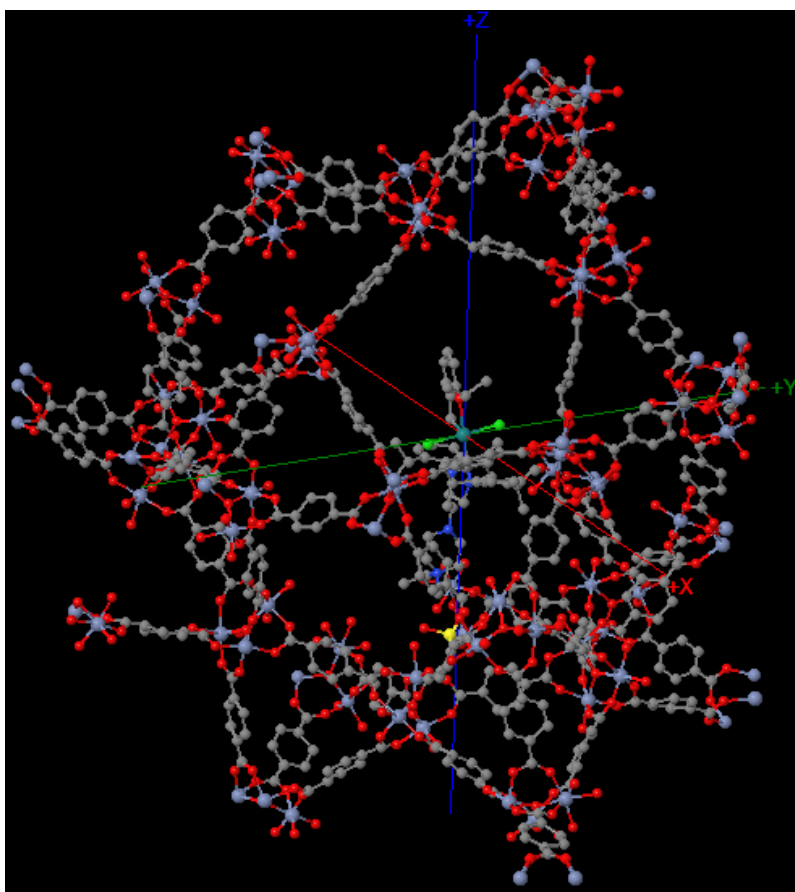


At 15.0 Å:

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

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

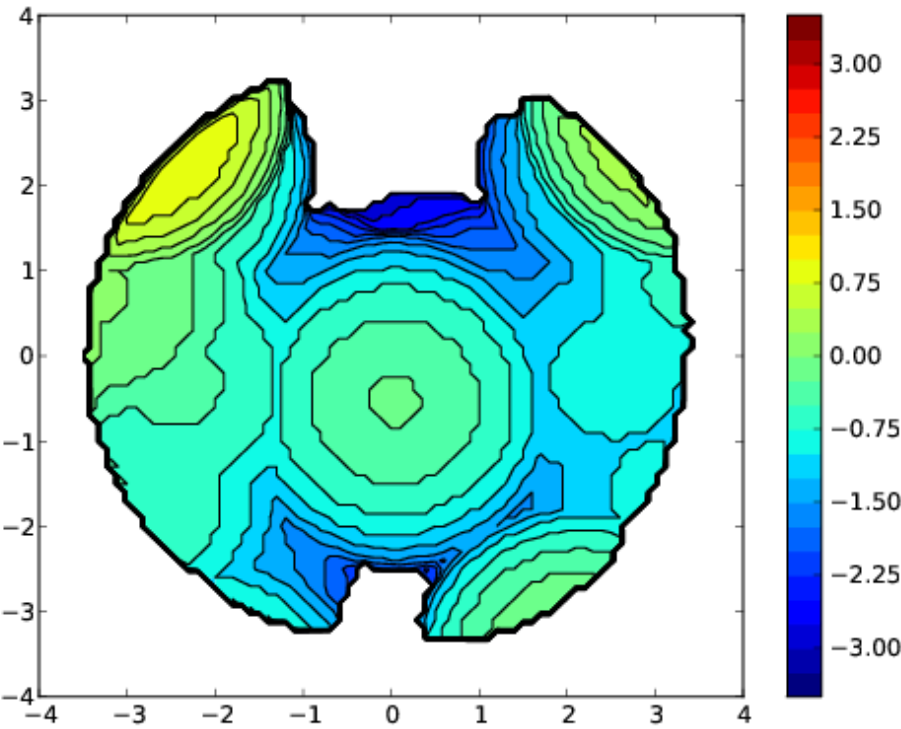




At 3.5 Å:

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

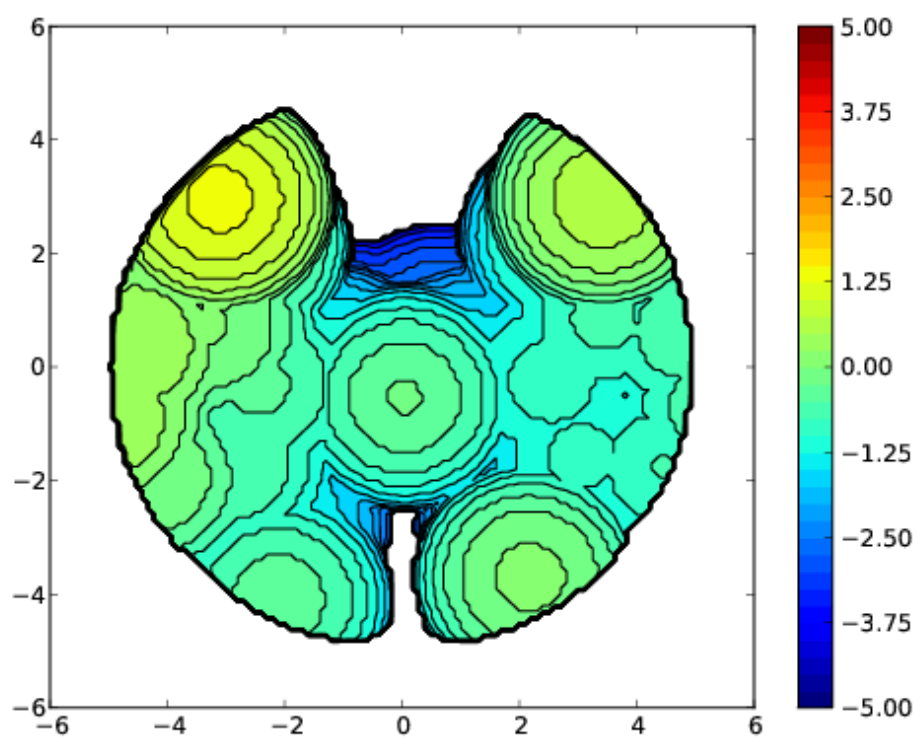
Quadrant	V f	V b	V t	%V f	%V b
SW	29.3	15.5	44.9	65.4	34.6
NW	28.3	16.6	44.9	63.1	36.9
NE	33.0	11.9	44.9	73.5	26.5
SE	29.8	15.1	44.9	66.4	33.6



At 5.0 Å:

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

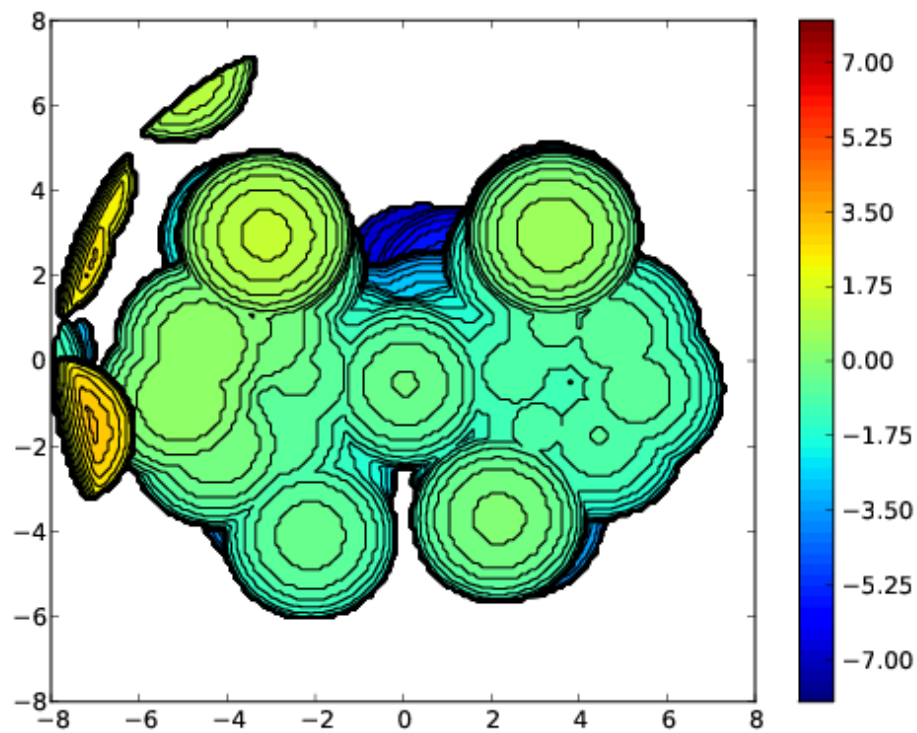
Quadrant	V f	V b	V t	%V f	%V b
SW	77.2	53.6	130.8	59.0	41.0
NW	74.6	56.2	130.8	57.0	43.0
NE	84.6	46.3	130.8	64.6	35.4
SE	79.9	50.9	130.8	61.1	38.9



At 8.0 Å:

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

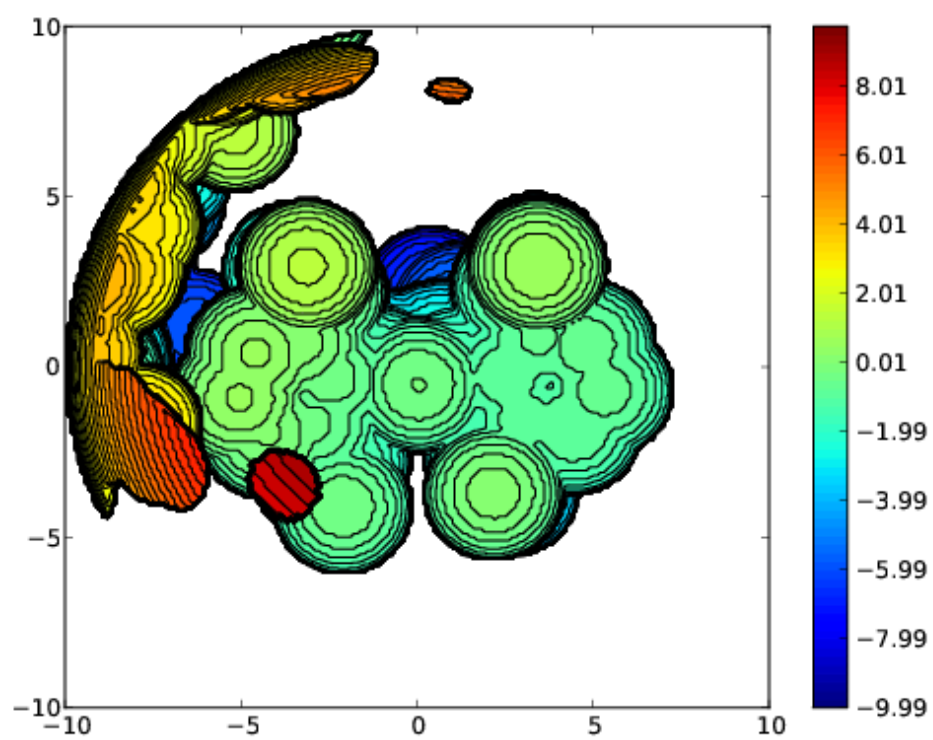
Quadrant	V f	V b	V t	%V f	%V b
SW	394.5	141.4	535.9	73.6	26.4
NW	414.1	121.8	535.9	77.3	22.7
NE	407.6	128.3	535.9	76.1	23.9
SE	395.8	140.1	535.9	73.9	26.1



At 10.0 Å:

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

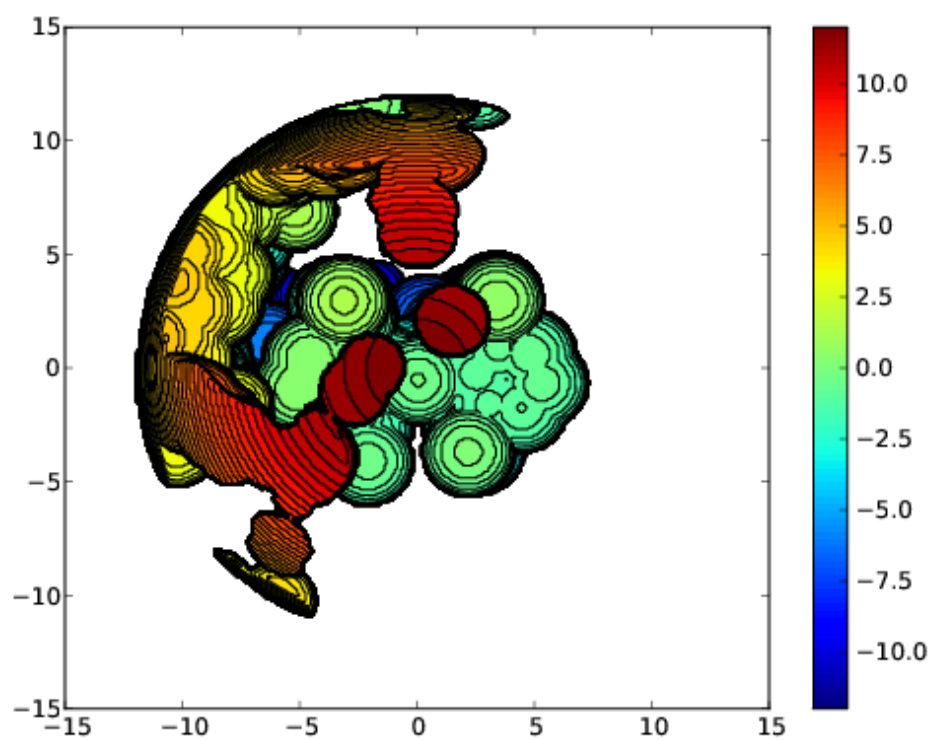
Quadrant	V f	V b	V t	%V f	%V b
SW	844.2	202.8	1046.9	80.6	19.4
NW	780.5	266.4	1046.9	74.6	25.4
NE	895.4	151.6	1046.9	85.5	14.5
SE	895.2	151.8	1046.9	85.5	14.5



At 12.0 Å:

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

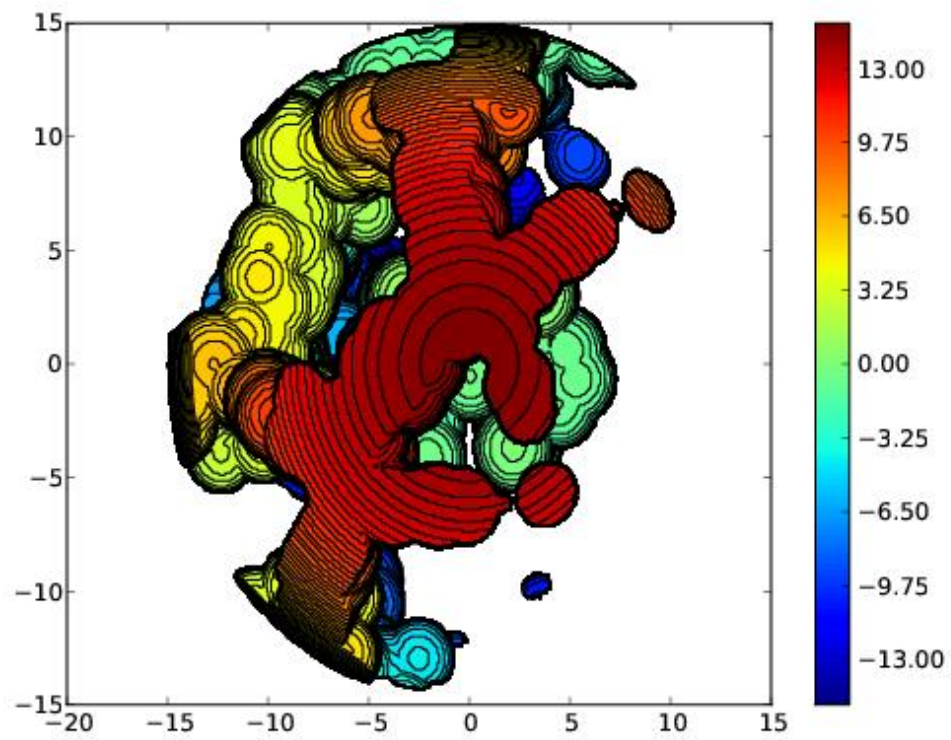
Quadrant	V f	V b	V t	%V f	%V b
SW	1439.1	370.3	1809.4	79.5	20.5
NW	1204.9	600.1	1805.0	66.8	33.2
NE	1583.8	216.7	1800.5	88.0	12.0
SE	1649.5	155.5	1805.0	91.4	8.6



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

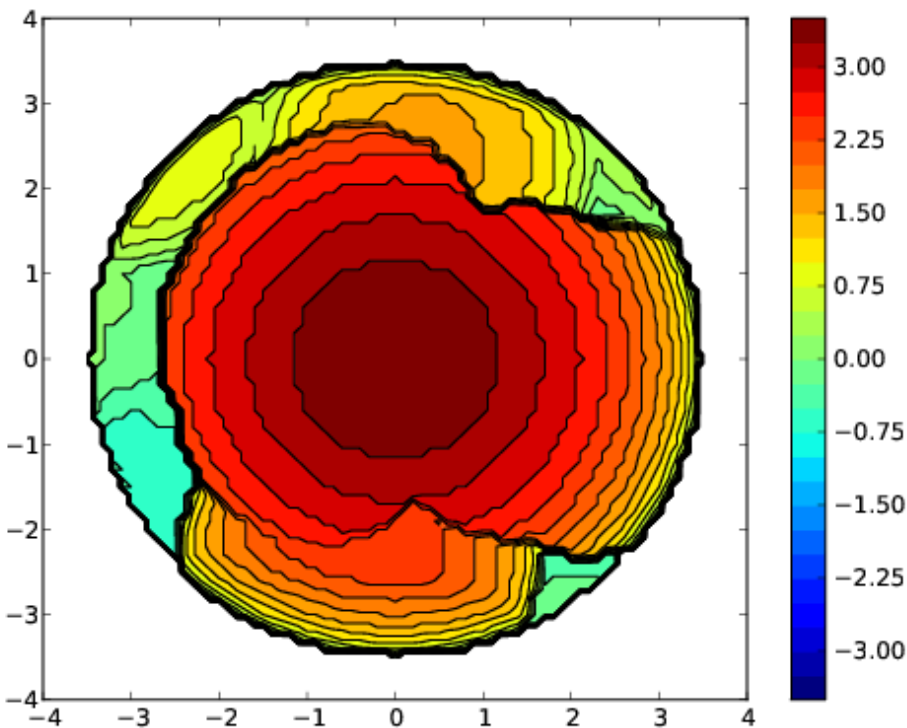


Including all the ruthenium catalyst and the MOF as well:

At 3.5 Å:

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

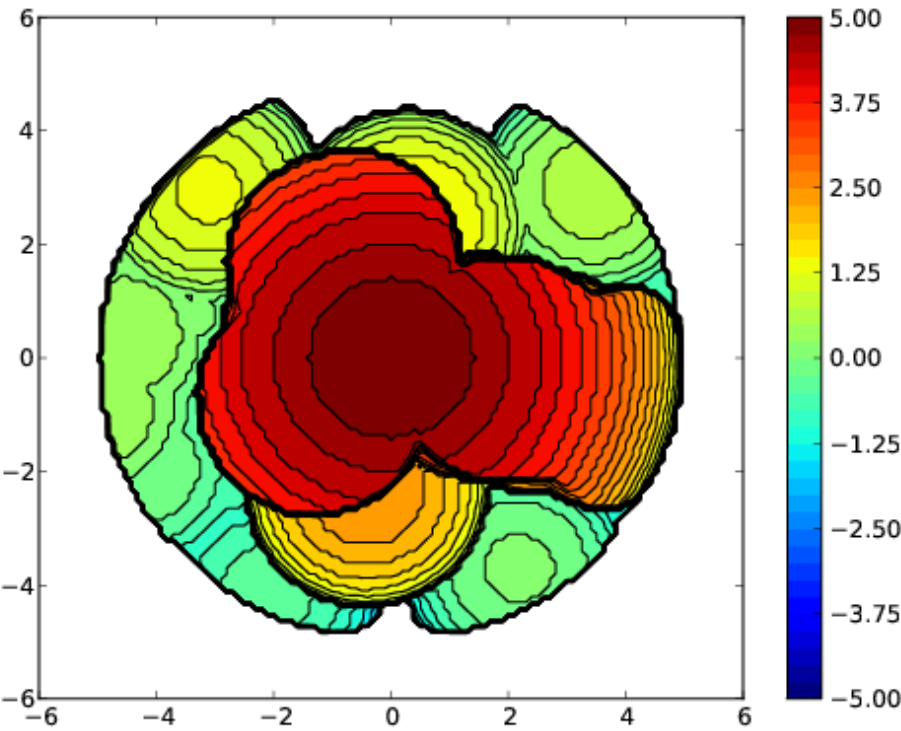
Quadrant	V f	V b	V t	%V f	%V b
SW	5.4	39.5	44.9	11.9	88.1
NW	5.7	39.2	44.9	12.7	87.3
NE	3.1	41.8	44.9	6.9	93.1
SE	1.9	43.0	44.9	4.2	95.8



At 5.0 Å:

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

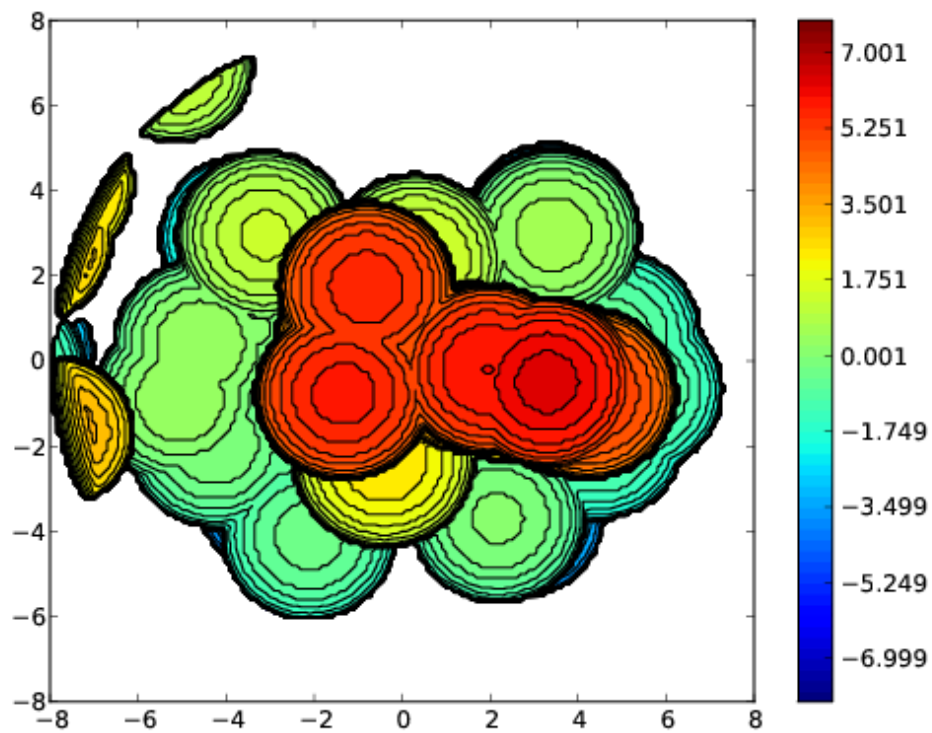
Quadrant	V f	V b	V t	%V f	%V b
SW	36.0	94.9	130.8	27.5	72.5
NW	35.1	95.7	130.8	26.8	73.2
NE	33.9	96.9	130.8	25.9	74.1
SE	28.1	102.8	130.8	21.4	78.6



At 8.0 Å:

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

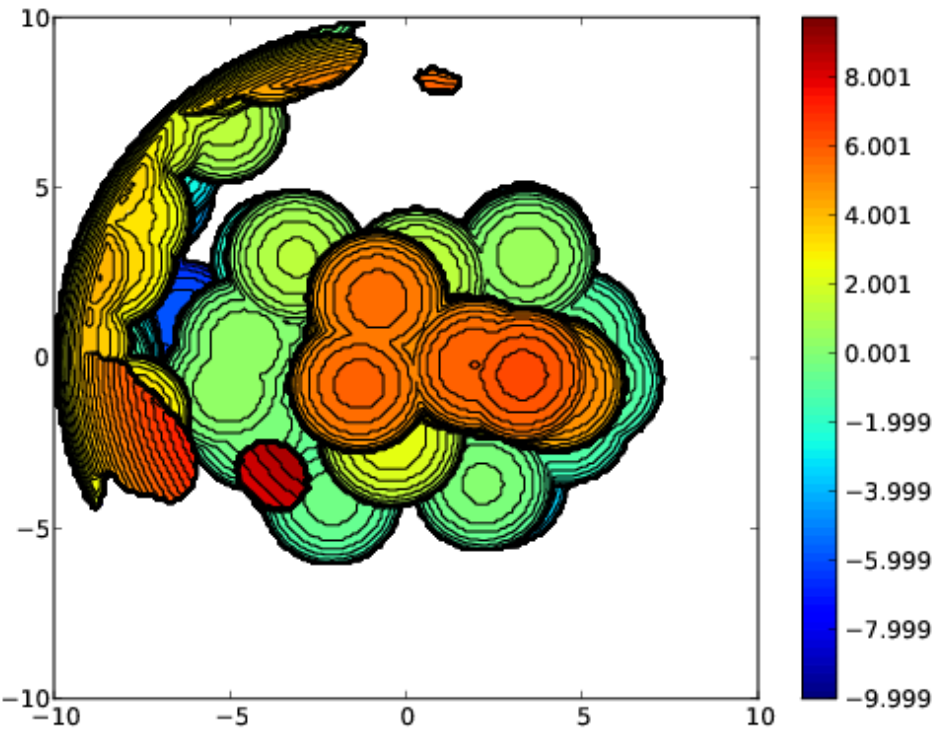
Quadrant	V f	V b	V t	%V f	%V b
SW	345.2	190.7	535.9	64.4	35.6
NW	365.3	170.5	535.8	68.2	31.8
NE	342.1	193.5	535.6	63.9	36.1
SE	312.1	223.7	535.8	58.3	41.7



At 10.0 Å:

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

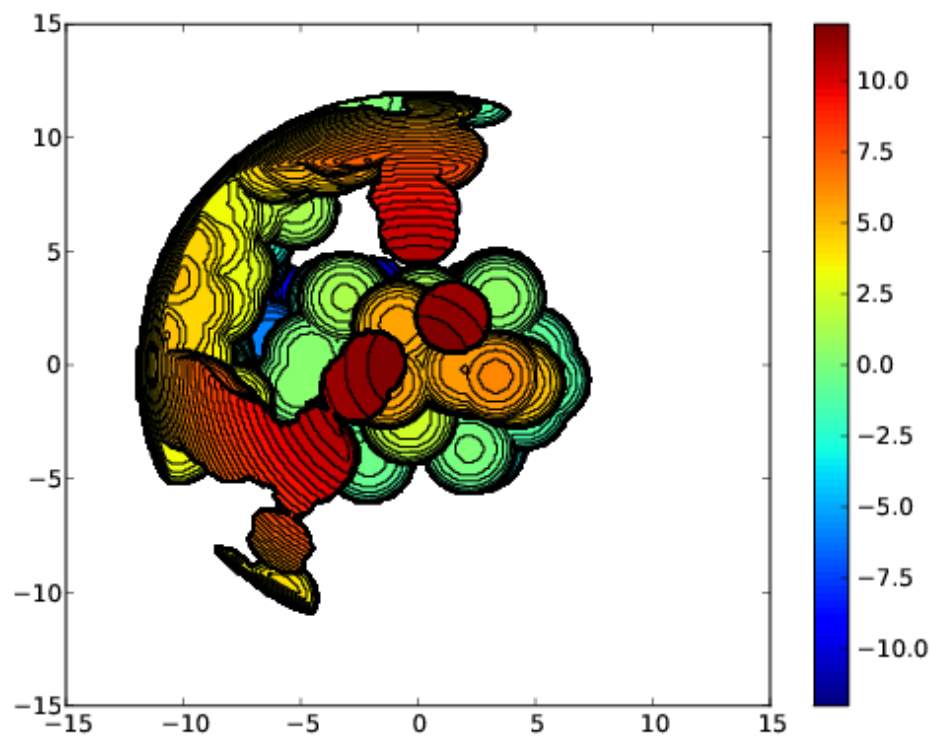
Quadrant	V f	V b	V t	%V f	%V b
SW	794.9	252.0	1046.9	75.9	24.1
NW	731.8	315.2	1046.9	69.9	30.1
NE	830.1	216.8	1046.9	79.3	20.7
SE	811.6	235.4	1046.9	77.5	22.5



At 12.0 Å:

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

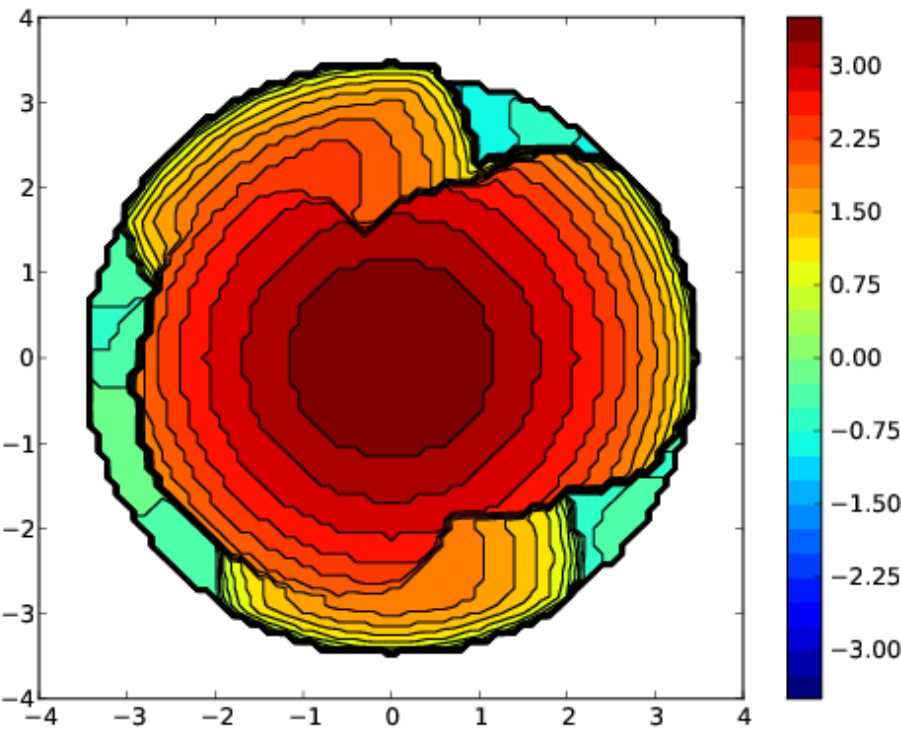
Quadrant	V f	V b	V t	%V f	%V b
SW	1389.5	419.6	1809.1	76.8	23.2
NW	1157.7	651.4	1809.1	64.0	36.0
NE	1525.7	283.5	1809.1	84.3	15.7
SE	1570.3	238.8	1809.1	86.8	13.2



AquaMet™ including all atoms:

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

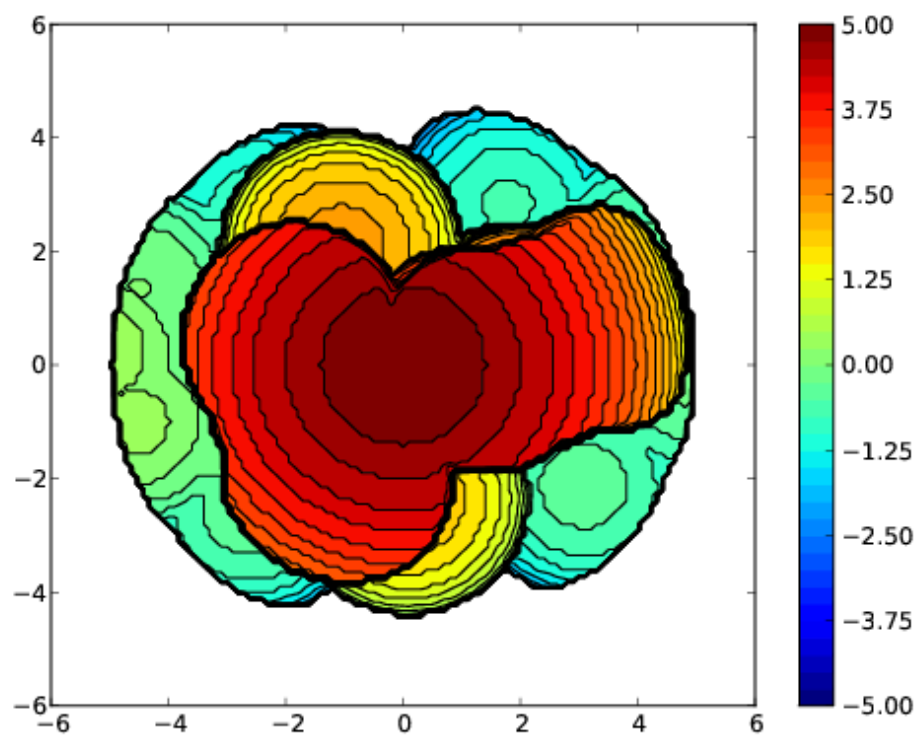
Quadrant	V f	V b	V t	%V f	%V b
SW	5.3	39.5	44.9	11.9	88.1
NW	3.6	41.3	44.9	7.9	92.1
NE	4.2	40.7	44.9	9.3	90.7
SE	4.3	40.5	44.9	9.7	90.3



At 5.0 Å:

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

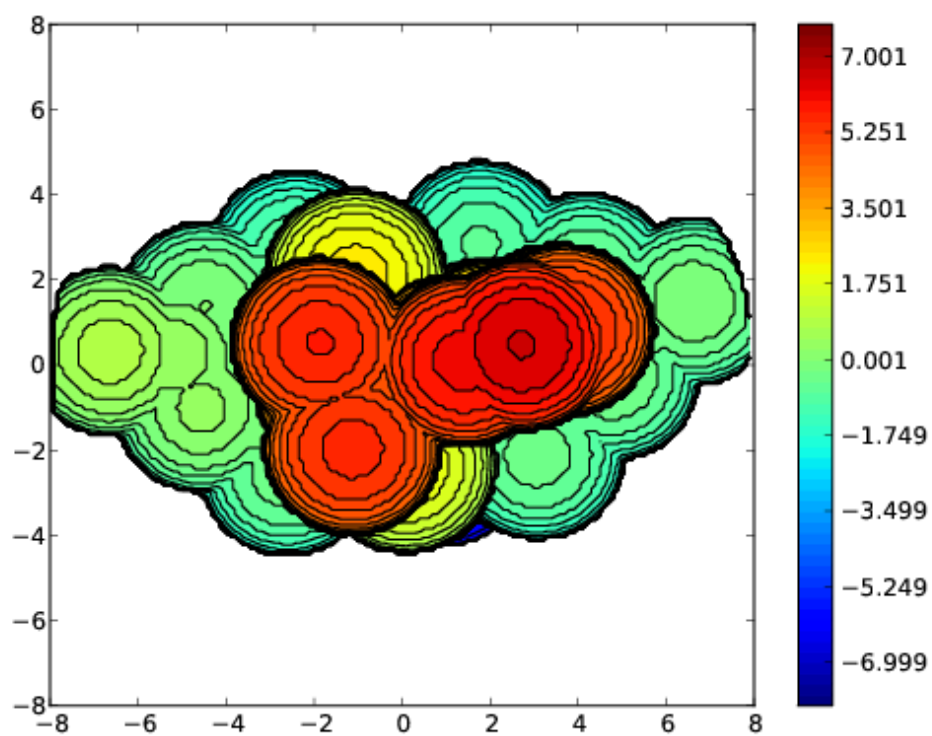
Quadrant	V f	V b	V t	%V f	%V b
SW	37.6	93.2	130.8	28.7	71.3
NW	39.1	91.8	130.8	29.9	70.1
NE	35.5	95.3	130.8	27.2	72.8
SE	44.6	86.2	130.8	34.1	65.9



At 8.0 Å:

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

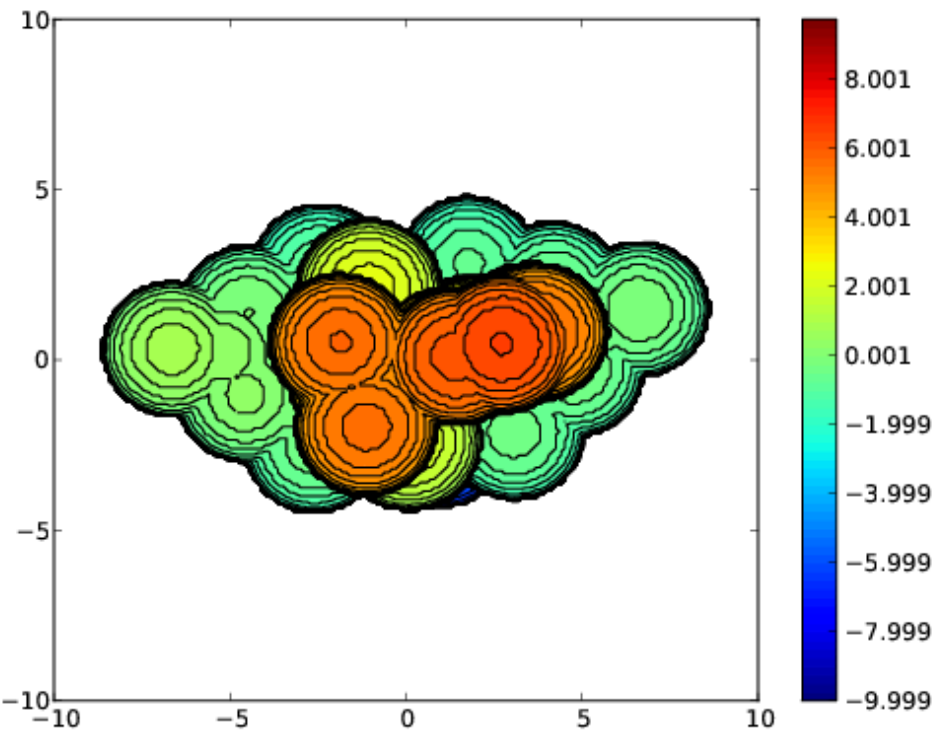
Quadrant	V f	V b	V t	%V f	%V b
SW	386.2	149.7	535.9	72.1	27.9
NW	388.6	147.2	535.8	72.5	27.5
NE	345.2	190.4	535.6	64.4	35.6
SE	381.6	154.2	535.8	71.2	28.8



At 10.0 Å:

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

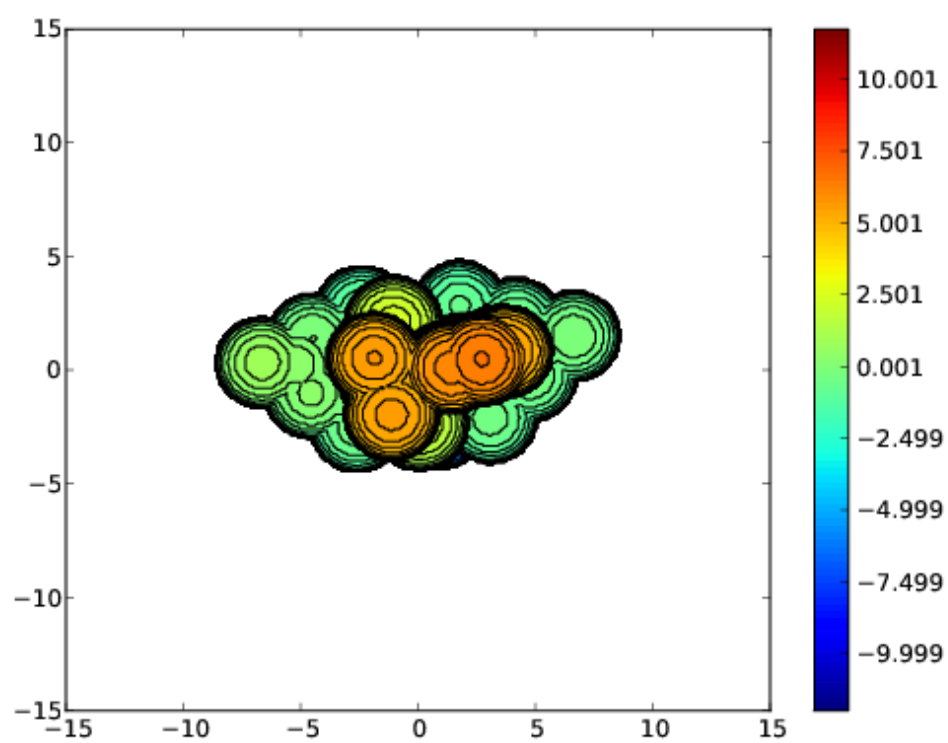
Quadrant	V f	V b	V t	%V f	%V b
SW	883.7	163.3	1047.0	84.4	15.6
NW	893.8	153.0	1046.8	85.4	14.6
NE	838.6	207.9	1046.5	80.1	19.9
SE	867.0	179.7	1046.8	82.8	17.2



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

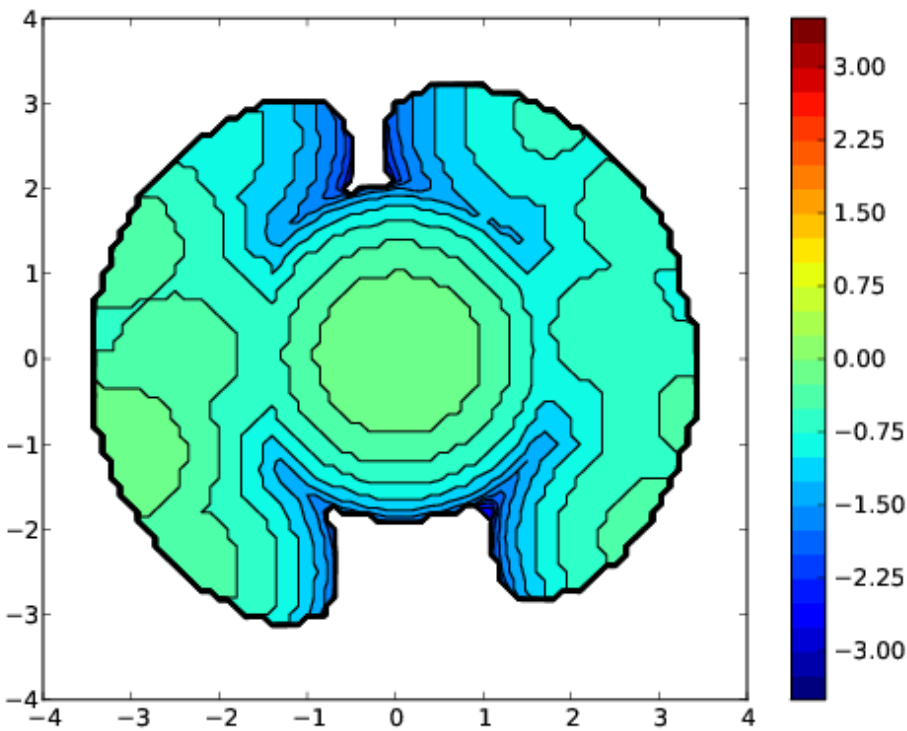


AquaMet™

At 3.5 Å:

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

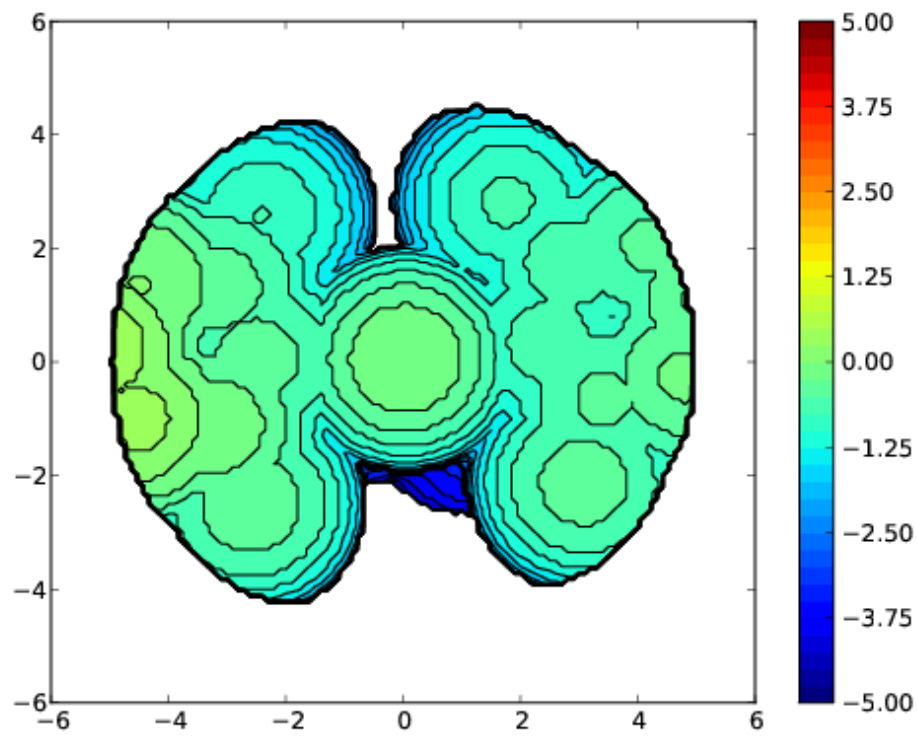
Quadrant	V f	V b	V t	%V f	%V b
SW	29.2	15.7	44.9	65.0	35.0
NW	29.9	15.0	44.9	66.6	33.4
NE	29.2	15.6	44.9	65.2	34.8
SE	31.4	13.4	44.9	70.0	30.0



At 5.0 Å:

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

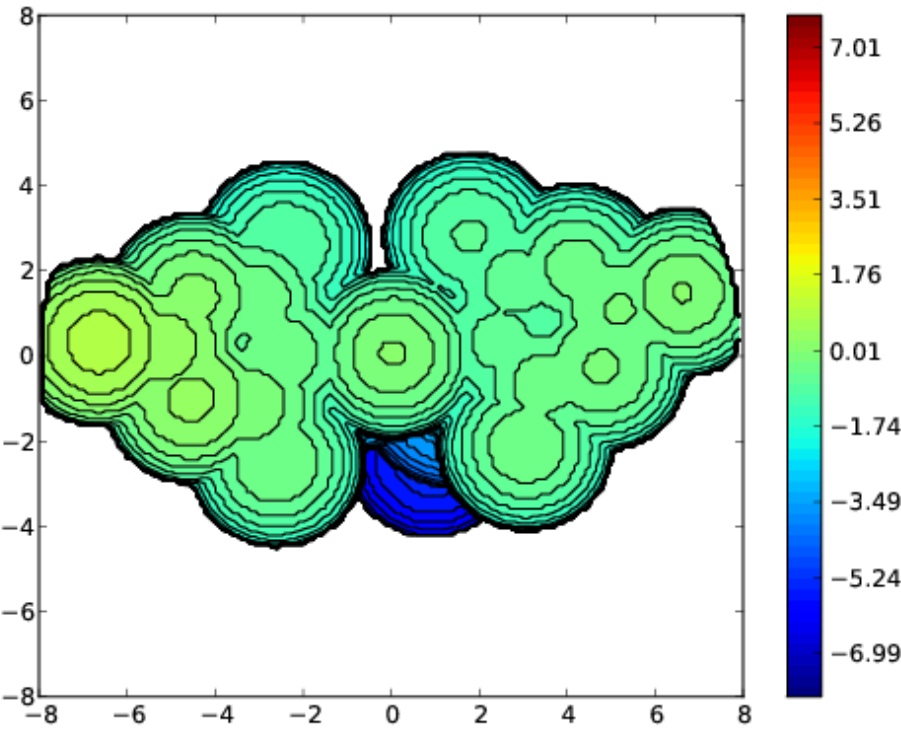
Quadrant	V f	V b	V t	%V f	%V b
SW	82.2	48.6	130.8	62.9	37.1
NW	83.9	46.9	130.8	64.2	35.8
NE	81.4	49.5	130.8	62.2	37.8
SE	89.5	41.4	130.8	68.4	31.6



At 8.0 Å:

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

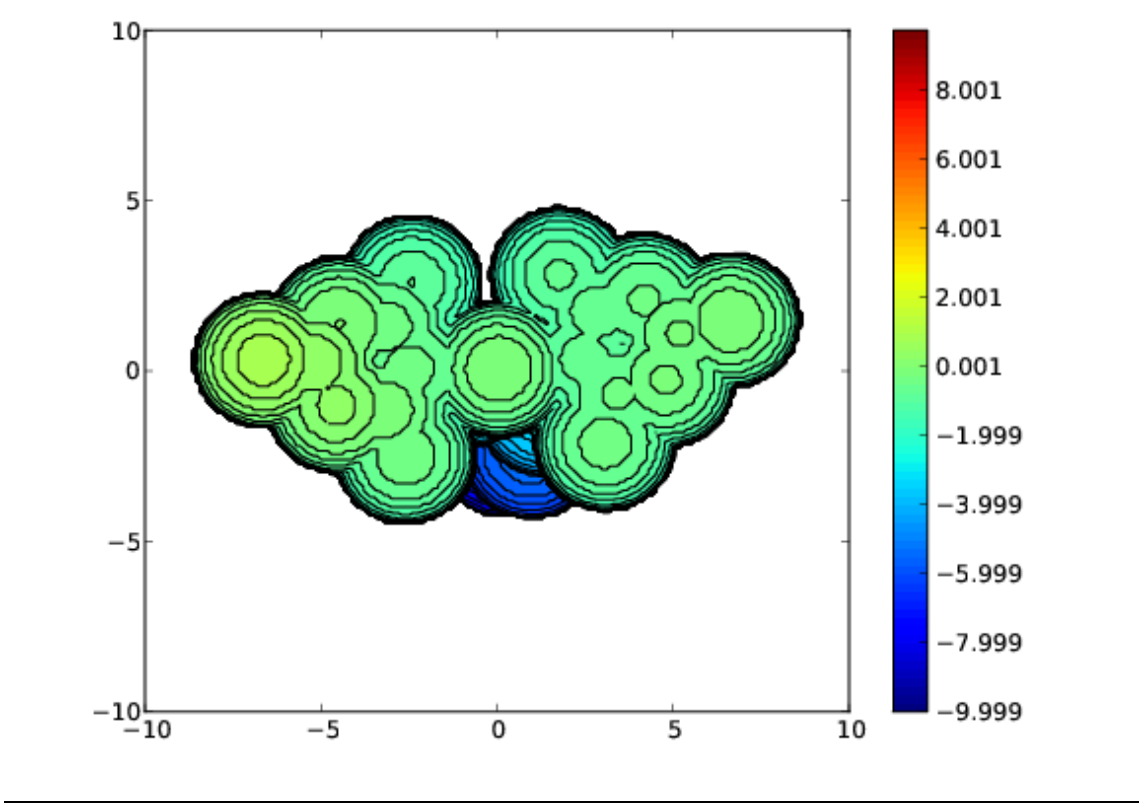
Quadrant	V f	V b	V t	%V f	%V b
SW	443.1	93.0	536.1	82.7	17.3
NW	439.9	94.2	534.1	82.4	17.6
NE	416.9	115.3	532.2	78.3	21.7
SE	437.3	96.8	534.1	81.9	18.1



At 10.0 Å:

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

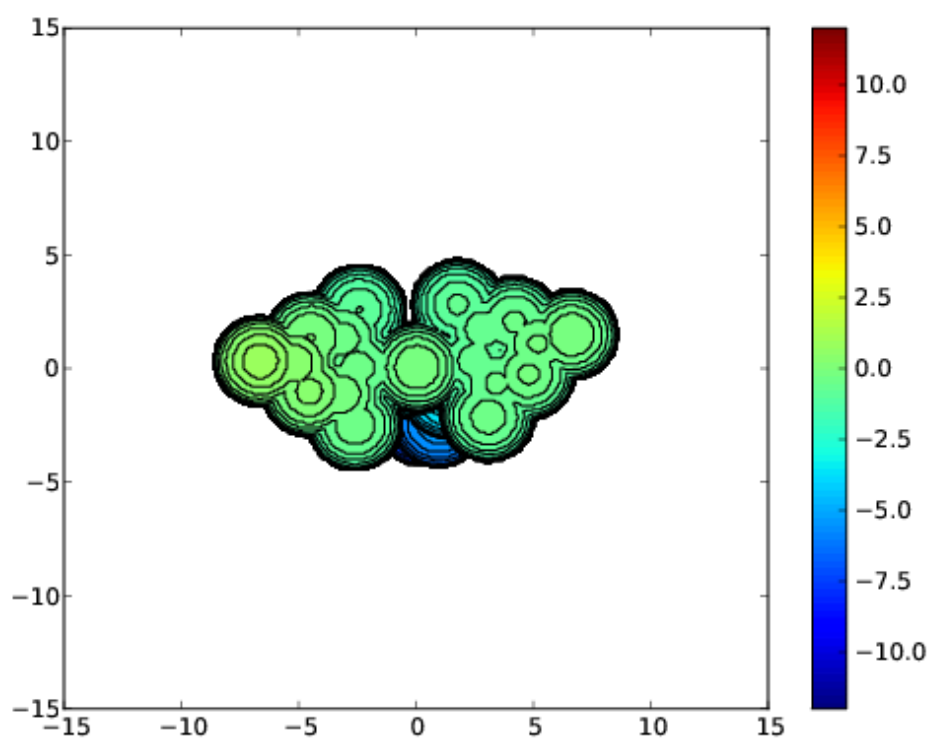
Quadrant	V f	V b	V t	%V f	%V b
SW	941.0	106.1	1047.0	89.9	10.1
NW	946.5	100.3	1046.8	90.4	9.6
NE	913.2	133.4	1046.5	87.3	12.7
SE	924.6	122.2	1046.8	88.3	11.7



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

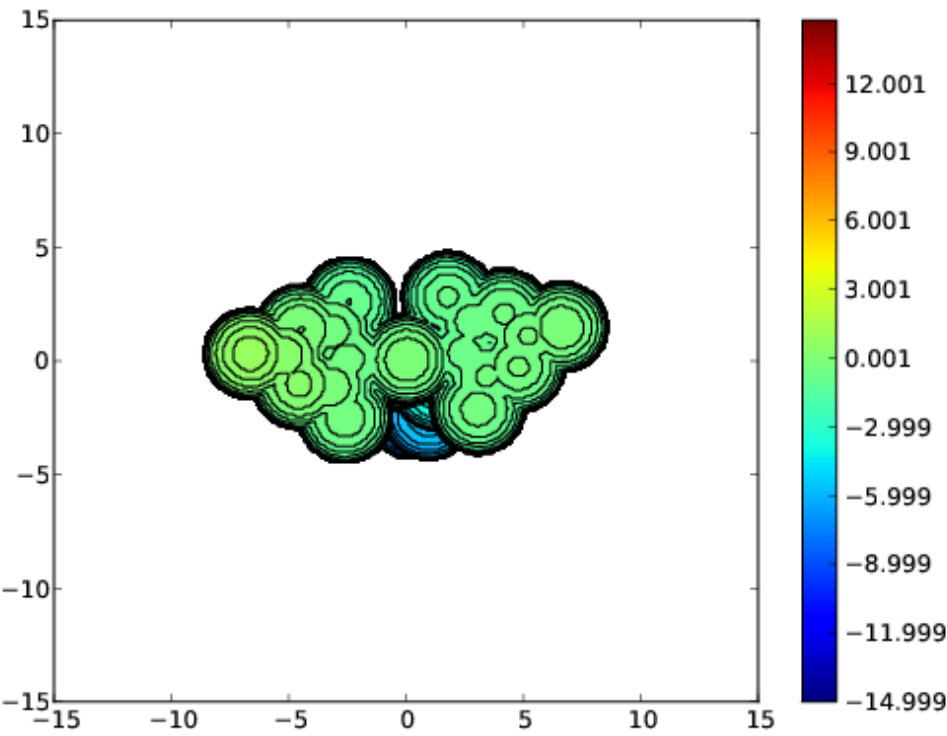
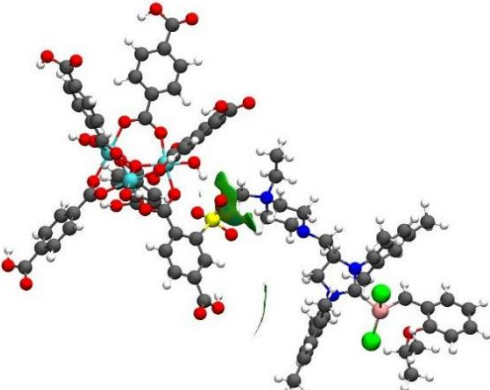
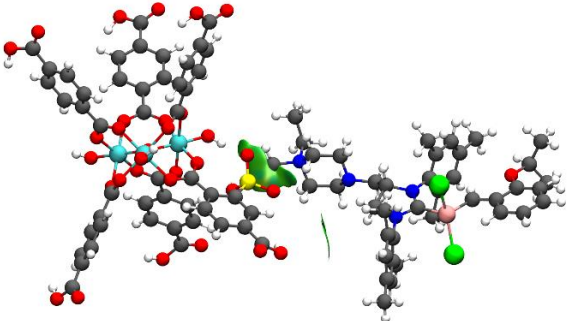
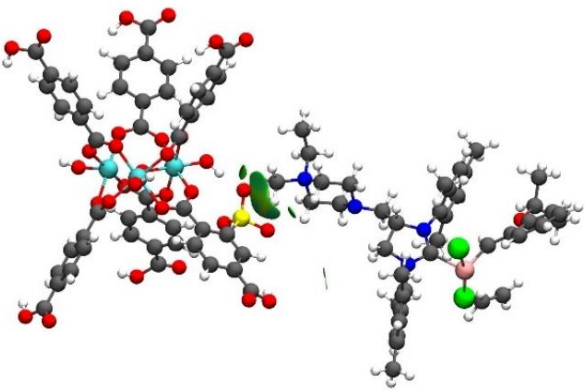
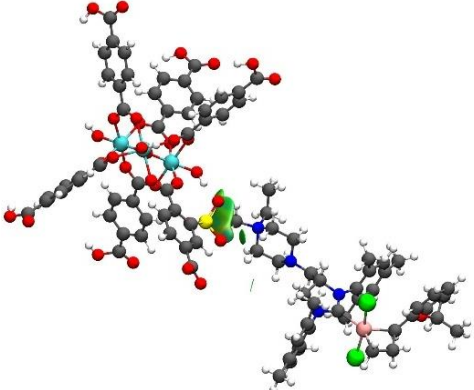
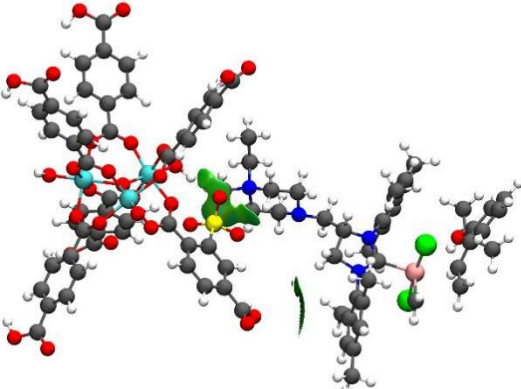
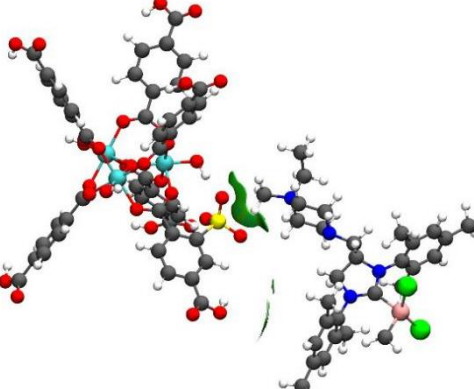


Table S1. NCI plots of the truncated MOF in combination with the Precat. Previously optimised geometries have been evaluated using the promolecular approach suitable for large structures.

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
C	27.3905992567	14.3763204450	21.1612618070	C	27.6445162092	14.3156987098	21.1636600355
C	28.1424246516	13.2603391648	20.7655216975	C	28.4072648329	13.2072550404	20.7658580832
C	27.2506333826	14.6804865887	22.5253324596	C	27.5042875648	14.6175905289	22.5281047571
C	28.7552021187	12.4590693060	21.7247476499	C	29.0220970737	12.4060478051	21.7237998596
C	28.6147666020	12.7581374811	23.0899712123	C	28.8719316900	12.6966374296	23.0901179375
C	27.8511066856	13.8696131710	23.4836526893	C	28.1066016127	13.8061791936	23.4849612941
C	29.2207574950	11.9093356497	24.1571984298	C	29.4636942125	11.8375407754	24.1572920741
H	26.6645908336	15.5507056508	22.8118938482	H	26.9147820350	15.4845814026	22.8170707404
C	26.7088771368	15.2012529764	20.1205799875	C	26.9533092995	15.1306927124	20.1215830307
C	22.4803551378	16.0791378058	20.4812780308	C	22.7537670297	15.9950646666	20.4821043280
C	21.7614868096	15.7085651434	21.7409087697	C	22.0492278150	15.6088709317	21.7415711207
C	22.1090562823	16.3019211244	22.9637682085	C	22.4106812013	16.1971209830	22.9621598591
C	21.4413237533	15.9363137198	24.1329339331	C	21.7519671931	15.8295571167	24.1343731897
C	20.4108999845	14.9798278441	24.0960521263	C	20.7178219325	14.8784582375	24.0986618962
C	20.0535279478	14.4038812938	22.8651771816	C	20.3498139207	14.3031682085	22.8707799808
C	20.7278720571	14.7566537011	21.7003752995	C	21.0166270277	14.6567013128	21.7024223877
H	22.9014318687	17.0460184969	22.9853276965	H	23.2054711722	16.9385144231	22.9773604568
H	20.4681662116	14.3080149226	20.7446247606	H	20.7508995253	14.2119819638	20.7461807408
C	19.6499571293	14.5486786734	25.3129625481	C	19.9571731802	14.4602546827	25.3167497364
O	22.1590313976	17.7176011544	17.7339239960	O	22.3948111423	17.6274472081	17.7331747582
O	23.9591671265	18.8944019550	18.4332304509	O	24.1875658594	18.8199854120	18.4317919978
H	28.2191405160	13.0279428999	19.7065334730	H	28.4889277905	12.9787141231	19.7061138467
C	24.0996463227	15.7146681112	14.9916773772	C	24.3458711072	15.6377493295	14.9828502878
C	23.9626965921	15.8211895332	13.5100636900	C	24.2072176782	15.7489144704	13.5027131358
C	24.9603981896	15.2615243231	12.6962198700	C	25.1984441835	15.1780626665	12.6888629472
C	24.8323975458	15.3103141064	11.3104923853	C	25.0677784401	15.2247143642	11.3037145301
C	23.7014704385	15.9062018547	10.7251823798	C	23.9411306292	15.8306345070	10.7207104384
C	22.7060411811	16.4626817099	11.5475194665	C	22.9545307998	16.4020919048	11.5426990096
C	22.8375463467	16.4351321977	12.9344206637	C	23.0884762216	16.3761257539	12.9290602828
H	22.0846302207	16.8779436729	13.5875803113	H	22.3422414104	16.8300966226	13.5823553545
H	25.8164330225	14.7841024436	13.1686912174	H	26.0502229665	14.6939550315	13.1625022525
C	22.7807408332	18.8044419036	17.9441512341	C	23.0079648035	18.7182269575	17.9421452307
C	22.0617650067	20.0855603906	17.6395546165	C	22.2749181913	19.9940523305	17.6347149570
C	20.7919817602	20.1823016934	17.0092611308	C	20.9965807091	20.0930268583	17.0142054985
C	20.2414419535	21.4580239187	16.8246010703	C	20.4473202046	21.3714871549	16.8400996778
C	20.8929472526	22.6265274237	17.2422192570	C	21.1090953612	22.5398470255	17.2457205023
C	22.1378234919	22.5221196776	17.8783414993	C	22.3620739441	22.4330056386	17.8635325840
C	22.7067173229	21.2679320544	18.0597459042	C	22.9257212048	21.1766728794	18.0443069181
S	19.7480886510	18.8189994453	16.3523186356	S	19.9568444151	18.7398392977	16.3138378092
C	27.0895658931	17.8175693238	17.4322203849	C	27.3611689378	17.7417673622	17.4406868453
C	28.0493647965	18.8295455551	16.9087413436	C	28.3237841023	18.7652345312	16.9307321817
C	28.3491922622	19.9711012759	17.6709150618	C	28.5979745370	19.9198449165	17.6834934684
C	29.2315610152	20.9230714602	17.1733540819	C	29.4697916496	20.8847970008	17.1868175814
C	29.8318016276	20.7423153799	15.9159039193	C	30.0889355591	20.7091179053	15.9372081582
C	29.5266676171	19.6000716657	15.1566674406	C	29.8168045242	19.5475705431	15.1922738767

C	28.6391073140	18.6462725383	15.6494504173	C	28.9413637227	18.5806362912	15.6841262189
H	28.3838014297	17.7597131655	15.0738005204	H	28.7157086717	17.6817069528	15.1146188369
H	27.8769625752	20.0922864781	18.6435139043	H	28.1132999600	20.0432258365	18.6498635196
O	20.9252661243	15.5561148917	17.1148490649	O	21.2240006706	15.4772292393	17.1204376757
O	27.3287080897	14.1546618269	16.4149823679	O	27.6159599997	14.0734501155	16.4023281614
O	25.3469815400	18.6719291182	20.6981290585	O	25.5802236382	18.6600839671	20.6862332648
H	24.6205019183	18.7773104691	21.3385378933	H	24.8315188664	18.7742837795	21.3006686093
H	28.1120721968	14.1529524600	16.9916685406	H	28.3739342818	14.0162996279	17.0063218156
H	20.4033624452	16.3980239942	17.2378818124	H	20.6847007350	16.3160066764	17.2135365484
H	27.7441501758	14.0748134751	24.5467118512	H	27.9974701275	14.0074588718	24.5485180682
H	29.3020173351	11.5734094182	21.4020251406	H	29.5762451928	11.5259425240	21.3978098993
O	28.7778522556	11.8219223315	25.2852397309	O	29.0115884677	11.7451082308	25.2816805357
O	30.3407272048	11.1949821005	23.8036565663	O	30.5785031059	11.1154546310	23.8056875728
H	30.6322480083	11.4666415879	22.9141557701	H	30.8831987770	11.3936073222	22.9226337624
H	29.4729004988	21.8216450842	17.7370723090	H	29.6860011906	21.7915320386	17.7478499004
H	29.9447948405	19.4624368280	14.1594782536	H	30.2508255500	19.4007806609	14.2029989299
C	30.7510592638	21.8159488417	15.4379482254	C	30.9883755615	21.8011822503	15.4490060005
O	30.7273942148	22.9536974765	15.8650975602	O	30.9555834579	22.9432517586	15.8671022313
O	31.6588964982	21.4690094891	14.4645287878	O	31.8911933448	21.4669285535	14.4653106933
H	31.6203919367	20.5069915766	14.3129989674	H	31.8689462186	20.5039391311	14.3159665792
C	23.4983661901	15.9366781641	9.2454294581	C	23.7341897969	15.8589298136	9.2427126031
H	21.8370201471	16.9150107256	11.0750153124	H	22.0909529752	16.8643146691	11.0698409518
H	25.5958760701	14.8379778455	10.6922772033	H	25.8247984166	14.7427710218	10.6850859885
O	22.4050768516	15.9477634640	8.7102308530	O	22.6394967109	15.8701998207	8.7096447558
O	24.6416006308	15.9445274712	8.4749167812	O	24.8766690061	15.8667211754	8.4723127667
H	25.4186506895	16.0427578350	9.0555933057	H	25.6541111741	15.9605176372	9.0532972836
H	20.7988430049	9.5698483044	17.9050243653	H	21.0641795421	9.4796102231	17.9648272513
H	24.9628049743	8.6271337041	18.5008679544	H	25.2445282534	8.5491623578	18.4495332585
C	22.3798950912	7.5262872810	18.4074854745	C	22.6568442197	7.4481909168	18.4096688851
O	21.2471449808	7.2289032660	18.7400873710	O	21.5276184729	7.1507552635	18.7475158688
O	23.3190609749	6.5371852310	18.2027948184	O	23.5798932698	6.4530325128	18.1988202571
H	24.1357191790	6.9352245774	17.8491750497	H	24.4046634964	6.8387297299	17.8497562886
H	21.7089328648	16.4329507591	25.0657071470	H	22.0272754138	16.3216077843	25.0671745067
H	19.2448862102	13.6764543816	22.8496773675	H	19.5379220722	13.5791059453	22.8612992786
O	20.2934020541	14.6985438648	26.5212415082	O	20.6006130550	14.6194914622	26.5232519809
H	21.2167241172	14.9708972459	26.3673623600	H	21.5272657083	14.8782914581	26.3664765871
O	18.5257968386	14.0830205337	25.2789088423	O	18.8300068446	14.0024997292	25.2816458634
C	20.3028441296	23.9895668501	17.0490928876	C	20.5290773189	23.9078624885	17.0500214089
H	19.2551172933	21.4844698448	16.3631598788	H	19.4559172727	21.4039389878	16.3895940325
H	22.6400569288	23.4258234619	18.2169501662	H	22.8760875086	23.3354738085	18.1877528113
O	19.3733844201	24.1153002642	16.0368158946	O	19.6050672164	24.0374232495	16.0341690159
H	19.3106306754	23.2678716366	15.5573120848	H	19.5410430955	23.1905086071	15.5538939490
O	20.6059248333	24.9588464588	17.7213698386	O	20.8383318484	24.8769166087	17.7199947395
O	19.3687867999	17.9563394150	17.4984629205	O	19.6045828718	17.8069925223	17.4170122151
O	20.5389239724	18.1289908361	15.3173865474	O	20.7671106119	18.1266286657	15.2443087569
O	18.5683081849	19.5294529487	15.7845220603	O	18.7491803171	19.4443668332	15.7907223236
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
Cl	9.8022865934	23.1840123374	16.9034435638	C	9.8489100066	19.5142149690	16.3544595672
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
H	15.1706855460	14.7867144368	16.0647882906	C	15.9618897778	17.4168491732	15.3784510303
H	16.8496992897	14.3522554833	15.6519796726	H	18.2705249112	16.0801593061	15.4687507966
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
H	17.9735756065	16.2380502288	15.5267242960	C	14.5039650150	17.7542710022	15.0815293278
H	16.2433229580	18.4452238714	15.5631824562	H	12.5927846510	19.8364538941	15.5349751748
H	14.0506716448	26.4486566982	16.3691987001	H	7.9090584865	17.9775412243	15.3294007365
H	15.4961458186	13.4692486642	14.9327126184	C	13.6414551519	24.5392422443	15.5852400113
C	14.1936930276	17.8636435820	15.0720543817	C	18.0928521495	16.5385027202	14.4913808459
H	12.3332958612	19.9613947226	15.5264651582	C	9.4985766052	19.3568090743	14.8950995271
H	7.6570840943	18.0840136734	15.2778571991	H	13.8794071861	16.8389576467	15.0535266461
C	8.2174450328	26.3929688393	15.8171506398	C	14.1627082171	25.8375331276	15.4696949566
C	13.2686828697	24.6296506447	15.5462893829	H	14.3827656933	21.3637353825	15.1577623935
C	17.8108844416	16.7112091318	14.5540494632	H	18.5161191457	17.5487960022	14.5046650061

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
H	9.3138824399	26.3588299488	15.8405255046	C	16.0190458708	15.2455783104	14.0496783434
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
H	14.0553163233	21.5694770593	15.1652277268	N	12.7487226351	22.5229220101	14.4684070373
O	7.9433718903	25.0507559780	15.2433393390	C	11.4180446868	22.1994815369	14.3413508420
H	18.2091409999	17.7313254065	14.5983153510	N	11.3449481892	20.8336786082	14.1592231987
C	8.1930164571	18.6160319297	14.4938525460	N	14.3824664779	18.5416136639	13.8498773380
C	5.4699788533	25.1687763199	15.1691219227	C	13.3098983541	23.8499796268	14.4004405175
N	16.3318955874	16.7898924545	14.2659802455	H	18.5435736809	15.9375470178	13.6951630544
C	15.7723410281	15.3882304030	14.0439150240	C	10.1768105883	20.0490561561	13.8700756253
C	6.7016598194	24.5516502461	14.9421153383	H	14.9802022208	15.3739301551	13.7304547480
C	12.3736197245	20.3115821455	14.4819233364	C	13.0073870993	19.0005197204	13.5805398434
C	4.2968919285	24.4988908488	14.7968133568	C	14.4040537708	26.4357391381	14.2298199954
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
N	12.4007050948	22.6493664576	14.4023224372	C	16.4048388199	17.4610074580	12.9732356688
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
N	11.0645139011	20.9344345827	14.1539116056	H	14.1509697058	21.3331930289	13.3947447895
N	14.1053818219	18.6743140084	13.8544444487	C	6.8860409860	17.4199504123	12.8589236122
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
Cl	9.9625468993	24.9796524845	12.8117579967	O	5.9177452927	21.6813084280	14.1503271388
C	8.4849753687	19.1782825831	12.1737521444	C	4.7173556467	20.9471303422	13.7516944377
H	12.7327642243	19.5095119705	12.5276604625	C	4.0103815224	21.5736690367	12.5496216639
H	16.6069525058	17.0697741145	12.1791996651	H	3.4634212210	22.4900561603	12.7956585457
H	14.6818795038	18.6244124176	11.8451382320	H	3.2884496268	20.8521551081	12.1417012307
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
H	8.1804778908	19.0839496873	11.1332786987	H	5.1785023099	20.0106495794	13.4098913902
H	12.6659264331	23.0035065214	16.8758372343	H	13.0809737086	22.9232273683	16.9270372821
H	12.5057784200	24.6062687596	17.5767690990	H	12.8723404352	24.5330912695	17.6045936853
H	14.1209256987	23.9060185516	17.3775393579	H	14.5090543142	23.8691267193	17.4293673777
H	13.4340030297	24.3566198036	10.9442968562	H	10.6200577657	20.2721257392	16.5250261649
H	12.0920848078	23.4090925117	11.6173005526	H	10.1782466505	18.5594114459	16.7888849762
H	13.7667480124	22.8340045154	11.7686936567	H	8.9631391375	19.8385108391	16.9196804663
H	14.8301277623	28.2205452167	13.1130419184	H	15.0965621810	28.1487537382	13.0981592618
H	15.6481359809	27.9352714813	14.6619480276	H	15.9209109418	27.9214018504	14.6556109153
H	14.0256255697	28.6350320219	14.6390567035	H	14.2714298197	28.5598307955	14.6150052379
H	10.4153813545	20.3092839408	16.5089766254	H	6.6799582605	17.4263820015	11.7811409098
H	9.8734280324	18.6258169531	16.7682324832	H	5.9590337830	17.6999400976	13.3808436640

H	8.7372095653	19.9780886068	16.8808250233	H	7.1120074497	16.3838231310	13.1509083807
H	6.4581529130	17.5575895510	11.7220918600	H	9.9847522028	20.4557774703	10.4450830182
H	5.7165585482	17.8800900397	13.3016869368	H	11.5117211799	20.4839061037	11.3477336740
H	6.8379528009	16.5294739887	13.1172562775	H	10.3436780695	21.7874205837	11.5702300590
H	9.7959548663	20.5112423710	10.3986773213	H	13.6034010637	24.2612712019	10.9836603457
H	11.3243617520	20.5385567791	11.2897023176	H	12.3153991778	23.3205859980	11.7618056252
H	10.1745708485	21.8600724098	11.4926802329	H	13.9957885152	22.7384782224	11.7921243232
Ci1				MCy			
223				223			
i =	66, E =	-1508.6173620635		i =	40, E =	-1508.6074468406	
Cr	26.4516294192	15.2706332079	17.2080594825	Cr	26.7537230533	15.3414571315	17.2160271641
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
O	25.5760566954	15.2452754130	15.4141674399	O	25.8991451691	15.3242028499	15.4210196345
O	27.3628862921	16.9677417642	16.7197033781	O	27.6848097078	17.0286097984	16.7172032658
O	27.4492901254	15.1563610383	18.9103345401	O	27.7704287541	15.1677968243	18.9064270023
O	23.6306825026	16.3971787419	15.6992810070	O	23.8956813004	16.3927304124	15.6726021837
O	22.7002764706	15.5594404385	19.4487081047	O	23.0243622274	15.5690934115	19.4534181875
O	23.3931471700	14.0707695679	17.3339395777	O	23.7133449762	14.0800449739	17.3346510038
O	26.2793424817	16.2408332129	20.5291795566	O	26.6780916986	16.3234957867	20.5333451939
O	27.0495738254	18.2570131337	18.5791464729	O	27.3787028079	18.2824878251	18.5886868809
O	23.7723599452	17.2535466097	20.5377487131	O	24.1017871791	17.2587583439	20.5414984215
C	24.3395083128	13.2533680092	17.6158921948	C	24.6725027577	13.2800451750	17.6200490606
C	23.9461745444	11.8228027168	17.8120753640	C	24.3043472667	11.8410910057	17.8223365907
C	22.5957811863	11.4338266106	17.7761012076	C	22.9559295799	11.4451334265	17.7826673142
C	24.9416894738	10.8636519113	18.0457308260	C	25.2996715075	10.8805957671	18.0623882945
C	24.5918889315	9.5299338882	18.2386853285	C	24.9485107147	9.5440005766	18.2552668856
C	23.2444163837	9.1332367114	18.2005209706	C	23.6000585545	9.1438608889	18.2148184906
C	22.487227596	10.1000838419	17.9763623627	C	22.6083852709	10.1118203404	17.9838407436
H	25.9794785819	11.1840049217	18.0750377467	H	26.3397814066	11.1970253046	18.0963769835
H	21.8356807086	12.1903396277	17.5934703766	H	22.1968535972	12.2009906549	17.5945687281
C	27.8014042204	14.5276105796	21.1574471066	C	28.1662878393	14.5812641149	21.1591696025
C	28.5548348261	13.4132260339	20.7540050756	C	28.9196235243	13.4657492718	20.7586503488
C	27.6603179640	14.8130428214	22.5253937411	C	28.0252953559	14.8700820045	22.5269675157
C	29.1700969464	12.6037110840	21.7069110179	C	29.5366068194	12.6584419259	21.7125347228
C	29.0364469814	12.8921050140	23.0758410918	C	29.4003901222	12.9488972539	23.0797315901
C	28.2652554966	13.9960704270	23.4765952744	C	28.6304432355	14.0546483238	23.4787777030
C	29.6610518498	12.0516997027	24.1456512842	C	30.0037168972	12.1031885171	24.1524952529
H	27.0739224037	15.6797025666	22.8209574212	H	27.4350254750	15.7338529009	22.8236036723
C	27.1274411264	15.3725864429	20.1232503969	C	27.4884412797	15.4241615273	20.1246100909
C	22.9648551099	16.2589437248	20.4788827179	C	23.2949840557	16.2641941318	20.4863765935
C	22.2501903260	15.8771696003	21.7366355438	C	22.5805444356	15.8834944774	21.7465983832
C	22.5986399920	16.4703863977	22.9583803158	C	22.9292094720	16.4735197063	22.9701924248
C	21.9342452699	16.1019529078	24.1280829082	C	22.2561924445	16.1126280570	24.1374478539
C	20.9087290063	15.1427078786	24.0927802315	C	21.2166968296	15.1667613033	24.0980482317
C	20.5498707792	14.5642863851	22.8634879612	C	20.8616220758	14.5887634137	22.8673756042
C	21.2207861918	14.9197528243	21.6971683099	C	21.5434599840	14.9349546603	21.7045402848
H	23.3887890839	17.2170346157	22.9785552967	H	23.7249250810	17.2139168398	22.9928540231
H	20.9602396457	14.4696412325	20.7413293629	H	21.2839417333	14.4880350491	20.7476511110
C	20.1494956514	14.7224010278	25.3101553747	C	20.4397068057	14.7635723350	25.3129924489
O	22.6158745326	17.8963052690	17.7299132036	O	22.9463762667	17.9072245368	17.7362050942
O	24.4124524015	19.0698945006	18.4314593383	O	24.7319492576	19.1191617662	18.4327265618
H	28.6373164152	13.1849077472	19.6943027342	H	28.9978402798	13.2356349333	19.6991313131
C	24.5505929537	15.8572228056	14.9806780008	C	24.8562323977	15.9050906052	14.9776653917
C	24.3928445622	15.9515283307	13.5023434557	C	24.7304878911	16.0034911843	13.4958313065
C	25.3770687678	15.3775939734	12.6830084684	C	25.7258129283	15.4344062559	12.6857637063
C	25.2505943665	15.4421888669	11.2984169185	C	25.6013739243	15.4876240750	11.2997711561
C	24.1337295783	16.0688185889	10.7206793611	C	24.4787392412	16.1003500127	10.7163643979
C	23.1396881825	16.6221297676	11.5474909087	C	23.4848341114	16.6632277644	11.5348012413
C	23.2705021832	16.5783628583	12.9341057462	C	23.6116993258	16.6278890382	12.9203941643
H	22.5205714636	17.0258865722	13.5875421443	H	22.8626655491	17.0758769272	13.5739180017
H	26.2255469763	14.8839314875	13.1508501449	H	26.5760563349	14.9497318071	13.1615425598
C	23.2330021004	18.9846795226	17.9426658482	C	23.5518529256	19.0055947856	17.9526274074
C	22.5155815510	20.2760093817	17.6474854691	C	22.8210449862	20.2900706303	17.6707832264
C	21.2449121412	20.3896577700	17.0175532232	C	21.5427301232	20.4017484074	17.0631109466
C	20.6974808828	21.6697303711	16.8476238453	C	21.0007495269	21.6807034611	16.8770715138
C	21.3509765014	22.8352892651	17.2742972940	C	21.6690287970	22.8464219876	17.2765212420
C	22.5962739194	22.7139273675	17.9084960243	C	22.9193671093	22.7301034708	17.9002537277
C	23.1608565271	21.4541310009	18.0806415145	C	23.4781544234	21.4705164119	18.0810967538

S	20.2093625514	19.0466139073	16.3244343477	S	20.5066449041	19.0545125368	16.3817636489
C	27.5646111407	18.0038521924	17.4298002176	C	27.9009223779	18.0504458016	17.4456812195
C	28.5046749523	19.0321937089	16.8961322187	C	28.8615312639	19.0711148085	16.9242480487
C	28.7637105926	20.1973329217	17.6374084642	C	29.1339293116	20.2277630427	17.6736031896
C	29.6371221639	21.1580183206	17.1393398218	C	30.0034307631	21.1931033298	17.1743194397
C	30.2694092006	20.9642907144	15.8996617370	C	30.6232110102	21.0170603923	15.9251401709
C	29.9958212911	19.8039348340	15.1554024190	C	30.3490685792	19.8550369521	15.1804561428
C	29.1186619014	18.8407110961	15.6495718995	C	29.4745397975	18.8876261348	15.6751273449
H	28.8943342356	17.9376787161	15.0857374628	H	29.2461302885	17.9895502034	15.1053015482
H	28.2704961498	20.3257773249	18.5989888037	H	28.6488260242	20.3513997512	18.6396335615
O	21.3894060575	15.7774083273	17.1922260131	O	21.7309261231	15.7915542358	17.1996309118
O	27.8337755347	14.3067792371	16.4097532258	O	28.1346766079	14.3942883408	16.4066675803
O	25.8041543698	18.8924144582	20.6884661127	O	26.0640252321	18.9829117964	20.6968269932
H	25.0618070789	19.0019724062	21.3103364360	H	25.3243973110	19.0317207627	21.3281709363
H	28.5883379889	14.2580771209	17.0198819229	H	28.9076828673	14.3580380998	16.9940530459
H	20.8907216756	16.6445382807	17.2631209025	H	21.2040370014	16.6389600718	17.2849702902
H	28.1553241893	14.1925435975	24.5405579047	H	28.5218964611	14.2500499786	24.5435963360
H	29.7158724432	11.7195472051	21.3770327653	H	30.0849660412	11.7756207359	21.3836018019
O	29.2312227280	11.9722861040	25.2793809504	O	29.5614793560	12.0501856775	25.2835429709
O	30.7906759720	11.3476160266	23.7964922210	O	31.1089339809	11.3562314879	23.8069336489
H	31.0647480890	11.5983586643	22.8949494874	H	31.4079080536	11.6105795073	22.9147342567
H	29.8477044572	22.0708324480	17.6928775212	H	30.2179827508	22.1013051609	17.7332589554
H	30.4331273496	19.6543296550	14.1677412254	H	30.7796668855	19.7071415796	14.1897211051
C	31.1961148600	22.0394061238	15.4307676187	C	31.5285248253	22.1096502100	15.4446377805
O	31.1805206766	23.1743767595	15.8627669165	O	31.4995358468	23.2502063185	15.8670748365
O	32.1122000636	21.6924795037	14.4623739872	O	32.4356950180	21.7761160180	14.4647404389
H	32.0559379191	20.7336677156	14.2934743364	H	32.4092433465	20.8140686021	14.3093706348
C	23.9456985639	16.1416048042	9.2411110561	C	24.2787548054	16.1542657818	9.2393610073
H	22.2754514325	17.0896379965	11.0796989340	H	22.6223524262	17.1256505067	11.0601711588
H	26.0046476686	14.9648640258	10.6724565381	H	26.3591186288	15.0072708148	10.6803073011
O	22.8555734521	16.1757249640	8.7034528279	O	23.1848892368	16.1804659483	8.7064008974
O	25.0932293778	16.1709473597	8.4761448129	O	25.4243885436	16.1767615853	8.4733472401
H	25.8672573768	16.2378197122	9.0652191677	H	26.1989013490	16.2479938044	9.0617481038
H	21.2103727348	9.7747463520	17.9633691020	H	21.5698044170	9.7883349900	17.9654593085
H	25.3806768072	8.8106578701	18.4571268000	H	25.7393876358	8.8258021128	18.4742346121
C	22.8175137049	7.7147970175	18.4066097772	C	23.1580871650	7.7255455481	18.4149737161
O	21.6944748750	7.3843685593	18.7393012947	O	22.0314142485	7.3963126194	18.7401029791
O	23.7800432786	6.7541232656	18.1991765717	O	24.1106865752	6.7579997209	18.2004532902
H	24.5811377882	7.1678494807	17.8294654424	H	24.9228241112	7.1672695590	17.8498647568
H	22.1998860943	16.5986435206	25.0614296490	H	22.5241959033	16.6078760604	25.0705476482
H	19.7423910394	13.8346829729	22.8514208738	H	20.0467640298	13.8681834172	22.8499362698
O	20.7596287473	14.9277921913	26.5239525345	O	21.0729437252	14.9305319690	26.5237877789
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
H	19.1046088077	21.6960919797	16.3871458770	H	20.0115780956	21.7096759172	16.4221331190
H	23.1044999466	23.6125026296	18.2534684677	H	23.4375578567	23.6286774284	18.2288580259
O	19.8176762311	24.3360732807	16.0965117686	O	20.1457869341	24.3376880815	16.0803180483
H	19.7301437104	23.4918448613	15.6149014707	H	20.0899718178	23.4970857664	15.5860785422
O	21.0757852028	25.1857676373	17.7356602093	O	21.3922718828	25.1918165304	17.7325115313
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
O	18.9739837233	19.7456917202	15.8655438870	O	19.2934180709	19.7574778565	15.8718099831
H	24.1285793187	21.3475949398	18.5645347034	H	24.4519109632	21.3630794644	18.5532942912
H	15.5172077157	15.2109835652	17.8857170621	Ru	9.2382494606	22.4880133808	14.7479610958
H	15.8537517300	17.3479992375	17.4955912931	C	11.0373655620	21.5508531312	14.7211796072
H	17.1668412668	14.7216034473	17.4197703886	N	12.2663528517	22.1120860017	14.7109447555
C	16.1133233505	14.7052962355	17.1166647969	N	11.1652919592	20.2035916342	14.8624303954
H	18.1022229725	16.6142999778	16.8330637017	C	12.5720493788	19.8212384371	15.1832753043
H	5.0484998633	23.7255149001	17.8621202844	C	13.3399216446	21.1025259830	14.8335469607
C	9.6093313307	19.5914782850	17.1603232056	H	14.0527463798	21.4051728481	15.6096234742
H	15.7941558860	13.6530238651	17.0991281320	H	13.8860514743	21.0074099998	13.8835140164
C	15.7182437919	17.7087299088	16.4702400289	C	10.1340073206	19.1933543237	14.8644439085
C	12.8099047705	24.2526044747	16.4409885469	C	12.6193356661	23.4782526515	14.4105837701
Cl	9.6526288098	23.3560813788	16.6805742492	C	12.7610990662	23.8574053069	13.0570766899
H	13.8617897945	18.6687248660	16.8242764410	C	13.1348883419	25.1777499106	12.7782744119
H	16.2821984907	18.6443771070	16.3582397550	C	13.4081023654	26.1037997901	13.7927359227
C	5.1673917070	23.0287078664	17.0355430418	C	13.373516074	25.6673194679	15.1202834208
C	17.8804632203	16.7691235165	15.7749404817	C	12.9634071009	24.3579222372	15.4577496716
C	14.2453335065	17.9063497375	16.1306317850	C	12.5916633452	22.8710487819	11.9292994658
H	7.2232449452	23.5587439508	16.6648670768	H	13.2325274559	25.4833570369	11.7380326039

H	3.1316141607	22.3024857103	17.1186420594	H	13.5967590439	26.3567408919	15.9226506157
H	13.6627058785	16.9841980611	16.3261774461	C	13.0172358753	23.9315241403	16.9037375245
H	18.2220673061	17.7754872629	15.5060635887	C	9.6838912226	18.6867891331	13.6207428474
C	4.0991094030	22.2229906956	16.6256872732	C	9.7341858627	18.5958373619	16.0801275614
C	15.8947512129	15.2845949143	15.7252272070	C	8.8696041852	17.5460428941	13.6268760428
C	6.3786394563	22.9433569914	16.3601239886	C	8.9263702516	17.4498551938	16.0223814508
H	12.2199234241	19.8864975092	16.1415176322	C	8.5196340403	16.8850718274	14.8100627023
N	16.3946920345	16.7130971995	15.5408510180	H	8.5350967762	17.1442719209	12.6717300780
H	8.0231892621	17.4694728407	16.7194182507	C	10.1595030488	19.1040932481	17.4357880879
C	9.2849468027	18.9627956273	15.8273622244	H	8.6303408079	16.9765095173	16.9576514161
H	13.4949461318	26.5521288139	15.2737273776	C	10.0818126026	19.3003149788	12.3045275427
H	18.3718900125	16.0087729087	15.1590283454	C	7.3087818342	21.9045381694	14.8652019655
H	13.7726927936	21.5411982006	15.4298587291	Cl	9.0255673376	22.6362734545	12.3855297262
C	8.4230390439	17.8553380723	15.7822030382	Cl	9.7447587173	22.6366067210	17.0846322886
H	8.9441377173	25.6317661104	15.5394450525	O	5.7601869372	19.6048976897	14.6249557578
C	12.8268246091	24.5358705932	14.9603858105	C	4.6502414782	18.8011265614	14.1048388376
H	14.8330713452	15.2723561563	15.4590810389	C	4.6425571068	17.37272721561	14.6507847637
C	12.2353498711	20.0027035274	15.0467270313	H	4.9373470078	18.7409838516	13.0468088796
H	16.4361267824	14.7012840927	14.9701727717	C	3.3043851318	19.5163461701	14.1873262845
C	13.2634265674	25.7962181638	14.5243800500	H	2.9435549778	19.6262301436	15.2159387045
C	4.2550251904	21.3085035955	15.5832227476	H	2.5585418902	18.9323026919	13.6298035152
N	14.0873558501	18.3773727268	14.7520145478	H	3.3663415469	20.5136172158	13.7331628874
C	6.5821523233	22.0431275325	15.2827200286	H	5.6436218813	16.9379083472	14.5654694596
C	13.0838022085	21.2126174857	14.6424278989	H	3.9511613825	16.7589781160	14.0557597957
C	8.8114176255	25.3492435874	14.4968133498	H	4.3258504297	17.3028730579	15.6970701731
N	10.8655269054	20.4278208568	14.6262810690	C	5.7520903240	20.1924226675	15.8643015847
C	16.1384093092	17.1867022654	14.1179260417	C	6.5922785785	21.3349697936	16.0276874772
N	12.0679438902	22.2518189878	14.3894805827	C	4.9889682867	19.7348895413	16.9542359700
C	12.6945655762	18.6930422294	14.3972467166	C	5.0421301539	20.3838954701	18.1883787170
Ru	9.2639198920	23.1449086873	14.3338536856	C	5.8598626111	21.5045224442	18.3620983147
C	10.7940252874	21.7693597076	14.3861254996	C	6.6149634608	21.9619962878	17.2890075396
C	9.8131480496	19.4485286411	14.6134316766	H	4.4400821719	20.0106151916	19.0142056316
C	5.4869045885	21.1800511463	14.9235875180	H	4.3466667621	18.8701833246	16.8421392645
H	6.7698142431	24.7181049264	14.7010610935	H	7.2721499815	22.8169181054	17.4234876172
C	7.8143522359	21.9732210903	14.5343240708	H	5.9094233262	22.0165806251	19.3199191802
H	11.9992454214	17.8730155842	14.6530228049	H	7.0508389434	21.4101907269	13.9251979479
C	12.5066214546	23.5671562421	13.9841704199	C	13.0426511124	18.5906757720	14.4020331230
H	3.4084064370	20.7036121477	15.2854456160	H	12.6230783424	19.6189730897	16.2643773940
H	16.6877328615	18.1314763865	14.0221099450	N	14.4713130307	18.3240287070	14.6304452813
H	5.2316914796	18.0761233210	15.2411307431	H	12.9161995103	18.7993632197	13.3309837546
H	3.5668849496	18.6934584041	15.2410225134	H	12.4036452272	17.7208954719	14.6399315552
C	8.0767262180	17.2306932734	14.5787758500	C	15.0258362587	17.4821434137	13.5698232643
C	14.6620655018	17.4066895579	13.8203689198	C	14.7522620440	17.7147251684	15.9360022926
C	7.6110222172	24.8612359438	14.0287335032	C	16.2564856142	17.5887420893	16.1612163153
C	4.3693571955	18.3082739698	14.6037068869	H	14.2470385062	16.7351338488	16.0532107450
H	13.6727210944	21.0167108819	13.7338913117	H	14.3629766543	18.3610628228	16.7359108532
C	13.4402145452	26.0970791384	13.1703018235	C	16.5306608660	17.3374274424	13.7415895263
H	14.1069317887	16.4489305530	13.8060068115	H	14.8614145496	17.9786061593	12.6015773050
C	7.2221087599	15.9847125050	14.5653070974	H	14.5293017023	16.4944449496	13.5054069942
H	9.5761031022	25.7022708852	13.7981091138	N	16.9286245130	16.7460552688	15.0852388720
H	16.5861409583	16.4463371584	13.4435762017	H	16.7512388513	18.5688603596	16.1227622380
H	7.8928246887	21.0923978188	13.8886681162	H	16.4871091883	17.1328549967	17.1301745251
O	5.7384687186	20.2961098104	13.9187585553	H	17.0050542739	18.3261568289	13.7079048535
C	13.9118786353	27.4640618347	12.7368964526	H	16.9739609955	16.7036361652	12.9639556003
C	9.4333822751	18.8824068610	13.3738871428	C	18.4228864434	16.8856677024	15.2088235757
H	12.6576418698	18.8198526768	13.3065478590	H	18.9029089452	16.2392217185	14.4683059764
H	4.0116205928	17.3710355474	14.1530020291	H	18.7418153740	16.6266019180	16.2218029394
C	8.5657967528	17.7819448789	13.3871407189	H	18.6798904086	17.9387168162	15.0420494661
C	12.7638507902	23.8070036007	12.6127946024	C	16.5489918222	15.2715317900	15.1555121823
C	4.7843337377	19.2664556567	13.4838489339	C	16.8921911351	14.5866192615	16.4724390510
H	14.6017288420	17.8178538805	12.8011632428	H	17.0909688386	14.8074299370	14.3220385387
C	13.2074209662	25.0801377393	12.2355453489	H	15.4779634828	15.1959691820	14.9421506579
H	7.4124553319	24.7791325091	12.9633814915	H	17.9546148332	14.6726511795	16.7304376066
H	2.8879916105	20.3753879665	13.2994990096	H	16.6670569683	13.5156529170	16.3646533699
Cl	9.2839349241	23.2025446247	11.9635861004	H	16.2946074019	14.9598293222	17.3126452414
C	3.6191629970	19.8444717621	12.6794296702	C	13.8030827318	27.5234473068	13.4648156907
H	5.4252486756	18.7063616985	12.7913705074	C	7.7875984678	15.5643880962	14.7805270246
C	9.9333437853	19.4264653463	12.0596543204	C	8.5152332701	24.3407294701	14.8768742270
C	12.6406086721	22.7256087100	11.5698068216	C	7.2128120298	23.5036371917	14.6860497053
H	8.2847549854	17.3291418683	12.4372938028	H	8.7288052580	25.0007281951	14.0339302316
H	13.3914706219	25.2759504380	11.1805277586	H	8.6213920613	24.7927602266	15.8660676414

H	3.0905749526	19.0210159084	12.1762782123	H	6.8508927356	23.6634090413	13.6650609884
H	3.9843107207	20.5358496762	11.9088738568	H	6.5029415883	23.8132922667	15.4601556742
H	12.4112695855	23.2616009256	16.6736931040	H	13.8194975975	27.6962154010	12.3815670728
H	12.1806601182	24.9769331277	16.9757746224	H	14.8015456024	27.7608088368	13.8601048408
H	13.8303542074	24.3363526813	16.8428015930	H	13.1012387466	28.2432841226	13.9103490248
H	10.1905596139	20.5151265819	17.0607789916	H	12.6483694760	22.9127371950	17.0546178297
H	10.1498717645	18.8884580900	17.8107993328	H	12.4002953553	24.5871975860	17.5333775423
H	8.6805405786	19.8634970030	17.6828014997	H	14.0519234153	23.9987144989	17.2721209170
H	6.9648984607	15.6845678187	13.5417315727	H	10.7231685335	20.0409195407	17.3851977497
H	6.2849478566	16.1248530361	15.1210013894	H	10.7519394264	18.3443772582	17.9663922344
H	7.7476633356	15.1419963761	15.0379188996	H	9.2725188169	19.3117807421	18.0526031760
H	14.0185742425	27.5268907102	11.6470019279	H	12.7240354266	23.3709512160	10.9618211615
H	14.8849358871	27.7093505143	13.1867463114	H	11.5986250736	22.4008880759	11.9366944089
H	13.2059393264	28.2458858546	13.0523206497	H	13.3501690519	22.0755145248	11.9882733953
H	12.8419567366	23.1345482870	10.5718652751	H	9.6370311508	18.7408902516	11.4727025898
H	11.6345974417	22.2862185680	11.5592778752	H	11.1716987796	19.3000708209	12.1637015215
H	13.3718495723	21.9223415022	11.7454946786	H	9.7532128480	20.3489467942	12.2243170516
H	9.5227192893	18.8461257623	11.2242539822	H	7.3633858241	15.3563402667	13.7898500761
H	11.0294704697	19.3861603968	11.9865352132	H	6.9747302499	15.5279165866	15.5184099945
H	9.6511857419	20.4830987320	11.9192003073	H	8.4735991517	14.7393573455	15.0246597645
Ci2				I14e			
223				197			
i =	16, E =	-1508.6061006353		i =	112, E =	-1421.7167583376	
Cr	26.1593888107	15.0119937981	17.2143948774	Cr	24.9697534923	15.0979232345	17.2067523356
Cr	22.8383848657	15.7220288634	17.5462033639	Cr	21.6544235467	15.7919158778	17.5408426571
Cr	25.1026255887	17.3608651752	19.4279042608	Cr	23.9264329623	17.4508571926	19.4227619827
O	24.6020440042	16.0975985747	18.1296228530	O	23.4154808682	16.1893891248	18.1237182771
O	25.2383063377	13.3015432795	17.7364799960	O	24.0461862832	13.3819879066	17.7312296119
O	25.3131368564	15.0042103069	15.4164875564	O	24.1111827691	15.0918563710	15.4105004627
O	27.0831475395	16.7085193519	16.7246568792	O	25.8951770039	16.7976552526	16.7135215127
O	27.1675207955	14.8527547685	18.9149994355	O	25.9756248163	14.9359748424	18.9044235016
O	23.3338405948	16.0867517459	15.6991448371	O	22.0940560776	16.1067729114	15.6906574985
O	22.3480301513	15.3141728157	19.4473084897	O	21.2262235966	15.3922897545	19.4490334707
O	23.0424899705	13.7674609835	17.3425382287	O	21.8542413041	13.8504787349	17.3376228802
O	26.0720508320	16.0149131685	20.5345965838	O	24.8790053380	16.1006128236	20.5252182726
O	26.7667958209	17.9644325787	18.5941899596	O	25.5864001400	18.0492934832	18.5846182704
O	23.4957505638	16.9499740684	20.5445413587	O	22.3228702482	17.0529419360	20.5435435419
C	24.0169922825	12.9791489352	17.6227572841	C	22.8254720836	13.0598928841	17.6166894374
C	23.6665679078	11.5416317815	17.8229476854	C	22.4637755644	11.6246366393	17.8117630244
C	22.3207093864	11.1451013510	17.7895109808	C	21.1161450829	11.2311514050	17.7827151095
C	24.6709100241	10.5882555077	18.0535719804	C	23.4693386992	10.6729385480	18.0353617816
C	24.3278962858	9.2492046113	18.2427300997	C	23.1271713405	9.3345993242	18.2232167331
C	22.9801526012	8.8502845856	18.2085105811	C	21.7799666587	8.9354370509	18.1940285325
C	21.9802925203	9.8126817091	17.9885421677	C	20.7782141793	9.8977000847	17.9806168539
H	25.7083628502	10.9135872618	18.0847173316	H	24.5060321963	11.0008503312	18.0607980365
H	21.5616977112	11.9034362331	17.6110156967	H	20.3552357326	11.9885427513	17.6088617067
C	27.5565469606	14.2803779226	21.1676896458	C	26.3524872388	14.3629716184	21.1578330185
C	28.3137704403	13.1691689750	20.7675468237	C	27.1028089973	13.2472027021	20.7582950229
C	27.4100191469	14.5703800597	22.5335584836	C	26.2030605074	14.6585230261	22.5220378776
C	28.9396995441	12.3699011095	21.7219862096	C	27.7152429972	12.4436512266	21.7157655208
C	28.8029336910	12.6603475119	23.0894987679	C	27.5756852171	12.7396037591	23.0819703254
C	28.0230867489	13.7609393563	23.4865325778	C	26.8036951715	13.8449820197	23.4777816845
C	29.4164647072	11.8169390542	24.1568736052	C	28.1977803172	11.9025026322	24.1518416099
H	26.8158760608	15.4321154988	22.8310265749	H	25.6131181564	15.5254543994	22.8107415255
C	26.8862499271	15.1151423229	20.1274209285	C	25.6888886338	15.1970798455	20.1166670897
C	22.6549329511	15.9850048746	20.4849329612	C	21.5011680106	16.0741597373	20.4860908282
C	21.9411682323	15.6064258802	21.7433629554	C	20.7876254910	15.6927389140	21.7437350455
C	22.2990541928	16.1909199092	22.9660644450	C	21.1439608300	16.2793210495	22.9668483974
C	21.6395137773	15.8211492403	24.1386044138	C	20.4799872167	15.9115641217	24.1367397571
C	20.6039765349	14.8701630034	24.1026120424	C	19.4449991182	14.9619283660	24.0979402806
C	20.2386533018	14.2987998119	22.8719838108	C	19.0793715201	14.3903592754	22.8670110832
C	20.9058191214	14.6555131061	21.7040527566	C	19.7508744107	14.7441295956	21.7008466745
H	23.0947429250	16.9317841388	22.9799846899	H	21.9394055107	17.0198837182	22.9869150932
H	20.6380079827	14.2117447081	20.7478554812	H	19.4851714189	14.3021767126	20.7431396269
C	19.8330262483	14.4529747486	25.3176344523	C	18.6783579329	14.5411559047	25.3127864832
O	22.3138732617	17.6099775949	17.7352533340	O	21.1468574472	17.6716795356	17.7303026259
O	24.1100713229	18.8092990134	18.4309654051	O	22.9280490142	18.8915214134	18.4271878234
H	28.3928656615	12.9427394300	19.7072607550	H	27.1818202303	13.0189914738	19.6982981407
C	24.2748215694	15.5915592727	14.9849959512	C	23.0561459442	15.6449290052	14.9749614372
C	24.1279650155	15.7109059435	13.5063961497	C	22.9135925345	15.7604661476	13.4963435381
C	25.1103648531	15.1427818244	12.6811444887	C	23.9085421893	15.1950760999	12.6832683108

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

H	15.9833959174	16.8200200914	16.2911483188	H	13.8558504879	14.6379051738	16.0730347310
H	15.3784301716	14.6998902791	16.1316389867	H	15.4669388227	14.0577042609	15.5731563393
H	17.0157514817	14.1864572855	15.6488100108	C	14.4452335616	14.2574516255	15.2302870191
C	15.9887665807	14.3366409257	15.2964835322	H	12.6259430066	18.3350968790	15.9124623489
H	14.0846414651	18.3847034819	15.9446859993	C	14.4094332904	17.3495478790	15.3323496317
C	15.8878171763	17.4226451457	15.3810961328	H	16.6768099700	15.9173676606	15.3860448253
H	18.1826230716	16.0609196271	15.4582934349	H	15.0442088214	18.2402344528	15.4451720373
H	16.5178109431	18.3168001137	15.5023656228	H	13.3358024882	26.2552017939	16.3853449627
H	14.2866348874	26.3663059024	16.4180022037	H	14.0038323579	13.2920585393	14.9392070728
H	15.5928373463	13.3504927954	15.0116367598	C	12.9568138661	17.7250560125	15.0594405525
C	14.4334585463	17.7814356646	15.0941165646	H	11.1066596667	19.8730170235	15.5324509016
H	12.4910896837	19.8317617214	15.5547001465	H	6.3682451072	18.2139127504	15.3555074249
H	7.9210737895	17.8794945813	15.4003340248	C	12.4455982141	24.4719403437	15.5797243775
C	13.4760321759	24.5507932376	15.6012060977	C	16.5067792108	16.4198730061	14.4289030757
C	17.9993979251	16.5146835258	14.4794470058	C	8.0142627809	19.5137408761	14.8978430842
C	9.4472310082	19.3141598073	14.9315348839	H	12.3065070638	16.8275655418	15.0468853384
H	13.7935547847	16.8760659769	15.0720199305	C	13.0499023848	25.7337115348	15.4728114778
C	14.0395310377	25.8321700019	15.5016389681	H	12.9665689723	21.3160115673	15.1497706709
H	14.2342857346	21.4301988178	15.2547243721	H	16.9530180075	17.4220720833	14.4790629787
H	18.4338208638	17.5209700815	14.4818088006	C	6.8997268213	18.7316893943	14.5580879475
C	8.4162511329	18.4241875261	14.5973935671	N	15.0209570099	16.5525703595	14.1875227282
N	16.5129608567	16.6297710296	14.2409059826	C	14.3902784872	15.1701867304	14.0135188626
C	15.9057409408	15.2382607317	14.0727280319	C	11.1734444828	20.2151248879	14.4864818412
C	12.5624940475	20.1904327755	14.5154726799	C	12.2071045843	21.3368215920	14.3588673682
C	13.5188219683	21.3863457896	14.4251169274	N	11.3853552820	22.5527025344	14.4673781814
N	12.6024938433	22.5452434878	14.4708558736	C	10.0442186196	22.2992789280	14.3122548989
C	11.3049775158	22.1788788772	14.2820927759	N	9.9134827575	20.9248700772	14.1489140018
N	11.2603256763	20.8177909609	14.1587679404	N	12.8417648725	18.5105834909	13.8276938802
N	14.3171507791	18.5669235548	13.8591340755	C	12.0475438267	23.8240992771	14.3939245327
C	13.1505613437	23.8723965743	14.4073408143	H	16.9412738898	15.8371014383	13.6096819286
H	18.4350851474	15.9029242334	13.6826222635	C	8.7029745483	20.1918236388	13.8665173620
C	10.0896579129	20.0186509644	13.8881347381	H	13.3521441257	15.3322073040	13.7072448343
H	14.8635393350	15.3757078374	13.7682090397	C	11.4804474532	19.0187557211	13.5785091964
C	12.9448674377	19.0290271064	13.5940828999	C	13.2681168882	26.3499351965	14.2346721403
C	14.3024741265	26.4344956239	14.2660517195	H	14.9199637865	14.7243316191	13.1621999608
H	16.4443392263	14.7991709905	13.2235351807	H	10.7076953644	18.2368801194	13.6901528809
H	12.1990961357	18.2164573472	13.6768893804	C	6.4555484031	18.5964643473	13.2395518221
C	8.0206788767	18.2013808446	13.2753082112	C	14.8111429740	17.3606570263	12.9135769895
C	16.3045953788	17.4368937730	12.9683651688	C	13.8527518330	27.7389991825	14.1528941831
C	14.8882879564	27.8236896461	14.1882379766	H	15.4269068121	18.2609238105	13.0287399683
H	16.9015695663	18.3480182015	13.0979841247	C	13.3522437440	17.7470095592	12.6905332637
C	14.8446891088	17.8021947037	12.729378674	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
C	11.301283085300	12.529949802300	8.529215664500	C	16.354896248300	17.574917670900	13.506784764400
C	12.317860155000	11.984982777800	7.730623479400	C	17.348997243400	17.011527481000	12.693649247100
C	12.198801959800	12.022990009800	6.343789175900	C	17.215062323700	17.057879950700	11.307674525900
C	11.063716043700	12.597466934500	5.748429821400	C	16.085564710000	17.659611318500	10.723756310700
C	10.041482529200	13.126072343000	6.553730720000	C	15.094365967000	18.222480528800	11.546333552600
C	10.161419840500	13.100109669500	7.938096322800	C	15.228483606500	18.190279553300	12.931358013200
H	9.380566950000	13.500709120900	8.580408426000	H	14.469963830100	18.623180657600	13.584852074100
H	13.179107220200	11.526591165400	8.210647550400	H	18.201721100800	16.528119329800	13.165476446100
C	10.204177829300	15.579529083100	13.036388222600	C	15.137095138000	20.538848619500	17.947313349900
C	9.558832752000	16.887853915100	12.755122738700	C	14.436876955700	21.838451745500	17.661968298900
C	8.279291548800	16.919483159600	12.179859773900	C	13.164735981300	21.958744881500	17.036904931600
C	7.663242042600	18.142738873500	11.929100515800	C	12.626724657800	23.240859995800	16.858260893900
C	8.316464337200	19.340986515500	12.260917359800	C	13.292359209000	24.402324009500	17.270783810700
C	9.589187596300	19.304458483700	12.853608220000	C	14.540509237700	24.278182172600	17.898779927800
C	10.214071450900	18.085348099800	13.089430652900	C	15.096113949000	23.015666304000	18.077601926800
H	11.203725282100	18.040387972800	13.537876226400	S	12.114657082700	20.618523051300	16.356833027200
H	7.782471627300	15.982409283300	11.941581359400	C	19.498587306500	19.595249026200	17.445520078400
C	14.471815519600	14.539977182700	12.445310609700	C	20.459752817200	20.615926691300	16.920294526800
C	15.433533514600	15.538465856100	11.908895709000	C	20.733005320800	21.770686777100	17.671182906900
C	15.774224645500	16.660776049700	12.681941521900	C	21.602667753500	22.735772954100	17.172473659700
C	16.664859930200	17.599743819900	12.177131454800	C	22.221118545800	22.560877113500	15.922375572200
C	17.230955619900	17.421958221500	10.904021644500	C	21.945458051600	21.399441326500	15.176257098100
C	16.884073650200	16.300972066800	10.132874313200	C	21.069848226700	20.432633808400	15.670434900800
C	15.987058750500	15.359922822800	10.632303492700	H	20.835194726900	19.536658504200	15.099470934500
H	15.698579847800	14.490011778400	10.047211984300	H	20.246215083000	21.891974151200	18.636682410100
H	15.330185908700	16.777496971200	13.668072405200	O	13.286082219200	17.188028291000	17.112440503400
O	8.256169219600	12.324266715900	12.105088719700	O	19.686635878600	15.951513038000	16.4111714510200
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
H	15.443778590000	10.915682019700	12.014881607000	H	12.735803126200	18.002001655800	17.128495348700
H	7.691957325700	13.043409324000	12.434535652800	H	20.125986053300	15.809322730000	24.545939693100
H	15.094737415800	10.794149035100	19.550759872600	H	21.705285909800	13.320005075800	21.400519187000
H	16.675264663000	8.277943031900	16.428999419900	O	21.155405778200	13.535059245400	25.283317881000
O	16.173241646300	8.592119474400	20.315869485600	O	22.716604564000	12.908174607100	23.801830084900
O	17.740614940800	7.962919731900	18.835640180500	H	23.011130809500	13.186040939000	22.915267486500
H	18.022415446700	8.220033508500	17.938825086700	H	21.818430628000	23.643144231800	17.731995144600
H	16.938867363000	18.485633159700	12.746005636700	H	22.373008307100	21.252200657500	14.184011933300
H	17.277062266300	16.172612330700	9.124470229200	C	23.125617068400	23.653623305800	15.443510567900
C	18.159633465000	18.486606314000	10.422663809800	O	23.100609189400	24.795289557500	15.865609672500
O	18.134982603200	19.621856988200	10.853944831400	O	24.035246690900	23.318016018100	14.464348098400
O	19.064885956200	18.130808301400	9.452248521600	H	23.995416454600	22.355380574400	14.308945608300
H	19.022774085400	17.168979772700	9.300738179700	C	15.877128596900	17.690289853800	9.246699011200
C	10.868639948900	12.639260472600	4.269340980200	H	14.222371364100	18.676778571800	11.080640377800
H	9.162713131100	13.545277328500	6.068425251800	H	17.970244955800	16.574165476900	10.688715877900
H	12.973594368800	11.560289745400	5.732931569500	O	14.786607726700	17.735528099200	8.708991847700
O	9.773344190800	12.658415878500	3.742672682200	O	17.024113470900	17.657002968900	8.474030890500
O	12.014374246500	12.656169015200	3.506346760600	H	17.797239350800	17.747054424900	9.060644438200
H	12.789925839500	12.749207803300	4.089251581500	H	13.190451622900	11.338454738000	17.956907060000
H	8.188818446000	6.340168081700	12.795143921400	H	17.365059364900	10.384447122300	18.468986411100
H	12.337121562000	5.423894361500	13.507405677700	C	14.805305097600	9.281086406300	18.409987240000
C	9.774894213300	4.333460191800	13.396210999900	O	13.686059333200	8.943654898200	18.744641844000
O	8.650021703400	4.050984233300	13.754559338400	O	15.769201453100	8.315864762600	18.200720128600
O	10.707128946300	3.346520390600	13.202356367200	H	16.565772380800	8.733175122400	17.827207705800

H	11.512493268900	3.727299957400	12.807035153200	H	14.137341668200	18.164413323300	25.072525024700
H	9.063718983800	13.225601808700	20.065774629800	H	11.653048474200	15.432028073000	22.846798819000
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
H	6.655889887800	18.154377706700	11.513481480100	H	15.059412807600	25.175411309600	18.229765882300
H	10.064554469600	20.245953760800	13.120571022900	O	11.819844031700	25.899621056100	16.023982772300
O	6.794690685200	20.786908336000	11.016699145000	H	11.722712138200	25.040486890400	15.569673117200
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