

Theoretical insights into the reaction mechanism between tetrachloro-*o*-benzoquinone and *N*-methyl benzohydroxamic acid

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Electronic supplementary information

The relevant calculations using the M06 function

To further testify the reliability of the B3LYP functional, the M06 function within the framework of density functional theory has been employed to investigate the reaction of the tetrachloro-*o*-benzoquinone (*o*-TCBQ) with neutral *N*-methyl benzohydroxamic acid (*N*-MeBHA) in the presence of one water molecule and the direct reaction of *o*-TCBQ with the anion of the *N*-MeBHA in combination with the 6-311++G(d,p) basis set. As a result, it was found that the optimized geometries including reactants and transition states are similar to those at the B3LYP/6-311++G(d,p) level. Correspondingly, the calculated energy barriers are 23.17 and -36.80 kcal/mol relative to the separated reactants for the former and the latter reactions, respectively, which are well consistent with the results at the B3LYP/6-311++G(d,p) level. So, both levels suggest that the reaction between *o*-TCBQ and neutral *N*-methyl benzohydroxamic acid is difficult to take place under mild conditions. Therefore, the relevant discussions will be mainly focused on the reaction of *o*-TCBQ with the anion of the *N*-MeBHA in this study. Moreover, considering the balance between the computational cost and accuracy, the B3LYP/6-311++G(d,p) level has been employed in this study. Actually, the relevant calculations at the M06/6-311++G(d,p) level are beyond our best computational ability if more water molecules are considered.

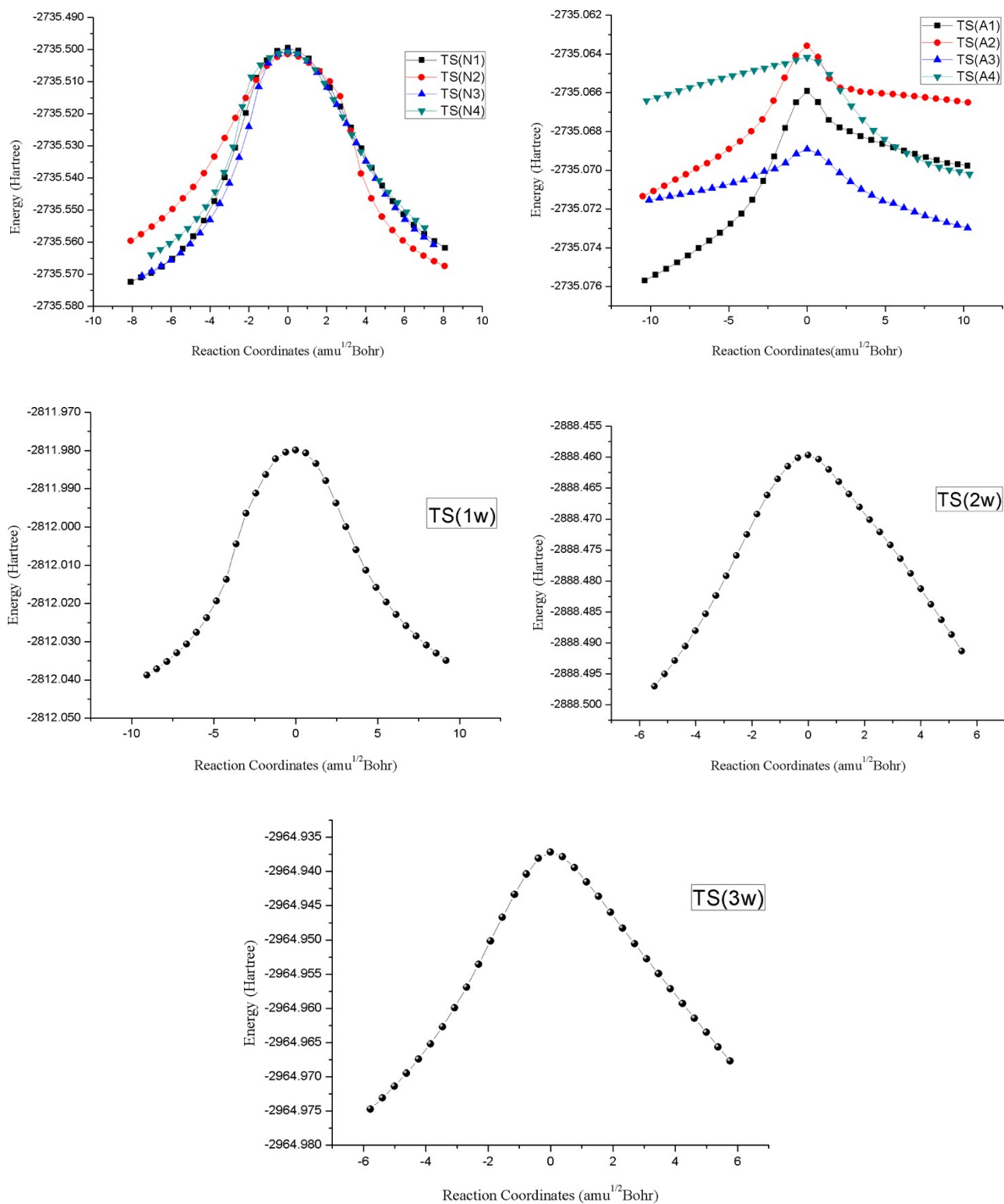


Figure S1. The IRC calculations on the basis of the optimized transition states at the B3LYP/6-311++G(d,p) level.

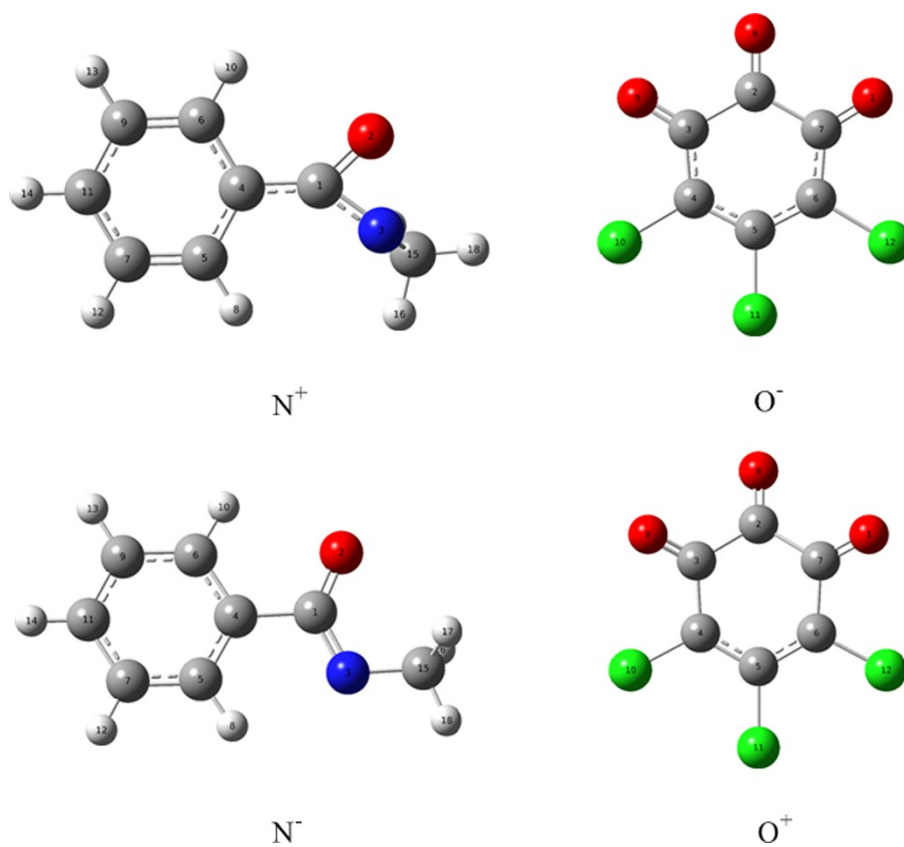


Figure S2. The products for the heterolytic cleavage of N-O bond of IM(A2) after the dissociation of Cl^- .

Cartesian coordinates of all the species mentioned in this study

<i>N</i> -MeBHA				<i>N</i> -MeBHA ⁻				<i>N</i> -MeBHA ⁻ (PCM)			
C	-1.30088900	1.18760000	0.42739300	C	1.03230500	0.59707300	-0.00004500	C	1.06264100	0.52539500	-0.29606500
C	-0.43401100	0.23244400	-0.11233400	O	1.31560400	1.83083000	-0.00007800	O	1.38151100	1.58159900	-0.92130900
C	-0.95400200	-0.97737400	-0.58380600	N	1.99110500	-0.35594700	0.00001800	N	1.95052100	-0.32765500	0.21456700
C	-2.32005900	-1.23237700	-0.50502100	O	1.81393000	-1.68799500	0.00009800	O	1.60241300	-1.41510000	0.96935600
C	-3.17571300	-0.28786100	0.06112600	C	-0.41466500	0.18889600	-0.00001400	C	-0.39595800	0.20290200	-0.11433700
C	-2.66334400	0.92216300	0.52736700	C	-0.91118500	-1.12877900	-0.00008800	C	-0.98205700	-0.90281100	-0.74171800
H	-0.89514400	2.13471400	0.76158100	C	-1.34642400	1.24456300	0.00004900	C	-1.20821400	1.08820500	0.60306700
H	-0.29860900	-1.70709800	-1.04490500	C	-2.28758800	-1.36458600	-0.00005300	C	-2.35602000	-1.12080600	-0.64894300
H	-2.71767200	-2.16536200	-0.88826100	H	-0.18715500	-1.93237700	-0.00018600	H	-0.36304600	-1.59232800	-1.30440200
H	-4.23847500	-0.49115300	0.13004000	C	-2.71574000	1.00251400	0.00006300	C	-2.58089300	0.86051600	0.71089300
H	-3.32639900	1.66251300	0.96029300	H	-0.94969600	2.25248500	0.00009500	H	-0.76512400	1.95485500	1.08151000
C	1.01028300	0.60468400	-0.25096600	C	-3.19852100	-0.30904900	0.00002400	C	-3.15907800	-0.24322200	0.08299200
O	1.35699200	1.72683300	-0.57953700	H	-2.64901100	-2.38945500	-0.00009800	H	-2.79953000	-1.97706100	-1.14535600
N	1.95830500	-0.40076000	-0.06766800	H	-3.41100200	1.83767400	0.00010000	H	-3.19725400	1.54766200	1.28020200
O	1.62644000	-1.36550100	0.91801200	H	-4.26763500	-0.50221700	0.00005900	H	-4.22650000	-0.41748300	0.16052300
H	1.56740500	-2.20242300	0.44058600	C	3.38862100	0.05111500	0.00001400	C	3.38447000	-0.12636100	0.06248100
C	3.36737500	-0.03149900	-0.00002900	H	3.87419300	-0.37219200	0.88668100	H	3.83441500	0.04525600	1.04503900
H	3.56956000	0.68683500	-0.79131500	H	3.87426900	-0.37262300	-0.88639500	H	3.82404300	-1.02893700	-0.37047200
H	3.61596200	0.41766900	0.96707300	H	3.46121800	1.13717700	-0.00025500	H	3.57861600	0.72672300	-0.58360800
H	3.96994600	-0.92771400	-0.15158400								
<i>o</i> -TCBQ				<i>o</i> -TCBQ(PCM)				H ₂ O			
C	-0.78016200	1.73275000	0.00008800	C	-0.00615600	-0.77922700	1.72052200	O	0.00000000	0.00000000	0.11704100
C	0.78016600	1.73275000	0.00009900	C	0.00615600	0.77922700	1.72052200	H	0.00000000	0.76348700	-0.46816500
C	1.45930400	0.41679400	0.00004400	C	0.00134300	1.45803800	0.41668000	H	0.00000000	-0.76348700	-0.46816500
C	0.74117500	-0.73400400	0.00002000	C	-0.00134300	0.74165100	-0.73493800				
C	-0.74117500	-0.73400400	0.00002200	C	0.00134300	-0.74165100	-0.73493800				
C	-1.45930400	0.41679600	0.00004100	C	-0.00134300	-1.45803800	0.41668000				
O	-1.36728800	2.78329500	-0.00010100	O	-0.01780900	-1.35840300	2.78245700				
O	1.36729200	2.78329300	-0.00009800	O	0.01780900	1.35840300	2.78245700				
Cl	3.18320400	0.45258600	0.00002000	Cl	0.00126600	3.18568700	0.45303500				
Cl	1.54775600	-2.26197700	-0.00003200	Cl	-0.00702500	1.54810100	-2.25734400				
Cl	-1.54776000	-2.26197500	-0.00002400	Cl	0.00702500	-1.54810100	-2.25734400				
Cl	-3.18320400	0.45258900	0.00001800	Cl	-0.00126600	-3.18568700	0.45303500				
<i>p</i> -TCBQ				<i>p</i> -TCBQ(PCM)							
C	-0.00000200	-1.45701500	-0.00068500	C	0.00000000	0.00000000	1.45197100				
C	-1.27939400	-0.67372300	-0.00017400	C	0.00000000	1.27688800	0.67273800				
C	-1.27939300	0.67372400	0.00003700	C	0.00000000	1.27688800	-0.67273800				
C	0.00000300	1.45701500	0.00033000	C	0.00000000	0.00000000	-1.45197100				
C	1.27939500	0.67372300	0.00004100	C	0.00000000	-1.27688800	-0.67273800				
C	1.27939300	-0.67372400	-0.00015000	C	0.00000000	-1.27688800	0.67273800				
O	-0.00000200	-2.66363700	0.00044000	O	0.00000000	0.00000000	2.66315600				
Cl	-2.71934100	1.61469000	0.00019600	Cl	0.00000000	2.71987500	-1.61251700				

Cl	2.71934500	1.61468600	0.00020500	Cl	0.00000000	-2.71987500	-1.61251700			
Cl	2.71934000	-1.61469000	-0.00005700	Cl	0.00000000	-2.71987500	1.61251700			
Cl	-2.71934500	-1.61468600	-0.00012700	Cl	0.00000000	2.71987500	1.61251700			
O	0.00000200	2.66363700	-0.00045000	O	0.00000000	0.00000000	-2.66315600			
MC(N1)				TS(N1)				IM(N1)		
C	-3.33030400	0.04513900	-1.68856000	C	1.90968900	2.15372900	1.60550700	C	-1.26200900	2.51246900
C	-3.09681600	-0.66149500	-0.50393600	C	2.33705900	1.31092900	0.57109400	C	-1.90995100	1.40984000
C	-3.51505800	-0.11624600	0.71464800	C	2.37212200	1.78929700	-0.74362800	C	-2.12731600	0.26184000
C	-4.14702100	1.12345300	0.74755200	C	1.97466700	3.09489300	-1.01751400	C	-1.68936000	0.21535800
C	-4.35149500	1.83590700	-0.43363300	C	1.52388400	3.92142500	0.01042700	C	-1.01835600	1.30339200
C	-3.94134800	1.29493400	-1.65160300	C	1.48926000	3.44825300	1.32243300	C	-0.80324900	2.45148500
H	-3.03447100	-0.39963100	-2.63097100	H	1.92051400	1.78431400	2.62372300	H	-1.13206400	3.41419600
H	-3.37485100	-0.66937100	1.63524500	H	2.72248100	1.15378600	-1.54620300	H	-2.65559900	-0.58415700
H	-4.48118100	1.53223300	1.69427600	H	2.01664300	3.46641100	-2.03471500	H	-1.87464800	-0.67110500
H	-4.83627100	2.80532100	-0.40514200	H	1.20695000	4.93466900	-0.20904600	H	-0.67312700	1.26127500
H	-4.10728500	1.84158800	-2.57294000	H	1.14656600	4.09140400	2.12461000	H	-0.29167900	3.30411000
C	-2.49677000	-2.02809700	-0.62468900	C	2.85937700	-0.02992900	0.96954700	C	-2.47567200	1.56844500
O	-2.77393100	-2.77432500	-1.54860200	O	3.49503400	-0.20760200	1.98963600	O	-3.24059000	2.47321000
N	-1.65306400	-2.46539900	0.39619800	N	2.66873800	-1.12188900	0.11047000	N	-2.05203400	0.70843800
O	-0.86091900	-1.45246400	0.98887000	O	1.60572400	-1.03047200	-0.81174100	O	-1.26235600	-0.42716100
C	-0.90361300	-3.70330300	0.20783900	C	3.09641100	-2.47517400	0.46531100	C	-2.71911000	0.56579800
H	-1.58438800	-4.45514100	-0.18480500	H	4.01648700	-2.36127800	1.03372200	H	-3.35266700	1.44208900
H	-0.07419000	-3.56831800	-0.49406700	H	2.34747500	-2.99130000	1.06423000	H	-1.97529000	0.54045300
H	-0.51508200	-4.02443000	1.17459200	H	3.30110700	-3.02831700	-0.45301900	H	-3.33569600	-0.33710600
C	2.01888800	-0.81749200	1.41213900	C	-1.82750600	-1.17521600	1.50382600	C	2.25826300	1.14033200
C	1.11215900	0.34589300	1.91300000	C	-0.46128400	-1.67978500	0.88367200	C	0.77929100	0.81546600
C	0.99389000	1.53475600	1.04433200	C	-0.16531000	-1.18824000	-0.45957600	C	0.08151900	-0.18618000
C	1.54833200	1.54222200	-0.19341400	C	-0.85967800	-0.18391700	-1.03654200	C	0.82055600	-1.02228600
C	2.30509300	0.38272800	-0.72096200	C	-2.08320500	0.34258700	-0.40764200	C	2.27571900	-0.84982100
C	2.52555800	-0.72756700	0.02478900	C	-2.54772700	-0.11620600	0.78515700	C	2.96020600	0.17431300
O	2.27800100	-1.72578600	2.15894100	O	-2.18738000	-1.67437400	2.53708900	O	2.76265700	2.13919100
O	0.54835300	0.23685300	2.97408000	O	0.23708100	-2.40352800	1.54358200	O	0.28824600	1.34031200
Cl	0.09688900	2.86087700	1.68436100	Cl	0.15283800	-3.04062400	-1.83989500	Cl	-3.49515300	-3.01395800
Cl	1.38038900	2.92666500	-1.21235300	Cl	-0.39727600	0.38675000	-2.60177500	Cl	0.04120600	-2.36582800
Cl	2.91302000	0.48202600	-2.33556600	Cl	-2.93939600	1.57831200	-1.25617200	Cl	3.08653800	-1.97884000
Cl	3.41958600	-2.08701100	-0.54811900	Cl	-3.98493800	0.48164200	1.53637700	Cl	4.64391000	0.45002300
H	-1.04984600	-1.48713400	1.93761000	H	1.59953800	-1.84789000	-1.41263500	H	-2.45234800	-2.24969400
MC(N2)				TS(N2)				IM(N2)		
C	-1.11255600	0.35479700	-1.91438300	C	1.70449300	-1.69874800	0.13012600	C	-1.42764100	-1.59487100
C	-2.02142300	-0.80749900	-1.41488300	C	3.15480000	-1.11586700	0.02042100	C	-2.94531200	-1.35604400
C	-2.52342500	-0.72094400	-0.02560600	C	3.26205700	0.33880700	-0.04519100	C	-3.44450600	0.02723300
C	-2.29754500	0.38615300	0.72326000	C	2.15421200	1.12629600	0.10007900	C	-2.59190600	1.03475400
C	-1.53913500	1.54527700	0.19732600	C	0.81317900	0.59808000	0.35397400	C	-1.13430900	0.81084700
C	-0.98859700	1.54052100	-1.04215900	C	0.63283000	-0.74110300	0.49845300	C	-0.58653700	-0.43225100

O	-0.55189100	0.24756300	-2.97726700	O	1.49612700	-2.85842100	-0.11649500	O	-0.99210100	-2.72068900	-0.33099400
O	-2.28585600	-1.71225800	-2.16410400	O	4.07307100	-1.89496700	-0.05792500	O	-3.64417300	-2.28774300	-0.78805200
Cl	-3.41967200	-2.07977200	0.54535900	Cl	4.84790800	0.97831700	-0.32589500	Cl	-5.14038400	0.25296700	-0.52942200
Cl	-2.90037800	0.48164400	2.34001400	Cl	2.31101600	2.84496500	0.00527100	Cl	-3.18615900	2.64199800	0.20383100
Cl	-1.36414600	2.92575900	1.22051600	Cl	-0.48899200	1.67878200	0.74231300	Cl	-0.13339700	2.19131100	0.39904700
Cl	-0.09007200	2.86640400	-1.68055500	Cl	0.02448500	-1.53291700	2.44904000	Cl	1.95541100	-4.08363400	-0.28875900
C	3.32331100	0.03666700	1.68633600	C	-3.81268000	1.34004600	-0.78009800	C	3.72181500	2.00673000	0.04318800
C	3.08946000	-0.67064100	0.50217100	C	-3.27055200	0.05291400	-0.67012200	C	3.11562500	0.74428700	0.07906400
C	3.51327400	-0.12916000	-0.71616300	C	-3.75894800	-0.82156000	0.30744800	C	3.16610100	-0.07691000	-1.05322600
C	4.15104300	1.10755700	-0.74933100	C	-4.76346600	-0.40624500	1.17564100	C	3.80149600	0.37224900	-2.20900900
C	4.35591000	1.82080200	0.43130100	C	-5.28042000	0.88450700	1.07880300	C	4.37087500	1.64329600	-2.25129100
C	3.94024500	1.28354800	1.64905200	C	-4.80540900	1.75637200	0.09810400	C	4.32904500	2.46138800	-1.12208300
H	3.02304200	-0.40532500	2.62865300	H	-3.44417600	2.00051100	-1.55513800	H	3.71626800	2.61843300	0.93724200
H	3.37284000	-0.68300100	-1.63630000	H	-3.38528100	-1.83537100	0.37653300	H	2.73841100	-1.06981200	-1.03104700
H	4.48943600	1.51337600	-1.69582400	H	-5.14328000	-1.09046400	1.92502500	H	3.85351500	-0.27639600	-3.07596900
H	4.84527600	2.78789900	0.40257800	H	-6.05747400	1.20824200	1.76182300	H	4.85502300	1.99151900	-3.15680700
H	4.10644600	1.83079400	2.56998800	H	-5.21237300	2.75749100	0.01703200	H	4.78209800	3.44593100	-1.14531700
C	2.48261500	-2.03417200	0.62341500	C	-2.25971500	-0.34567400	-1.68465200	C	2.56613200	0.30418900	1.40162300
O	2.75381800	-2.78038800	1.54908800	O	-2.24190100	0.08225800	-2.81780000	O	3.15182300	0.53428600	2.44445800
N	1.63943600	-2.46895600	-0.39905800	N	-1.34446400	-1.38977400	-1.35338800	N	1.31583500	-0.32030100	1.48040600
O	0.85331700	-1.45303400	-0.99478400	O	-0.85748400	-1.30535100	0.00095900	O	0.73755200	-0.74169900	0.23871900
H	1.04453300	-1.48957700	-1.94298800	H	-0.96192200	-2.14899000	0.49802000	H	0.79085900	-3.50212500	-0.29990500
C	0.88363700	-3.70303900	-0.21073900	C	-0.35911600	-1.81146300	-2.34861600	C	1.01864300	-1.25584900	2.56340700
H	1.55997900	-4.45769700	0.18415200	H	-0.90979000	-1.94892100	-3.27691400	H	1.56366800	-0.90777900	3.43759800
H	0.05345000	-3.56327500	0.48932200	H	0.41705700	-1.05944000	-2.51477800	H	-0.05111000	-1.24064600	2.77932500
H	0.49552400	-4.02336700	-1.17791100	H	0.07731800	-2.75648600	-2.03641100	H	1.33548900	-2.26947500	2.30274000
MC(N3)				TS(N3)				IM(N3)			
C	-1.11256100	-0.34656000	1.91298800	C	0.53578900	-1.16418700	-2.09549500	C	-1.54484300	1.64382800	1.79010200
C	-2.01898300	0.81708100	1.41217700	C	1.97303700	-0.95787900	-1.53207500	C	-2.67180100	1.64840900	0.71328000
C	-2.52493400	0.72778200	0.02451400	C	2.12362700	-0.85929000	-0.05538500	C	-2.58584600	0.62584700	-0.35666200
C	-2.30439500	-0.38233300	-0.72148300	C	1.04400700	-0.90771800	0.75642500	C	-1.52220800	-0.20557300	-0.40874400
C	-1.54826300	-1.54220700	-0.19389200	C	-0.30232700	-1.11363300	0.19415200	C	-0.39615000	-0.15154300	0.56140400
C	-0.99440200	-1.53527800	1.04411600	C	-0.56950300	-1.17580200	-1.12843200	C	-0.42528000	0.69580900	1.62507700
O	-0.54891900	-0.23781200	2.97418400	O	0.38513000	-1.29365600	-3.28591000	O	-1.63236900	2.41392500	2.71324900
O	-2.27845500	1.72505100	2.15924600	O	2.90454300	-0.88179300	-2.28904000	O	-3.56296500	2.45257700	0.78635600
Cl	-3.41834900	2.08764000	-0.54835300	Cl	3.73162400	-0.67196600	0.53667500	Cl	-3.88860200	0.57604600	-1.48246700
Cl	-2.91159200	-0.48094800	-2.33640700	Cl	1.20956500	-0.76103400	2.47083200	Cl	-1.42631100	-1.41308800	-1.65622600
Cl	-1.38034700	-2.92642700	-1.21313000	Cl	-1.21798600	-2.83891600	1.44196100	Cl	-0.53564000	-4.93543400	-0.12622100
Cl	-0.09821400	-2.86190800	1.68424500	Cl	-2.15049300	-1.44991200	-1.78015200	Cl	0.76304000	0.77868600	2.88725700
C	3.33036900	-0.04454500	-1.68838800	C	-0.28914400	2.84360900	-1.12270700	C	3.07314300	1.95181300	-0.64972800
C	3.09661900	0.66167500	-0.50356400	C	-0.79697600	2.31971700	0.07238500	C	2.57294000	0.65126400	-0.78428600
C	3.51488200	0.11613600	0.71488500	C	-0.06364700	2.44864300	1.25655200	C	1.96115300	0.26610400	-1.98191600
C	4.14711100	-1.12343400	0.74745500	C	1.17413000	3.08645500	1.23938100	C	1.84046500	1.17906800	-3.02732400
C	4.35183800	-1.83548000	-0.43393600	C	1.69135100	3.57959300	0.04280300	C	2.31246300	2.48195800	-2.87798300

C	3.94168500	-1.29421400	-1.65177400	C	0.95915100	3.45607900	-1.13857200	C	2.92746300	2.86729300	-1.68693700
H	3.03451500	0.40046300	-2.63068100	H	-0.87959500	2.76720100	-2.02761500	H	3.57720900	2.23202400	0.26713200
H	3.37451500	0.66895200	1.63564200	H	-0.46152300	2.07111800	2.18998700	H	1.59675600	-0.74515900	-2.10743000
H	4.48128800	-1.53244500	1.69407100	H	1.73419100	3.19674000	2.16054100	H	1.38079800	0.87064800	-3.95931700
H	4.83681300	-2.80480200	-0.40569800	H	2.66066500	4.06461300	0.03122000	H	2.20899400	3.19260600	-3.69010700
H	4.10782500	-1.84053600	-2.57327200	H	1.35695800	3.84383600	-2.06898000	H	3.30314000	3.87723700	-1.57018900
C	2.49628800	2.02818300	-0.62392100	C	-2.17774300	1.75279200	0.03486100	C	2.84501500	-0.30330000	0.33955800
O	2.77327700	2.77472800	-1.54763200	O	-3.09260700	2.27902000	-0.56527200	O	3.94156500	-0.39236900	0.86060000
N	1.65256700	2.46503400	0.39716100	N	-2.44847800	0.57948900	0.74827700	N	1.79880700	-1.05682600	0.85873100
O	0.86054100	1.45178000	0.98945300	O	-1.35964700	-0.19125600	1.21203300	O	0.55458200	-1.05605800	0.19394800
H	1.04939700	1.48612700	1.93822000	H	-1.69370900	-1.01202700	1.72097100	H	-0.84629700	-3.75502200	-0.54457900
C	0.90293800	3.70291000	0.20932600	C	-3.75941600	-0.05243000	0.84335800	C	1.97533600	-2.22122600	1.71168900
H	1.58345500	4.45479700	-0.18367400	H	-4.47138100	0.68781500	0.48514600	H	3.01713800	-2.22139300	2.02459900
H	0.07310900	3.56792000	-0.49209600	H	-3.82155800	-0.94780900	0.22639100	H	1.33168700	-2.14455800	2.58992500
H	0.51494800	4.02396500	1.17632200	H	-3.97412900	-0.29107000	1.88805100	H	1.74902800	-3.13726800	1.16060800
MC(N4)				TS(N4)				IM(N4)			
C	-1.11206300	-0.34693100	1.91290600	C	-3.31630900	-0.64698800	0.16009300	C	-3.22901900	0.91831900	0.63786600
C	-2.01859300	0.81687200	1.41263000	C	-3.35654300	0.90861000	0.24683300	C	-3.55490900	-0.46922300	-0.00355300
C	-2.52492600	0.72793200	0.02508100	C	-2.09421000	1.65174300	-0.03912800	C	-2.41903900	-1.24495900	-0.55460400
C	-2.30470400	-0.38205100	-0.72120900	C	-0.95215600	0.99446500	-0.33999300	C	-1.16621900	-0.72635300	-0.56295600
C	-1.54854500	-1.54211700	-0.19406400	C	-0.94613500	-0.47707500	-0.45448900	C	-0.88514300	0.64752600	-0.08552800
C	-0.99431100	-1.53550200	1.04377700	C	-2.02799100	-1.24658400	-0.13212100	C	-1.84122700	1.40396000	0.50941200
O	-0.54805300	-0.23841000	2.97392800	O	-4.33670100	-1.27000400	0.35410200	O	-4.11109500	1.54326000	1.16833500
O	-2.27783100	1.72465900	2.15999800	O	-4.37986900	1.46698700	0.54182900	O	-4.69235500	-0.86268700	-0.00510800
Cl	-3.41835500	2.08800000	-0.54723700	Cl	-2.18678900	3.37080700	0.04020300	Cl	-2.78371900	-2.83592800	-1.11161400
Cl	-2.91239500	-0.48025300	-2.33597000	Cl	0.52211600	1.83585100	-0.64581800	Cl	0.17524600	-1.69181900	-1.05862200
Cl	-1.38108000	-2.92617700	-1.21362600	Cl	-0.19800100	-0.93691600	-2.52557900	Cl	0.60578300	-1.45113500	2.90845200
Cl	-0.09812100	-2.86236900	1.68339400	Cl	-1.96482500	-2.97823800	-0.29435200	Cl	-1.50639000	2.98778400	1.11670600
C	3.33029600	-0.04504200	-1.68831900	C	3.76680500	1.08476000	0.84267200	C	3.88361400	-0.73262200	-0.85371000
C	3.09671700	0.66154800	-0.50369800	C	3.08419700	-0.13015000	0.69940500	C	3.01789300	0.31011000	-0.50341600
C	3.51508300	0.11636800	0.71488600	C	3.47630100	-1.03187600	-0.29697700	C	3.01040800	0.78464200	0.81371400
C	4.14724200	-1.12322100	0.74777200	C	4.52502700	-0.71211300	-1.15342000	C	3.84910500	0.20706800	1.76729600
C	4.35180600	-1.83564600	-0.43342700	C	5.18196000	0.51032500	-1.02472300	C	4.68148500	-0.85760200	1.41996300
C	3.94155000	-1.29473900	-1.65138400	C	4.80342600	1.40698400	-0.02415100	C	4.69559900	-1.32685900	0.10711300
H	3.03436700	0.39967300	-2.63072800	H	3.47195600	1.76436600	1.63276600	H	3.91479300	-1.06632100	-1.88375200
H	3.37486100	0.66951900	1.63546900	H	2.99676900	-2.00003100	-0.38188900	H	2.36990500	1.60938300	1.09534900
H	4.48150100	-1.53196900	1.69447400	H	4.83070500	-1.41752400	-1.91681100	H	3.85935000	0.59774400	2.77878100
H	4.83672800	-2.80498500	-0.40493000	H	5.99352400	0.76105700	-1.69811100	H	5.32355800	-1.31021900	2.16693700
H	4.10755700	-1.84134800	-2.57273500	H	5.32050000	2.35348700	0.08123200	H	5.34849500	-2.14598300	-0.17108800
C	2.49650100	2.02808200	-0.62433200	C	2.02701200	-0.44452400	1.69378500	C	2.25267400	0.95408400	-1.62187400
O	2.77355900	2.77442800	-1.54817400	O	2.04985900	-0.07304300	2.84482000	O	2.77596300	1.17741000	-2.69820600
N	1.65283600	2.46515800	0.39672200	N	0.99976600	-1.36836700	1.30342700	N	0.89743900	1.25889100	-1.47129600
O	0.86057800	1.45204300	0.98898800	O	0.49112500	-1.06881900	-0.03750100	O	0.38272800	1.15654100	-0.13552800
H	1.04962200	1.48613400	1.93771700	H	0.69463400	-1.74632500	-0.72956000	H	1.67494700	-1.02015300	2.32156800

C	0.90328900	3.70304700	0.20867800	C	-0.02109800	-1.71489300	2.29388300	C	0.29939800	2.36198400	-2.22233400
H	1.58380400	4.45478800	-0.18460100	H	0.53045900	-2.03375000	3.17714300	H	0.79616100	2.38704700	-3.18914400
H	0.07335900	3.56792900	-0.49260200	H	-0.65448900	-0.86892400	2.56734400	H	-0.76444100	2.17411200	-2.37063000
H	0.51543600	4.02437100	1.17564000	H	-0.61194800	-2.54643800	1.92217700	H	0.43986700	3.31417800	-1.70289000
MC(1w)				TS(1w)				IM(1w)			
C	0.77300800	-0.26711600	-1.90754200	C	-0.58246100	-0.70159000	2.32027900	C	1.61560300	-0.72722200	-1.15044700
C	1.89665400	0.70197300	-1.43745700	C	-1.90336200	-1.07991300	1.59353900	C	2.26832600	0.68167100	-1.04753700
C	2.58404800	0.37698700	-0.17198200	C	-1.82034500	-1.38541500	0.13825200	C	1.71885700	1.60715600	-0.04010000
C	2.29872900	-0.76990400	0.49215400	C	-0.65128200	-1.27659100	-0.52336500	C	0.64100400	1.24223400	0.69008100
C	1.29234600	-1.73410100	-0.00896800	C	0.60434200	-0.91096200	0.18009800	C	-0.03946200	-0.07291400	0.52608600
C	0.57677100	-1.50698900	-1.14025500	C	0.61447700	-0.57624300	1.50419700	C	0.42498200	-1.01081700	-0.34718100
O	0.12361700	0.02232400	-2.88664300	O	-0.61399200	-0.51950300	3.51764900	O	2.11844300	-1.53201300	-1.90575200
O	2.17427000	1.64976800	-2.12939800	O	-2.94025200	-1.11655700	2.20234100	O	3.17820300	0.96056400	-1.78814400
Cl	3.76040300	1.51539400	0.37031200	Cl	-3.29188900	-1.85558300	-0.63116600	Cl	2.50886200	3.12753300	0.12724100
Cl	3.11415800	-1.14566200	1.96782100	Cl	-0.56338000	-1.57367900	-2.22868200	Cl	-0.00595400	2.31183100	1.88554500
Cl	1.03971400	-3.18047800	0.89734600	Cl	1.96226000	-2.63003900	-0.25731200	Cl	4.17050000	-1.16169300	1.26127500
Cl	-0.60286000	-2.60555300	-1.74842000	Cl	2.08648800	-0.24288400	2.37190300	Cl	-0.24230000	-2.59422000	-0.60092600
C	-3.19180400	-0.51584500	1.70922700	C	-0.99692000	2.94347600	0.57512200	C	-3.95669300	-0.48582400	-1.46083300
C	-2.79111300	0.60326600	0.97032900	C	-0.13113800	2.42859200	-0.39701100	C	-3.44490700	-0.13816500	-0.20478800
C	-3.28379000	0.78071700	-0.32760800	C	-0.62279100	2.10872200	-1.66662600	C	-3.36176900	1.21073700	0.15784700
C	-4.15787200	-0.15347400	-0.87700100	C	-1.97195700	2.29479600	-1.95636600	C	-3.77387500	2.19825900	-0.73426600
C	-4.53347800	-1.27922700	-0.14502800	C	-2.83739100	2.77983500	-0.97741800	C	-4.25345800	1.84862900	-1.99523500
C	-4.04707700	-1.45979700	1.14937400	C	-2.34861000	3.10176800	0.28898400	C	-4.34299600	0.50481600	-2.35752300
H	-2.83321800	-0.62627500	2.72542400	H	-0.60234300	3.21305200	1.54718800	H	-4.05120900	-1.53302400	-1.72051700
H	-3.00821600	1.65451000	-0.90385100	H	0.04319800	1.73514200	-2.43440400	H	-2.99548400	1.49250800	1.13619700
H	-4.54544400	-0.00107100	-1.87786800	H	-2.34667900	2.05806000	-2.94529600	H	-3.72154700	3.24075200	-0.44194200
H	-5.20817500	-2.00878600	-0.57917600	H	-3.88986300	2.91046700	-1.20138400	H	-4.56418300	2.62032600	-2.69041300
H	-4.34278900	-2.32920700	1.72575900	H	-3.01898000	3.48083400	1.05131800	H	-4.72360800	0.22835500	-3.33399100
C	-1.93193300	1.61074200	1.67300000	C	1.32083300	2.36689900	-0.05477500	C	-3.13103700	-1.26592800	0.73236000
O	-2.05563100	1.83231100	2.86883300	O	1.90637200	3.26532400	0.51418900	O	-3.87999300	-2.21505600	0.87517000
N	-1.02830400	2.34756200	0.91872700	N	2.06914300	1.24605100	-0.43419100	N	-1.91091600	-1.27783600	1.39871800
O	-0.46931900	1.69755000	-0.19902800	O	1.39221900	0.09328900	-0.85514300	O	-1.10935900	-0.11863800	1.35912500
H	-0.70996600	2.23088100	-0.98970000	H	1.93893500	-0.35977700	-1.64874500	H	4.08671500	-1.58995000	-2.02542200
C	-0.06973200	3.20834400	1.59863500	C	3.50166300	1.11056400	-0.15366200	C	-1.62110600	-2.11429000	2.55243600
H	0.31823400	3.93188900	0.88093400	H	4.08676600	1.44728600	-1.01438100	H	-1.66341700	-1.52655500	3.47364500
H	-0.58515700	3.72604400	2.40433200	H	3.73910000	1.73271300	0.70616200	H	-2.38175800	-2.89162700	2.57207400
H	0.76104400	2.63081300	2.01883700	H	3.72406100	0.07282200	0.08235800	H	-0.63592400	-2.57141500	2.44438500
O	-0.85462900	2.72831500	-2.70951900	O	2.66191000	-1.02451100	-2.69413800	O	4.97074000	-1.57498500	-1.61858400
H	-0.45378100	1.94584400	-3.12311200	H	2.67592200	-1.90604400	-2.26367100	H	4.62351100	-1.39068200	0.02312800
H	-0.32347200	3.47391600	-3.00788700	H	3.57633200	-0.77774300	-2.87713200	H	5.38942800	-0.78153200	-1.97140800
MC(2w)				TS(2w)				IM(2w)			
C	0.68530200	0.70757600	-1.74485400	C	-1.07229400	0.08953300	2.37629000	C	1.29809700	-2.31677100	1.39200300
C	1.91348400	1.14512200	-0.89697500	C	-1.86061400	-1.09465300	1.75226900	C	2.36553200	-2.44339400	0.26427800
C	2.61149100	0.10658400	-0.12440500	C	-1.22301800	-1.82009500	0.61390300	C	2.27733900	-1.47997100	-0.85631600

C	2.17345800	-1.17804700	-0.14530400	C	-0.03793600	-1.41574400	0.12261700	C	1.32617700	-0.52062700	-0.84962000
C	0.99074600	-1.59284700	-0.93244700	C	0.72021000	-0.27911400	0.71708900	C	0.33475100	-0.36536400	0.24582100
C	0.28156800	-0.70960200	-1.67882300	C	0.18025000	0.44804700	1.75278800	C	0.30157600	-1.22864700	1.29459200
O	0.14283700	1.52757100	-2.44518100	O	-1.54940500	0.64464500	3.34578500	O	1.32165600	-3.11188200	2.29697400
O	2.26849900	2.30221700	-0.93371900	O	-2.94135000	-1.40433400	2.18000300	O	3.20200700	-3.30520900	0.33145700
Cl	3.98740700	0.62102900	0.78177600	Cl	-2.10270400	-3.15911800	-0.03145900	Cl	3.43278800	-1.66206800	-2.12083200
Cl	2.99517100	-2.38595700	0.77351000	Cl	0.66549900	-2.21697100	-1.25289300	Cl	1.22221500	0.59943600	-2.17286800
Cl	0.52756000	-3.25546400	-0.88163600	Cl	2.62792800	-1.05828000	1.19726500	Cl	3.13763700	2.02247100	1.25826200
Cl	-1.08763500	-1.15525200	-2.62117800	Cl	1.10062000	1.69202200	2.56407400	Cl	-0.83973200	-1.20479300	2.60256900
C	-3.18407400	-1.49845900	0.90340900	C	-2.45969400	2.03519400	-0.75709900	C	-4.33356600	-0.70950000	0.13565200
C	-2.61311500	-0.25323600	1.19290500	C	-1.21254700	1.77183600	-1.33484600	C	-3.23768000	0.08226200	-0.23407900
C	-3.13647500	0.89774100	0.59091600	C	-1.11595000	0.86361400	-2.39350900	C	-2.78986600	0.05030600	-1.56013800
C	-4.20827900	0.79614600	-0.29240900	C	-2.25797900	0.22007200	-2.86438200	C	-3.42320300	-0.76697100	-2.49429600
C	-4.75724500	-0.44939400	-0.59405000	C	-3.49395300	0.46196200	-2.26751200	C	-4.49359800	-1.57213000	-2.11187000
C	-4.24137000	-1.59810700	0.00505300	C	-3.59268700	1.36858500	-1.21182200	C	-4.94627800	-1.54270100	-0.79309700
H	-2.79450900	-2.37843000	1.40046500	H	-2.52971700	2.75904900	0.04567500	H	-4.69732400	-0.65611600	1.15396600
H	-2.72945100	1.87400800	0.81859800	H	-0.15974900	0.67191300	-2.86461100	H	-1.96080000	0.66638200	-1.87819900
H	-4.61575600	1.69350100	-0.74420700	H	-2.18097700	-0.47304100	-3.69414000	H	-3.07746500	-0.77314800	-3.52163400
H	-5.58828800	-0.52325000	-1.28686800	H	-4.37879100	-0.05176900	-2.62550400	H	-4.97693300	-2.21474100	-2.83896500
H	-4.66956500	-2.56863500	-0.21909200	H	-4.55213300	1.55914700	-0.74548300	H	-5.78272800	-2.16194800	-0.49038100
C	-1.53732900	-0.23115700	2.23702600	C	-0.05114200	2.58674200	-0.86320700	C	-2.70717400	0.99564500	0.83322600
O	-1.52626300	-1.03770800	3.15746500	O	-0.11393200	3.79118800	-0.70808000	O	-3.45191000	1.53899700	1.63191400
N	-0.58197700	0.77231600	2.19080200	N	1.17079800	1.96146800	-0.61895900	N	-1.34172700	1.17755700	0.98403100
O	-0.22540400	1.27384500	0.92688700	O	1.25179600	0.57377300	-0.59077700	O	-0.47208000	0.70891900	-0.01905600
H	-0.48382000	2.22922100	0.93461400	H	2.14784300	0.23018800	-1.25641500	H	-0.15287600	2.71407400	-1.39243600
C	0.52802000	0.75033100	3.13306900	C	2.36141000	2.70820100	-0.20593900	C	-0.73720900	2.15304600	1.88095000
H	0.97198600	1.74548700	3.16742500	H	2.90563800	3.07204500	-1.08405300	H	-0.46858500	3.06987300	1.34958600
H	0.14027400	0.48240700	4.11341200	H	2.05199300	3.56202400	0.39218700	H	-1.47814300	2.37235000	2.64591900
H	1.29338500	0.02095600	2.84595400	H	2.99098900	2.05749400	0.39612800	H	0.15323000	1.72563300	2.34201500
O	-0.96289700	3.86360100	0.74594300	O	3.05416300	-0.03155600	-2.08254400	O	-0.11176200	3.67579300	-1.47721700
H	-0.51649200	4.20014200	-0.06698900	H	3.53358600	-0.88948400	-1.85323000	H	1.31242700	4.36253500	-0.58228600
H	-0.85893500	4.53985900	1.42170600	H	3.71857600	0.66398300	-2.15871100	H	-1.01836000	3.99530400	-1.42172600
O	0.39116600	4.44066200	-1.54271800	O	4.28465800	-2.16055700	-1.26203100	O	2.07789300	4.56316000	-0.00825000
H	-0.11389100	4.15351100	-2.31168300	H	4.21854700	-3.04507000	-1.63728600	H	2.68767200	5.09311100	-0.53137700
H	1.11574100	3.79353900	-1.48902300	H	3.89399500	-2.19720800	-0.36933500	H	2.71672900	3.15869500	0.70684700
MC(3w)				TS(3w)				IM(3w)			
C	2.22049900	-0.32493500	-1.62827000	C	-1.52570100	0.36109000	2.25410000	C	0.38489800	2.25347200	-1.62648100
C	1.96776300	1.19551700	-1.38892600	C	-1.76194400	-1.13680200	1.91379200	C	1.33178500	2.79681500	-0.51340100
C	2.07915900	1.68968700	0.00021300	C	-0.76656300	-1.80479800	1.02369000	C	1.29075600	2.11167600	0.80044800
C	2.43517600	0.85222200	1.00516200	C	0.26692100	-1.11322800	0.51107700	C	0.51261900	1.02082900	0.96718400
C	2.75449600	-0.57416700	0.75889300	C	0.50546300	0.31905200	0.84334800	C	-0.32858200	0.44924600	-0.11541000
C	2.68208900	-1.12196000	-0.47965700	C	-0.37980100	0.99708200	1.65118800	C	-0.42381800	1.05536000	-1.32799200
O	2.02109000	-0.78666600	-2.72608300	O	-2.30368600	0.90108100	3.01605700	O	0.34493700	2.83703100	-2.68037500
O	1.69871800	1.89652400	-2.33015600	O	-2.71212900	-1.72456500	2.36004300	O	2.04023100	3.74153100	-0.74183000

Cl	1.74393500	3.36255500	0.24297500	Cl	-1.04398300	-3.47633800	0.68046500	Cl	2.28268300	2.77246100	2.04617000
Cl	2.54337600	1.43481900	2.62618300	Cl	1.37965400	-1.87225200	-0.58987400	Cl	0.46816400	0.20255000	2.50147300
Cl	3.23159500	-1.53579600	2.10657700	Cl	2.45278900	0.46927100	1.49306300	Cl	3.26436900	-0.52050600	-1.26616200
Cl	3.05907200	-2.78019700	-0.79732800	Cl	-0.04355500	2.62602300	2.19394000	Cl	-1.46251300	0.55041700	-2.62217600
C	-4.11236200	-0.00992300	1.79597800	C	-3.11647200	0.61459200	-1.28116900	C	-4.90749800	-0.61674600	-0.41753700
C	-3.78738100	0.12066600	0.44125500	C	-1.80923700	0.80413400	-1.74327100	C	-3.71743300	-1.03361100	0.19109700
C	-3.84793100	-1.00076900	-0.39360900	C	-1.21151100	-0.17076400	-2.54687900	C	-3.51096000	-0.77011400	1.54995400
C	-4.21820400	-2.23919900	0.12508500	C	-1.91395700	-1.32682600	-2.87959500	C	-4.47939500	-0.08782300	2.28302000
C	-4.51326700	-2.37091200	1.48181800	C	-3.20529200	-1.52510500	-2.39468100	C	-5.64860900	0.35108100	1.66468100
C	-4.45830500	-1.25431400	2.31734400	C	-3.80405000	-0.55410500	-1.59177400	C	-5.86016700	0.08656800	0.31183300
H	-4.09891500	0.87087500	2.42692100	H	-3.58375400	1.38733500	-0.68286800	H	-5.07566000	-0.85553200	-1.46035400
H	-3.61978100	-0.90575500	-1.44833200	H	-0.20861100	-0.02294700	-2.92752100	H	-2.60904500	-1.10874600	2.04173300
H	-4.26986200	-3.10098900	-0.53002400	H	-1.45037400	-2.07401300	-3.51352700	H	-4.31969100	0.09936200	3.33881700
H	-4.79502000	-3.33749800	1.88442300	H	-3.74456600	-2.43233800	-2.64218100	H	-6.39533200	0.89066900	2.23631000
H	-4.70007600	-1.34988700	3.37001800	H	-4.80778800	-0.70464700	-1.21188400	H	-6.77137400	0.41889900	-0.17207200
C	-3.48254700	1.49662300	-0.07486700	C	-1.16779600	2.12927700	-1.46878200	C	-2.78844600	-1.85834900	-0.65013200
O	-4.13759900	2.46835700	0.27094000	O	-1.76517200	3.17703800	-1.64032300	O	-3.20249600	-2.71853800	-1.40893600
N	-2.47099900	1.62015700	-1.01039500	N	0.15098600	2.17156600	-1.03043600	N	-1.42805400	-1.60436100	-0.61498400
O	-1.40571800	0.69834400	-0.91298300	O	0.81941000	1.00951600	-0.69099800	O	-0.94004300	-0.68358800	0.33260300
H	-1.37243200	0.19386000	-1.77027500	H	2.00643900	1.01433500	-1.15777000	H	2.38221900	-1.84212400	1.78980500
C	-2.02967500	2.94491800	-1.42619100	C	0.88630300	3.42342900	-0.87435800	C	-0.40570100	-2.48531400	-1.15979200
H	-1.47843300	2.85020400	-2.36149700	H	1.56321100	3.58054000	-1.72032100	H	0.21124900	-2.89011900	-0.35416000
H	-2.91200900	3.56329400	-1.57598800	H	0.15652000	4.22884000	-0.84476300	H	-0.93142800	-3.28552400	-1.67625600
H	-1.38903100	3.40990700	-0.67002800	H	1.43761400	3.40814100	0.06376100	H	0.22417600	-1.94800800	-1.87220400
O	-1.06263700	-0.90977500	-3.00540900	O	3.06753500	1.13527100	-1.58751800	O	2.63896600	-2.28573700	0.97305900
H	-0.88407400	-1.75734300	-2.54158400	H	3.55512800	0.25202500	-1.77593800	H	3.47893500	-2.77854300	1.15956000
H	-0.25944700	-0.71486600	-3.50358800	H	3.57456500	1.58131400	-0.89337500	H	2.93953000	-1.32003000	-0.20377800
O	-0.57872300	-3.02574700	-1.29294800	O	4.36606300	-1.02980400	-1.92504800	O	5.05493000	-3.40936700	1.25676700
H	0.24010800	-3.52903100	-1.34340500	H	5.16157300	-1.06938800	-2.46485500	H	5.24011300	-4.34423200	1.12737900
H	-0.55094300	-2.54846500	-0.43781300	H	4.56945600	-1.43378400	-1.04522700	H	5.60665900	-2.91982700	0.60936600
O	-0.58290800	-1.28584500	0.90804400	O	4.70285900	-1.80654700	0.62397300	O	6.24333700	-1.85865800	-0.67839100
H	-1.21348500	-1.50669500	1.60267500	H	4.66826800	-2.70082100	0.97939900	H	6.97116800	-1.23881200	-0.56803400
H	-0.98007600	-0.52443800	0.44172500	H	4.00482400	-1.30761100	1.08139900	H	5.51331400	-1.35047800	-1.06740600
MC(A1)				TS(A1)				IM(A1)			
C	-1.19354200	-1.51764300	1.30368300	C	-1.58294700	0.81221200	-1.62639600	C	2.93109700	0.12387500	1.41828100
O	-1.19168800	-2.75679600	1.32115500	O	-1.57206100	1.85530300	-2.27776400	O	3.71881100	0.52581400	2.27136700
N	-0.06085300	-0.84279000	1.70166800	N	-0.50204000	-0.04009500	-1.64716800	N	1.61448600	-0.06027900	1.79981600
O	0.05676100	0.47173900	1.74944100	O	-0.47774200	-1.17839100	-0.91223000	O	0.80979000	-0.88810900	0.98645900
C	-2.43192900	-0.76614300	0.90570000	C	-2.81345500	0.43140500	-0.84750200	C	3.38445000	-0.05541100	-0.01035100
C	-2.73741000	0.54789000	1.28693500	C	-3.31515100	-0.87224700	-0.77988000	C	2.74877100	-0.79620300	-1.01900100
C	-3.38468200	-1.49843800	0.18042000	C	-3.55776300	1.47839400	-0.29173900	C	4.60379100	0.57843600	-0.30857700
C	-3.96818700	1.10742700	0.94621600	C	-4.54039900	-1.11961000	-0.16345800	C	3.32261200	-0.88422800	-2.28782400
H	-2.00460800	1.12629600	1.82953700	H	-2.74379700	-1.68938400	-1.19671100	H	1.81518700	-1.30955600	-0.84998300
C	-4.60209100	-0.92949100	-0.17385100	C	-4.76758300	1.22605800	0.34606700	C	5.16423000	0.49372800	-1.57621400

H	-3.14732800	-2.52013300	-0.08835800	H	-3.17300200	2.48729100	-0.37279600	H	5.09695500	1.13460400	0.47808300
C	-4.90042800	0.37872100	0.21197200	C	-5.26483500	-0.07611700	0.40918700	C	4.52265800	-0.24177600	-2.57433300
H	-4.18659300	2.12705600	1.24495900	H	-4.92188700	-2.13419900	-0.12085100	H	2.80705900	-1.45821600	-3.04919700
H	-5.32068800	-1.50572000	-0.74788600	H	-5.32534400	2.04432800	0.78924300	H	6.10075100	0.99993900	-1.78585400
H	-5.85082500	0.82576400	-0.06225400	H	-6.21104800	-0.27538000	0.90175900	H	4.95660600	-0.31092700	-3.56664000
C	1.02100900	-1.63954000	2.29335900	C	0.55952600	0.10840900	-2.63630000	C	1.25638100	-0.17502400	3.20842100
H	1.77430500	-0.93414000	2.63206000	H	1.51877500	0.29559300	-2.15203300	H	0.20229200	0.08105600	3.32011200
H	0.63633500	-2.22154300	3.13580200	H	0.62875900	-0.81525700	-3.21703500	H	1.42222000	-1.19302300	3.57418300
H	1.44305600	-2.33704800	1.56794400	H	0.30765800	0.94831500	-3.27922800	H	1.87004000	0.52726500	3.76608600
C	0.51569200	2.06839400	-0.08662600	C	1.52449600	-1.98507100	0.21010000	C	-1.46871600	-1.51404400	0.88450800
C	1.84324700	1.73421800	0.59745100	C	2.79901300	-1.28348300	-0.34088900	C	-2.86162300	-1.28302500	0.27683000
C	2.50469200	0.47992800	0.17788000	C	2.92256000	0.09082900	0.00621500	C	-3.12463500	0.09751300	-0.20170600
C	1.97821300	-0.34547200	-0.76698500	C	1.90941400	0.78024200	0.69602100	C	-2.19348200	1.07965700	-0.10357600
C	0.72705000	-0.01714000	-1.43230300	C	0.68025500	0.22379900	1.06303400	C	-0.81163200	0.81219400	0.29666900
C	0.04653300	1.12001600	-1.11873400	C	0.35706600	-1.10212600	0.65176900	C	-0.44585200	-0.43349500	0.67961200
O	-0.05684400	3.11529400	0.15572800	O	1.47698900	-3.18509200	0.27618200	O	-1.27269300	-2.42018500	1.66432500
O	2.35365400	2.51461800	1.37930700	O	3.60899800	-1.96306400	-0.96658800	O	-3.72789300	-2.12355400	0.36154100
Cl	4.03753000	0.14761900	0.94038300	Cl	4.39517200	0.89845100	-0.51844900	Cl	-4.75096600	0.40671200	-0.73719800
Cl	2.80804700	-1.81388900	-1.22610800	Cl	2.20529100	2.45505000	1.11556800	Cl	-2.61400900	2.72518300	-0.51324000
Cl	0.15141200	-1.08326000	-2.69188000	Cl	-0.51703400	1.16869100	1.93949600	Cl	0.36838900	2.08471400	0.07109100
Cl	-1.39238500	1.58740100	-1.97646800	Cl	-0.80792900	-1.99789000	1.64242400	Cl	-0.88370400	-2.01743800	-1.69427000
MC(A2)				TS(A2)				IM(A2)			
C	2.35429300	-1.93645900	-0.62974300	C	2.59965700	-1.37194900	-0.91773000	C	2.93111000	-0.12249300	-1.41842000
O	2.87614100	-3.01363900	-0.94264700	O	3.32767900	-2.34977900	-1.10093800	O	3.71890000	-0.52322200	-2.27201300
N	0.98503700	-1.81073300	-0.53278900	N	1.24261200	-1.47879900	-1.11721100	N	1.61448500	0.06203600	-1.79970200
O	0.36813600	-0.64210800	-0.47794400	O	0.37561600	-0.48224600	-0.84170900	O	0.80985100	0.88906200	-0.98547500
C	3.21095600	-0.72742100	-0.39343300	C	3.19241900	-0.04933400	-0.51994600	C	3.38448700	0.05533900	0.01035900
C	3.02179000	0.16867800	0.66266700	C	2.69210600	1.19595700	-0.91685500	C	2.74884500	0.79514200	1.01975300
C	4.32158500	-0.56942000	-1.23237100	C	4.38349000	-0.10075600	0.21581400	C	4.60376800	-0.57892100	0.30794800
C	3.92541500	1.21086500	0.86375900	C	3.36571700	2.36490600	-0.57002400	C	3.32272200	0.88189600	2.28864500
H	2.18338100	0.05436200	1.33408900	H	1.77171900	1.25457200	-1.47915900	H	1.81521300	1.30860000	0.85131200
C	5.21016500	0.48468400	-1.04272300	C	5.04649600	1.06799200	0.57318200	C	5.16424900	-0.49547200	1.57564800
H	4.47851100	-1.28875100	-2.02735000	H	4.77611300	-1.07055200	0.49546700	H	5.09687400	-1.13433300	-0.47928000
C	5.01444500	1.37930800	0.01014400	C	4.53808100	2.30640800	0.17990700	C	4.52274600	0.23910700	2.57449600
H	3.76521900	1.89528100	1.68946000	H	2.95371200	3.32225800	-0.86771200	H	2.80716400	1.45509500	3.05061000
H	6.05794200	0.60372900	-1.70991200	H	5.95787700	1.01386200	1.15956900	H	6.10074100	-1.00194800	1.78477000
H	5.70840300	2.19933400	0.16579500	H	5.04851500	3.22083400	0.46400700	H	4.95669800	0.30723800	3.56687100
C	0.13833200	-2.97089400	-0.80399400	C	0.65480600	-2.70385000	-1.64329800	C	1.25636900	0.17830600	-3.20818900
H	-0.62937500	-3.02988900	-0.03518800	H	-0.12651800	-2.42173000	-2.35110800	H	1.42194100	1.19676100	-3.57280800
H	-0.33934900	-2.84577300	-1.78193100	H	1.43596500	-3.28049700	-2.13424400	H	1.87024000	-0.52319900	-3.76660600
H	0.75100800	-3.86859400	-0.80163900	H	0.21028800	-3.30151300	-0.84349700	H	0.20235900	-0.07791600	-3.32020500
C	-1.23228200	-0.77996500	1.51461800	C	-0.23631100	0.88104900	1.08923700	C	-1.46860100	1.51487800	-0.88292900
C	-0.45060600	0.52627700	1.60358800	C	-1.09809200	1.93894300	0.34633800	C	-2.86157300	1.28330100	-0.27562000
C	-0.78097200	1.56699000	0.61260000	C	-2.37422500	1.46337500	-0.06394300	C	-3.12467600	-0.09765900	0.20161600

C	-1.78328700	1.41459900	-0.29312300	C	-2.72466700	0.10616200	0.03952700	C	-2.19354200	-1.07969600	0.10266100
C	-2.61008200	0.21813800	-0.29688400	C	-1.86811400	-0.90390100	0.49403600	C	-0.81163200	-0.81192600	-0.29728600
C	-2.35863200	-0.80817700	0.55803800	C	-0.50332300	-0.58195000	0.75211100	C	-0.44573800	0.43413700	-0.67898100
O	-0.98392200	-1.70497200	2.27135400	O	0.57284600	1.21974700	1.91227500	O	-1.27254000	2.42169200	-1.66196400
O	0.35630400	0.70539600	2.50408100	O	-0.66310900	3.08378600	0.24795800	O	-3.72780000	2.12394000	-0.35960400
Cl	0.18592800	3.00903800	0.67756100	Cl	-3.46977700	2.65215800	-0.75666300	Cl	-4.75107800	-0.40736100	0.73658000
Cl	-2.12728800	2.66987700	-1.45971100	Cl	-4.34401200	-0.35653100	-0.44833300	Cl	-2.61416100	-2.72558000	0.51074000
Cl	-3.95816200	0.14124200	-1.40807500	Cl	-2.37186600	-2.59125800	0.48777100	Cl	0.36817700	-2.08490200	-0.07305500
Cl	-3.37641700	-2.22399100	0.61720000	Cl	0.44221600	-1.69472200	1.73406800	Cl	-0.88359100	2.01596200	1.69617400
MC(A3)				TS(A3)				IM(A3)			
C	1.13693300	-1.68642200	-1.03458600	C	1.09419500	-0.61569200	1.92442900	C	2.46615800	-0.71006400	1.42804700
O	1.19731700	-2.90902000	-0.88983900	O	1.17495800	-0.21513100	3.08505000	O	3.01721700	-1.03956200	2.47469200
N	-0.05871400	-1.12007900	-1.46553200	N	-0.08801900	-1.14080400	1.46209600	N	1.09123100	-0.91167900	1.35476100
O	-0.21197300	0.15044300	-1.74062600	O	-0.22006400	-1.60392000	0.19622300	O	0.53662300	-0.95414500	0.03496800
C	2.35410100	-0.83422700	-0.81688300	C	2.31037700	-0.60745600	1.03890300	C	3.25852000	-0.09340900	0.30889500
C	2.61629300	0.37717400	-1.47077300	C	2.65645600	-1.67615700	0.20488800	C	2.75198400	0.53284600	-0.83883000
C	3.33897900	-1.38019500	0.01953000	C	3.20404600	0.45880900	1.18914400	C	4.65338200	-0.15837600	0.48458100
C	3.84155000	1.01771500	-1.29092100	C	3.87952000	-1.67536700	-0.46235500	C	3.62679700	1.07953700	-1.77805000
H	1.85736100	0.81131000	-2.10458200	H	1.96380400	-2.49578400	0.07199600	H	1.69484200	0.61506500	-1.04485800
C	4.54991300	-0.72622500	0.21308800	C	4.41126000	0.47196500	0.49766100	C	5.51749900	0.38061700	-0.45869200
H	3.13095300	-2.32288300	0.50943000	H	2.93947200	1.26907100	1.85732500	H	5.03677100	-0.63700900	1.37632900
C	4.80841900	0.47561700	-0.44704800	C	4.75550600	-0.59960200	-0.32650800	C	5.00394600	1.00537600	-1.59759900
H	4.03389900	1.95287400	-1.80667500	H	4.14177800	-2.51273200	-1.10047300	H	3.20230400	1.55712200	-2.65370500
H	5.29236300	-1.15365600	0.87892500	H	5.08584200	1.31451100	0.60639000	H	6.58981800	0.31497700	-0.30679900
H	5.75421500	0.98744300	-0.29978600	H	5.70022400	-0.59510100	-0.86050100	H	5.67605700	1.42828500	-2.33754700
C	-1.09516800	-2.05494200	-1.93643900	C	-1.13757600	-1.47508000	2.43182600	C	0.48509400	-1.89088500	2.25502600
H	-0.71727500	-2.61967200	-2.79537100	H	-0.68232200	-1.95148000	3.30364800	H	0.86209300	-1.69533800	3.25489500
H	-1.36856600	-2.76207200	-1.15400300	H	-1.67970200	-0.58857400	2.76383300	H	-0.59637400	-1.76011700	2.24094700
H	-1.94931800	-1.45179900	-2.22889500	H	-1.82483400	-2.15557400	1.93691000	H	0.73494700	-2.91516500	1.95999600
C	-1.83427300	-1.15808600	1.29150000	C	-2.59671100	1.07125500	0.53804300	C	-3.10909700	-1.19919100	-0.52859700
C	-0.49693900	-0.68319600	1.89446500	C	-1.45623600	2.09560600	0.32847700	C	-3.57127900	0.19102900	-0.00071400
C	0.01842100	0.60215500	1.42453900	C	-0.34746300	1.72090400	-0.59587200	C	-2.53006000	1.11009300	0.47100800
C	-0.62507200	1.33771900	0.46910400	C	-0.29956900	0.51089000	-1.18585200	C	-1.21268400	0.78109400	0.41724600
C	-1.90764100	0.90672500	-0.06994000	C	-1.28509300	-0.55639300	-0.83550700	C	-0.77720500	-0.56480300	-0.02640000
C	-2.49821600	-0.24628600	0.36987200	C	-2.45859600	-0.15454600	-0.15541400	C	-1.68208200	-1.49039400	-0.44823900
O	-2.29286800	-2.24251600	1.61773700	O	-3.52968600	1.40077800	1.27271800	O	-3.94436700	-1.98356700	-0.92683400
O	0.05718600	-1.36326200	2.74178200	O	-1.48015200	3.17342000	0.87770100	O	-4.75490600	0.45119300	0.01277200
Cl	1.49925200	1.15096200	2.16639300	Cl	0.83790500	2.96344300	-0.90158800	Cl	-3.07982500	2.66671700	1.01711400
Cl	-0.01024200	2.89728200	-0.00438900	Cl	0.95763600	0.13226800	-2.32369600	Cl	-0.01888900	1.88538800	1.00702000
Cl	-2.76769800	1.98267300	-1.13586200	Cl	-1.50113600	-1.78114700	-2.12511900	Cl	-0.37391000	1.10158100	-2.41267700
Cl	-4.06623700	-0.75864000	-0.21824800	Cl	-3.76318600	-1.32366400	0.06696100	Cl	-1.17216700	-3.07475800	-0.95636600
MC(A3)(PCM)				TS(A3)(PCM)				IM(A3)(PCM)			
C	1.13014500	-1.64170100	-0.89920600	C	0.97521800	-0.62233800	1.92630000	C	-2.55435600	-1.47631300	-1.03519100
O	1.13699200	-2.84578700	-0.61456700	O	1.00169600	-0.16428900	3.07559500	O	-3.20044200	-2.22747900	-1.76295200

N	-0.04441800	-1.09516900	-1.42621100	N	-0.18552700	-1.19903900	1.46411900	N	-1.19601700	-1.71196400	-0.89933200
O	-0.17279200	0.16177500	-1.72418900	O	-0.31191200	-1.62756500	0.20318700	O	-0.64086000	-1.11948100	0.28153700
C	2.36603800	-0.81261200	-0.76314900	C	2.20974400	-0.63911400	1.08136300	C	-3.21064400	-0.33368200	-0.32564300
C	2.68206200	0.27345800	-1.59345300	C	2.60660500	-1.77669800	0.36683700	C	-2.63095000	0.92723000	-0.13261300
C	3.31823400	-1.25404500	0.16970800	C	3.06757100	0.46634700	1.14633000	C	-4.52690600	-0.55617700	0.10712000
C	3.92182400	0.90105900	-1.48456700	C	3.84226300	-1.80179800	-0.27657600	C	-3.35948500	1.94471500	0.47991500
H	1.96821200	0.61864700	-2.32620200	H	1.96065100	-2.64354500	0.32553600	H	-1.62758300	1.13198400	-0.47411200
C	4.54649100	-0.61217100	0.28866400	C	4.29097100	0.44758000	0.48175900	C	-5.24200500	0.45588300	0.74041400
H	3.08655300	-2.10298300	0.80024000	H	2.77095700	1.33865800	1.71602900	H	-4.98034700	-1.52730500	-0.04733300
C	4.85325600	0.46801900	-0.54062100	C	4.68210200	-0.68818100	-0.22935000	C	-4.66077500	1.71124400	0.92451700
H	4.15881300	1.73111000	-2.14051500	H	4.14838700	-2.69120200	-0.81557900	H	-2.90607100	2.92049300	0.60997200
H	5.26546100	-0.95702500	1.02308400	H	4.94084000	1.31420400	0.52455900	H	-6.25226000	0.26635300	1.08418100
H	5.81268800	0.96574600	-0.45439200	H	5.63911700	-0.70738900	-0.73863800	H	-5.21952300	2.50342900	1.40981600
C	-1.04721400	-2.03765800	-1.96413300	C	-1.24456600	-1.54663000	2.42263100	C	-0.65681100	-3.04835200	-1.17445600
H	-0.60855200	-2.58808300	-2.80067800	H	-0.80110700	-2.05355700	3.28142100	H	-1.03157900	-3.35682300	-2.14637600
H	-1.36655200	-2.74691400	-1.20296800	H	-1.78071600	-0.66308600	2.77047900	H	0.42930100	-2.99165000	-1.22174700
H	-1.88701500	-1.44306400	-2.30948100	H	-1.93072900	-2.21618800	1.91242800	H	-0.96621100	-3.76214600	-0.40682200
C	-1.70308900	-1.20826400	1.21957200	C	-2.35809600	1.24698700	0.58525600	C	2.77711600	-0.88050400	1.57145600
C	-0.38504400	-0.67589500	1.77923400	C	-1.11159900	2.10137500	0.32540400	C	3.52165600	-0.29480800	0.33646800
C	0.01251500	0.65494000	1.37703300	C	-0.14571300	1.63637700	-0.68845500	C	2.71304500	0.04766800	-0.84417800
C	-0.70767700	1.37904200	0.46235700	C	-0.27792700	0.43006700	-1.28087500	C	1.37652100	-0.18220100	-0.86558200
C	-1.97978300	0.88739900	-0.03982600	C	-1.36806300	-0.49553000	-0.87756100	C	0.68905600	-0.85166900	0.26955600
C	-2.47028100	-0.32348200	0.37096000	C	-2.43937400	0.03699600	-0.11796800	C	1.35190300	-1.14038800	1.42368100
O	-2.06858300	-2.34579700	1.52822300	O	-3.20720600	1.69827400	1.38351800	O	3.41897800	-1.12648400	2.57092800
O	0.26186300	-1.38193600	2.55795800	O	-0.95372500	3.14675100	0.93390600	O	4.71723000	-0.12413000	0.40402000
Cl	1.46725400	1.28689300	2.10535800	Cl	1.14592900	2.73490300	-1.07490800	Cl	3.55763800	0.80649700	-2.14701300
Cl	-0.19222100	2.97196200	0.00437500	Cl	0.85402400	-0.09965400	-2.47762000	Cl	0.44098200	0.37210800	-2.20330900
Cl	-2.93290300	1.92047300	-1.05764300	Cl	-1.77434700	-1.73033300	-2.07440500	Cl	0.34353200	5.15493200	0.80207600
Cl	-4.02468200	-0.91496500	-0.16270400	Cl	-3.88762700	-0.93330600	0.14544500	Cl	0.54272700	-1.88388200	2.76511200
MC(A4)				TS(A4)				IM(A4)			
C	-2.35407400	1.93625400	0.63038100	C	2.34231300	-1.73622400	-0.43620200	C	-2.77698800	0.98091200	-0.73116900
O	-2.87583000	3.01335200	0.94380100	O	3.05438900	-2.72276200	-0.23979900	O	-3.63648500	1.84132700	-0.89150200
N	-0.98485200	1.81055300	0.53319000	N	0.98467700	-1.89834400	-0.58852700	N	-1.48313000	1.27102900	-1.06111600
O	-0.36798600	0.64194200	0.47818100	O	0.13155800	-0.84066500	-0.71563000	O	-0.53568700	0.23556300	-1.02143700
C	-3.21087500	0.72742100	0.39361200	C	2.96661400	-0.37845400	-0.58683200	C	-3.12702400	-0.35679200	-0.13546000
C	-3.02194500	-0.16804200	-0.66307900	C	2.48728300	0.61408200	-1.44820400	C	-2.67848900	-1.58163100	-0.64154400
C	-4.32139800	0.56904800	1.23260300	C	4.17438000	-0.16836700	0.08951000	C	-4.04842200	-0.34905500	0.91856200
C	-3.92571400	-1.20999600	-0.86470600	C	3.20364800	1.79595200	-1.62144600	C	-3.13964700	-2.77675100	-0.09173100
H	-2.18356100	-0.05344900	-1.33448300	H	1.54888500	0.47080500	-1.96381400	H	-1.97587200	-1.60659600	-1.46292300
C	-5.21012900	-0.48483300	1.04240500	C	4.87752800	1.02057900	-0.06943600	C	-4.48831100	-1.54289000	1.48073900
H	-4.47814100	1.28792100	2.02803000	H	4.54911800	-0.95378300	0.73402900	H	-4.41296200	0.60279100	1.28452100
C	-5.01465300	-1.37882300	-0.01104200	C	4.39378600	2.00710000	-0.92904000	C	-4.03565100	-2.76168100	0.97502300
H	-3.76571200	-1.89392900	-1.69084300	H	2.81661100	2.56238700	-2.28366800	H	-2.78982100	-3.72023700	-0.49605300
H	-6.05783100	-0.60422500	1.70962900	H	5.80175100	1.17869000	0.47652900	H	-5.18672200	-1.52298300	2.31029700

H	-5.70873600	-2.19866700	-0.16710100	H	4.93701800	2.93828900	-1.05174200	H	-4.38068800	-3.69392900	1.40938300
C	-0.13822700	2.97071700	0.80441300	C	0.42608000	-3.22796400	-0.79957400	C	-1.09978100	2.45381500	-1.82839400
H	0.33958600	2.84570200	1.78232800	H	-0.03839500	-3.61666100	0.10917900	H	-0.02077300	2.40778300	-1.99959200
H	0.62949500	3.02969000	0.03562600	H	-0.32784200	-3.15505100	-1.58486000	H	-1.63621000	2.47413700	-2.78057600
H	-0.75089000	3.86842500	0.80211300	H	1.23373800	-3.89307100	-1.10007000	H	-1.35009700	3.34443800	-1.25070200
C	0.45048600	-0.52650900	-1.60358300	C	-1.16428900	2.21983000	0.44869100	C	1.72588300	0.85335000	1.92575100
C	1.23216200	0.77975200	-1.51482000	C	-2.49496900	1.91146500	-0.27336200	C	2.81488900	-0.18842900	1.53713300
C	2.35858600	0.80806100	-0.55835700	C	-2.93243300	0.48379600	-0.34731500	C	2.59602900	-0.95104600	0.30696500
C	2.61027600	-0.21823800	0.29651300	C	-2.15537500	-0.51121500	0.10969200	C	1.53462600	-0.68985500	-0.49322600
C	1.78348300	-1.41469300	0.29306600	C	-0.76615400	-0.25938700	0.64021500	C	0.49117100	0.30349000	-0.12592300
C	0.78086900	-1.56701600	-0.61234400	C	-0.43518000	1.10019900	0.90148900	C	0.56938300	0.99883700	1.04251800
O	-0.35642800	-0.70582400	-2.50399500	O	-0.86216700	3.40896100	0.58382500	O	1.86439400	1.47223700	2.95974700
O	0.98376200	1.70465600	-2.27166500	O	-3.17140500	2.79297100	-0.75084900	O	3.76779300	-0.34699500	2.26808600
Cl	3.37609800	2.22406500	-0.61756900	Cl	-4.50175200	0.20541000	-1.05993800	Cl	3.79903500	-2.13865000	-0.09208300
Cl	3.95861700	-0.14121500	1.40741400	Cl	-2.70985900	-2.15974500	0.02091800	Cl	1.22438600	-1.67375700	-1.88735900
Cl	2.12760400	-2.66976500	1.45979500	Cl	-0.34197900	-1.41063200	1.98521700	Cl	2.33152600	1.71677300	-2.03514700
Cl	-0.18652400	-3.00878900	-0.67661500	Cl	1.07288300	1.44852100	1.74172000	Cl	-0.62383300	2.14543800	1.60628500
<i>p</i> -MC(A1)				<i>p</i> -TS(A1)				<i>p</i> -IM(A1)			
C	-1.41097700	-0.38874600	1.62041700	C	-1.27812800	-1.14890100	1.27042400	C	1.97016700	-1.22193200	-1.17030000
C	-2.44254000	-0.20210300	0.57789200	C	-2.55403100	-0.85306500	0.48281000	C	3.04979500	-0.37334800	-0.59339900
C	-2.32067300	0.71912800	-0.40714300	C	-2.80224100	0.33014300	-0.10453000	C	2.84506300	0.41484600	0.47838100
C	-1.17363900	1.66327900	-0.48891400	C	-1.82531500	1.44702300	-0.00627800	C	1.56297900	0.33154400	1.24590000
C	-0.14654400	1.47520500	0.56797600	C	-0.43720800	1.09729000	0.54474800	C	0.41026500	-0.31938400	0.52495900
C	-0.25414300	0.53166900	1.53428400	C	-0.30912500	-0.11946000	1.25787200	C	0.62582600	-1.09906400	-0.55698700
O	-1.52110800	-1.22414700	2.50756400	O	-1.20098900	-2.23071900	1.85904600	O	2.18016000	-1.95264100	-2.12221500
Cl	-3.53817600	0.93826400	-1.62456500	Cl	-4.28319400	0.69517500	-0.95648100	Cl	4.08170700	1.38181100	1.19271900
Cl	1.15325500	2.62328600	0.54098500	Cl	0.27947100	2.56546700	1.31623400	Cl	0.77954900	2.50404200	-0.12627100
Cl	0.92809700	0.35359100	2.80082200	Cl	1.15193800	-0.43214100	2.18967600	Cl	-0.63715000	-1.93908400	-1.41953100
Cl	-3.81750400	-1.27031300	0.69292900	Cl	-3.69074700	-2.15676900	0.41307200	Cl	4.57534300	-0.44106600	-1.42852300
O	-1.16425500	2.61523700	-1.25417400	O	-2.10905300	2.56396700	-0.37216300	O	1.51782700	0.52276600	2.44373200
C	1.17814900	-1.83846100	-0.78549800	C	1.59407800	-0.76631800	-1.69284100	C	-2.98005200	-0.96063900	1.03533900
O	1.21589000	-3.02955900	-0.45535600	O	1.55683900	-1.77094600	-2.40474800	O	-3.79280100	-1.76779600	1.47913900
N	0.00531100	-1.31354900	-1.29083400	N	0.52105100	0.09068300	-1.67290100	N	-1.64397400	-1.17928500	1.32455200
O	-0.12938700	-0.07388500	-1.72230500	O	0.48958900	1.21153500	-0.89836300	O	-0.75163600	-0.09122500	1.20290700
C	2.41506800	-0.99005700	-0.69943200	C	2.83636100	-0.44539900	-0.90879800	C	-3.43192400	0.15341600	0.12566700
C	2.70028400	0.09159300	-1.54319500	C	3.31035000	0.85108200	-0.68079600	C	-2.72446400	1.31904600	-0.20382100
C	3.39202300	-1.41324900	0.21374900	C	3.61225600	-1.53637400	-0.49914200	C	-4.72393400	-0.02258500	-0.40160200
C	3.93952300	0.72661800	-1.47236100	C	4.53849100	1.04587600	-0.05158500	C	-3.30026000	2.27023000	-1.04696900
H	1.94450400	0.43467000	-2.23453900	H	2.71374000	1.70106000	-0.97836200	H	-1.73261600	1.51940100	0.17128300
C	4.61639800	-0.76065100	0.29884900	C	4.82651900	-1.33894600	0.14865500	C	-5.28690500	0.92447100	-1.24639300
H	3.16997300	-2.26472100	0.84468000	H	3.24455300	-2.53516500	-0.69774000	H	-5.26986100	-0.91718700	-0.13151300
C	4.89708400	0.31137900	-0.54979000	C	5.29590000	-0.04418900	0.37196100	C	-4.57357400	2.07971500	-1.57281000
H	4.14796300	1.56086500	-2.13404900	H	4.89617200	2.05575800	0.11907300	H	-2.72613200	3.15725600	-1.28894000
H	5.35405700	-1.08944900	1.02365100	H	5.40686300	-2.19385700	0.47944400	H	-6.28100900	0.76270400	-1.64998000

H	5.85371700	0.82060300	-0.48834600	H	6.24370500	0.11327500	0.87669100	H	-5.00936100	2.82245300	-2.23334400
C	-1.06775500	-2.26580900	-1.61030600	C	-0.54267500	-0.04574700	-2.66279200	C	-1.24946000	-2.07481100	2.40401200
H	-0.73846200	-2.94585800	-2.40357700	H	-0.88801700	0.95776800	-2.91398000	H	-1.26290700	-1.55756800	3.36854900
H	-1.33166100	-2.86261300	-0.73792600	H	-0.14232500	-0.54759600	-3.54290000	H	-1.94865600	-2.90637300	2.41663200
H	-1.91636100	-1.68067400	-1.95196800	H	-1.38147700	-0.63427700	-2.28284600	H	-0.24180000	-2.44051500	2.20239200
<i>p</i> -MC(A2)				<i>p</i> -TS(A2)				<i>p</i> -IM(A2)			
C	1.25460900	-0.21641700	1.67903100	C	-2.16702700	1.20110600	-0.32318200	C	-2.49392400	1.56470600	-0.19495100
C	0.16346900	0.74979500	1.42496000	C	-0.87728500	1.91311700	0.09197600	C	-3.16218100	0.23921900	-0.16489900
C	0.16721400	1.58343600	0.35663700	C	0.01923000	1.38677700	0.94553900	C	-2.49754600	-0.88476300	0.16453300
C	1.26896300	1.61047200	-0.64102900	C	-0.19659000	0.03720600	1.52540100	C	-1.08289100	-0.85372500	0.68063000
C	2.35549400	0.62952100	-0.38298200	C	-1.27879400	-0.81998200	0.84993900	C	-0.37359300	0.46821700	0.52876800
C	2.35522800	-0.19762400	0.68902400	C	-2.31261500	-0.10966700	0.17598000	C	-1.06636500	1.57842900	0.17753300
O	1.26707300	-0.95374700	2.65515900	O	-2.97202000	1.82066300	-1.02659200	O	-3.09457900	2.58144000	-0.49818700
Cl	-1.06025700	2.78619800	0.12033600	Cl	1.40930800	2.25511600	1.54235600	Cl	-3.26386700	-2.42875400	0.25378500
Cl	3.66815300	0.67228600	-1.51965100	Cl	-1.80979800	-2.11229300	1.98512100	Cl	-0.51970800	-1.39479300	-1.91705100
Cl	3.65528100	-1.31696300	1.00481400	Cl	-3.80193200	-0.94839100	-0.27212500	Cl	-0.27934600	3.13246600	0.10571300
Cl	-1.09933600	0.77534000	2.62375700	Cl	-0.68155400	3.50428400	-0.56017100	Cl	-4.83462400	0.23533500	-0.64410400
O	1.35768200	2.47564700	-1.49861800	O	0.45457700	-0.36543100	2.46096600	O	-0.66208100	-1.74031400	1.39598100
C	-1.11850600	-1.91314000	-0.69333300	C	1.05285600	-0.88269900	-1.86379800	C	2.95734500	-0.41085400	1.44436100
O	-1.12985200	-3.08794600	-0.30664700	O	1.16971200	-0.55369400	-3.04505000	O	3.69443600	-0.70034600	2.38061200
N	0.03925900	-1.39560200	-1.24085900	N	-0.15873000	-1.33830700	-1.41312500	N	1.59852300	-0.25232500	1.69383000
O	0.15377800	-0.18192600	-1.74346500	O	-0.32757800	-1.80075000	-0.13271200	O	0.95160800	0.64865100	0.79695000
C	-2.36910400	-1.08423600	-0.62470600	C	2.24603100	-0.81376300	-0.94742400	C	3.48931600	-0.26821900	0.05404600
C	-2.68023800	-0.02987900	-1.49336300	C	2.52151700	-1.73828600	0.06702500	C	2.76811200	-0.59064900	-1.09886700
C	-3.33168700	-1.50108500	0.30707200	C	3.19398500	0.17540000	-1.24208900	C	4.82423000	0.14792900	-0.05765600
C	-3.93010300	0.58506200	-1.42766800	C	3.72143000	-1.66557500	0.77230000	C	3.37820700	-0.48804100	-2.34789300
H	-1.93703800	0.30644000	-2.20139000	H	1.79544300	-2.49955000	0.31188300	H	1.74198500	-0.93615200	-1.05714900
C	-4.56714700	-0.86942000	0.38483000	C	4.38087200	0.25731200	-0.52311800	C	5.42155800	0.26544900	-1.30722500
H	-3.08834200	-2.33133700	0.95803300	H	2.98349300	0.86825000	-2.04722500	H	5.37877000	0.37018700	0.84592400
C	-4.87341400	0.17584000	-0.48809500	C	4.64962200	-0.66720300	0.48661300	C	4.69711000	-0.05403600	-2.45777000
H	-4.15863400	1.39858100	-2.10823500	H	3.92124400	-2.38528300	1.55866100	H	2.80240400	-0.74715500	-3.22905100
H	-5.29327800	-1.19330100	1.12338300	H	5.09599700	1.04099600	-0.74967900	H	6.45039700	0.60113200	-1.38486600
H	-5.83869100	0.66910500	-0.43205200	H	5.57469000	-0.60548100	1.05057700	H	5.16249100	0.03337800	-3.43438800
C	1.12313600	-2.34724900	-1.52303200	C	-1.19762400	-1.67860600	-2.38723600	C	1.17362100	-0.05534700	3.07542000
H	1.96597100	-1.76609200	-1.88495200	H	-1.87863300	-2.37305200	-1.90213000	H	1.44962600	0.94161400	3.43650500
H	1.39033100	-2.90918000	-0.62923700	H	-1.75169300	-0.79449700	-2.70661500	H	0.09864600	-0.20390700	3.13749800
H	0.80263600	-3.05833300	-2.29240000	H	-0.73301700	-2.13852100	-3.26211300	H	1.67122700	-0.81047100	3.67785700
<i>p</i> -MC(A2)(PCM)				<i>p</i> -TS(A2)(PCM)				<i>p</i> -IM(A2)(PCM)			
C	1.40042800	-0.46985400	1.57603300	C	1.73140200	1.42920100	0.62010700	C	-2.49454700	-0.76095200	1.34548100
C	0.24574300	0.44795900	1.56774100	C	0.38117500	1.93097200	0.14203900	C	-3.07825700	-0.49608600	-0.00906000
C	0.11167000	1.42577800	0.64039200	C	-0.27877900	1.39628300	-0.90390700	C	-2.29486600	-0.40521200	-1.09788400
C	1.12158300	1.66083100	-0.41763500	C	0.26901700	0.22703900	-1.61971300	C	-0.80459000	-0.51168200	-0.99501400
C	2.30548200	0.76881100	-0.36463300	C	1.46077900	-0.46875900	-0.96290300	C	-0.23974600	-0.94526100	0.32505600
C	2.43818400	-0.20741500	0.56391100	C	2.22715000	0.29463700	-0.03903300	C	-1.03258800	-1.00808800	1.41530400

O	1.50102400	-1.38508300	2.39235700	O	2.31822800	2.06784000	1.51966300	O	-3.19620900	-0.80182800	2.33441700
Cl	-1.21912300	2.53504200	0.65654500	Cl	-1.73945200	2.07291700	-1.56037200	Cl	-2.90585200	-0.09714200	-2.67888700
Cl	3.52643400	1.08495100	-1.55199100	Cl	2.37521000	-1.41093100	-2.17484800	Cl	-1.40616300	5.37231700	0.37372200
Cl	3.82966400	-1.24870200	0.62809500	Cl	3.83855600	-0.24703300	0.43794600	Cl	-0.39485100	-1.39238500	2.97399800
Cl	-0.90883700	0.20993500	2.84593300	Cl	-0.23352500	3.30920500	0.98324700	Cl	-4.79008100	-0.31483000	-0.06104300
O	1.07273000	2.63894400	-1.16481300	O	-0.21482300	-0.18259200	-2.65562300	O	-0.09098300	-0.22962600	-1.93204900
C	-1.12050800	-1.77930300	-0.83386200	C	-0.75042300	-1.36213900	1.67842200	C	3.06229500	-1.43827400	-0.75897200
O	-1.10225200	-2.97218000	-0.48136400	O	-0.79788600	-1.27721600	2.91409300	O	3.84705200	-2.22137900	-1.29155000
N	0.00772900	-1.22488900	-1.39042800	N	0.43026900	-1.71821700	1.08835300	N	1.75473500	-1.84013900	-0.56407200
O	0.09478800	0.04900100	-1.72648500	O	0.57044400	-1.77389200	-0.26125700	O	1.09500700	-1.13105600	0.49165900
C	-2.37582800	-0.97229000	-0.72540800	C	-1.98695800	-1.15763200	0.85949500	C	3.49098900	-0.06583400	-0.34745900
C	-2.80089700	-0.09368500	-1.73162000	C	-2.33211400	-1.99616100	-0.20819400	C	2.73543400	1.08776800	-0.59056800
C	-3.22554100	-1.23019600	0.35915700	C	-2.90256900	-0.19083500	1.29685600	C	4.75837600	0.04872500	0.24044800
C	-4.05006000	0.51792700	-1.64630200	C	-3.57344900	-1.86315600	-0.82816800	C	3.24479100	2.33817100	-0.24616900
H	-2.16175600	0.10221400	-2.58125900	H	-1.64284500	-2.75910000	-0.54279000	H	1.76852900	1.01500000	-1.06842600
C	-4.46206200	-0.59731700	0.45537200	C	-4.13319900	-0.04737300	0.66295200	C	5.25237200	1.29846300	0.60470600
H	-2.91046500	-1.92620600	1.12669300	H	-2.64428600	0.44707200	2.13346000	H	5.34736400	-0.84273500	0.41891100
C	-4.87897400	0.27726900	-0.54954100	C	-4.47322800	-0.88675700	-0.39953700	C	4.49763500	2.44633000	0.35884200
H	-4.37495200	1.18468800	-2.43715700	H	-3.83810100	-2.52559900	-1.64452400	H	2.66094200	3.22809300	-0.45089300
H	-5.10240500	-0.79202100	1.30828300	H	-4.82809400	0.71303000	1.00062200	H	6.22638400	1.37611900	1.07382200
H	-5.84574500	0.76353000	-0.48135600	H	-5.43532500	-0.78238900	-0.88849000	H	4.88535600	3.42064700	0.63386800
C	1.09730400	-2.12534700	-1.80292500	C	1.51533300	-2.27131200	1.90587400	C	1.41316000	-3.26503900	-0.57998800
H	1.88814000	-1.50493100	-2.21313200	H	2.22441400	-2.73940800	1.22857900	H	1.82416800	-3.77927900	0.29275700
H	1.47142700	-2.70217700	-0.95831600	H	2.01783700	-1.49514800	2.48340000	H	0.32928900	-3.36670800	-0.59998900
H	0.73383700	-2.81616600	-2.56828600	H	1.10856200	-3.01880200	2.58900700	H	1.82123500	-3.69252600	-1.49213200
N ⁺				O ⁻				N ⁻			
C	1.15295000	0.37256400	0.23238800	O	2.39909800	1.93559600	-0.00038700	C	1.31202600	0.31857100	-0.00001000
O	1.94025600	1.36719300	0.21320100	C	-0.00055400	2.05862700	-0.00002300	O	1.71249300	1.52041000	-0.00004600
N	2.32693900	-0.25800900	0.48837500	C	-1.35692600	1.28405600	0.00008800	N	2.02711600	-0.78960700	0.00011200
C	-0.22222400	0.14252900	0.11057300	C	-1.24516900	-0.13638500	-0.00008500	C	-0.19767800	0.08999500	-0.00003600
C	-0.72778300	-1.17561200	0.22315400	C	0.00018800	-0.78336100	-0.00008700	C	-0.76509400	-1.19192500	-0.00005400
C	-1.08572600	1.24282200	-0.11744600	C	1.24529000	-0.13587200	0.00004400	C	-1.05786200	1.19427800	0.00001100
C	-2.08866200	-1.38282500	0.10412800	C	1.35641400	1.28456800	-0.00017400	C	-2.14810000	-1.36319600	-0.00002700
H	-0.05801800	-2.00601100	0.41451000	O	-0.00074800	3.26165100	0.00001300	H	-0.08591300	-2.03604100	-0.00007700
C	-2.44246500	1.01247200	-0.23691200	O	-2.40003300	1.93449000	0.00029200	C	-2.44360900	1.02792600	0.00005600
H	-0.68078500	2.24522200	-0.19393700	Cl	-2.75825400	-1.03925900	-0.00001600	H	-0.60009800	2.17715800	-0.00000400
C	-2.93904100	-0.29344000	-0.12668400	Cl	0.00059000	-2.53924200	-0.00014900	C	-2.99782700	-0.25267500	0.00001600
H	-2.49736700	-2.38141400	0.19212300	Cl	2.75872300	-1.03818700	0.00028700	H	-2.56913600	-2.36540900	0.00000800
H	-3.12087900	1.83791300	-0.41158200					H	-3.09407400	1.89887600	0.00001600
H	-4.00574900	-0.46425100	-0.21803100					H	-4.07606200	-0.38557300	0.00000900
C	3.11882200	-0.81373100	-0.59530900					C	3.45738100	-0.56112000	-0.00000700
H	3.01083600	-1.90009000	-0.45490400					H	3.79907600	0.01473500	-0.87789300
H	2.77987600	-0.52410100	-1.59099700					H	3.79921300	0.01457000	0.87795800
H	4.16623300	-0.56742800	-0.42476100					H	3.98181300	-1.52546700	-0.00011400

O ⁺				·N(CH ₃)-COAr				o-CBQ·			
O	2.32370500	1.89166700	0.38348900	C	1.25526200	0.38675400	0.15546000	O	2.38495600	1.90141800	-0.00015200
C	0.00030200	2.10607800	-0.17871200	O	1.73026200	1.51365700	0.27584100	C	0.00023400	2.09478300	0.00010000
C	-1.30262300	1.33532300	0.11404400	N	2.07292400	-0.73369300	0.17440400	C	-1.33185600	1.30646000	-0.00012800
C	-1.21975700	-0.18524300	0.04316900	C	-0.20861600	0.12509800	0.08071300	C	-1.23339900	-0.16182700	-0.00001200
C	-0.00016000	-0.89201500	0.01233300	C	-0.72888100	-1.17335600	0.16121800	C	-0.00010700	-0.83739900	0.00001500
C	1.21966300	-0.18559600	0.04330600	C	-1.07664600	1.21099400	-0.09238200	C	1.23340400	-0.16211800	-0.00001200
C	1.30314200	1.33515000	0.11347800	C	-2.10250800	-1.38014600	0.06720400	C	1.33214300	1.30615100	-0.00003600
O	0.00020600	3.22656700	-0.57338900	H	-0.05383400	-2.00609600	0.31198800	O	0.00039200	3.29079200	0.00039400
O	-2.32274100	1.89219000	0.38514500	C	-2.44700600	0.99995300	-0.18631400	O	-2.38454100	1.90193900	-0.00036200
Cl	-2.68595500	-0.96796000	-0.04723600	H	-0.65888600	2.20879600	-0.15028900	Cl	-2.72181000	-1.01059300	0.00007200
Cl	-0.00040500	-2.60238200	-0.05020000	C	-2.96176400	-0.29595900	-0.10697800	Cl	-0.00034400	-2.56822300	0.00004000
Cl	2.68560900	-0.96881000	-0.04654500	H	-2.50302100	-2.38513500	0.13577900	Cl	2.72162700	-1.01115400	-0.00003100
				H	-3.11619300	1.84203700	-0.32139400				
				H	-4.03148300	-0.45859200	-0.17871100				
				C	3.39581500	-0.59871300	-0.36664900				
				H	3.53425500	-1.39962800	-1.10560500				
				H	3.59449100	0.37687000	-0.81796000				
				H	4.12816800	-0.79940700	0.42501100				
P1				TS				P2			
O	2.02218300	-2.74389900	1.17947800	O	-0.42649600	2.70534900	-1.26643000	O	-0.64280500	-0.86425800	-2.73429900
C	0.72071200	-0.93785400	2.02343600	C	-0.65463700	0.36504700	-1.71707500	C	-2.38830100	0.01419300	-1.35861000
C	-0.14257400	0.25725900	1.57273000	C	-0.04059100	-1.03138700	-1.44395500	C	-2.45210600	0.87236100	-0.07654300
C	0.39728000	1.09041200	0.37028500	C	1.24019500	-1.05983400	-0.67142900	C	-1.52042300	0.49540200	1.02138300
C	1.32024300	0.31996500	-0.56373900	C	1.90341300	0.11438200	-0.29167700	C	-0.57495900	-0.46635900	0.89711900
C	1.84144100	-0.90165800	-0.30326800	C	1.22810700	1.35240100	-0.23227700	C	-0.30249000	-1.24238000	-0.37810700
C	1.58877500	-1.64220500	0.95963200	C	-0.00144800	1.60154200	-1.05331300	C	-1.06342200	-0.71796600	-1.62415300
O	0.68873300	-1.32369600	3.15529400	O	-1.55317200	0.49170400	-2.49577900	O	-3.30532900	-0.03714500	-2.12604100
O	-1.12959300	0.56658600	2.17046600	O	-0.53322700	-2.01660600	-1.92416800	O	-3.24756500	1.77188800	0.00601300
Cl	1.55776400	2.19644000	1.36206000	Cl	2.05665600	-2.56744500	-0.69394200	Cl	-1.78201200	1.33234400	2.50868500
Cl	1.70040900	1.13470100	-2.04179600	Cl	3.53910100	0.02450400	0.27206300	Cl	0.36394900	-0.96918000	2.25788600
Cl	2.87931400	-1.71619700	-1.42103200	Cl	2.01898800	2.75857100	0.32030500	Cl	-1.12250000	-2.90183000	-0.15013100
C	-1.95834800	1.42864400	-0.41305800	C	-0.58362100	-0.17669500	1.46735900	C	2.12338500	-0.67674400	-0.30126200
O	-2.84507800	2.24610000	-0.55085900	O	0.03811800	0.92204500	1.62027500	O	1.02011700	-1.50713900	-0.66239400
N	-0.62094000	1.86360900	-0.28752400	N	-0.01646700	-1.37860700	1.63665400	N	3.19638700	-1.20109100	0.07663200
C	-2.25527500	-0.03949200	-0.50082100	C	-2.00594000	-0.15945300	1.00439400	C	1.96662300	0.79034100	-0.47768200
C	-1.57590400	-0.87829000	-1.38925500	C	-2.68924800	-1.34201900	0.68052600	C	2.38443000	1.64746600	0.54771500
C	-3.33620000	-0.54343700	0.23361000	C	-2.68139400	1.06773100	0.93062700	C	1.47828200	1.33303100	-1.67332100
C	-1.95457400	-2.21542400	-1.52100000	C	-4.01308100	-1.28923100	0.26084200	C	2.28272700	3.02623400	0.39251000
H	-0.78583000	-0.48444300	-2.01615500	H	-2.16905600	-2.28781800	0.75315200	H	2.78811700	1.22349700	1.45862000
C	-3.69882900	-1.87888100	0.11378400	C	-4.00871300	1.11402700	0.51997200	C	1.38944200	2.71483400	-1.82762500
H	-3.87319000	0.11752200	0.90226200	H	-2.15430300	1.97543400	1.19525800	H	1.20335300	0.68058600	-2.49149300
C	-3.00655700	-2.71914000	-0.76173700	C	-4.67460000	-0.06298800	0.17784000	C	1.78074400	3.56289600	-0.79292500
H	-1.43357400	-2.85507200	-2.22399400	H	-4.53015700	-2.20391700	-0.00511300	H	2.59787200	3.68232500	1.19569100

H	-4.52407400	-2.26694900	0.69949200	H	-4.52155800	2.06684200	0.45961500	H	1.02478400	3.12707800	-2.76144100
H	-3.29527700	-3.75956700	-0.85754700	H	-5.70659000	-0.02555100	-0.15256500	H	1.70422600	4.63744800	-0.91340200
C	-0.41479900	3.29843700	-0.56660600	C	1.17282100	-1.45802700	2.44792700	C	3.34053000	-2.63313100	0.26736700
H	0.62287400	3.47952300	-0.82884000	H	1.85500800	-2.20630400	2.03465300	H	3.94097100	-2.80154300	1.16386900
H	-1.05275300	3.56976700	-1.40398300	H	1.68540100	-0.50765600	2.61363000	H	2.39112000	-3.16856500	0.34823500
H	-0.69118200	3.90914600	0.29549200	H	0.85650700	-1.85940500	3.42179900	H	3.90229100	-3.04370400	-0.57740900