

Supporting Information for

Aquation and Dimerization of Osmium (II) Anticancer Complexes: A Density Functional Theory Study

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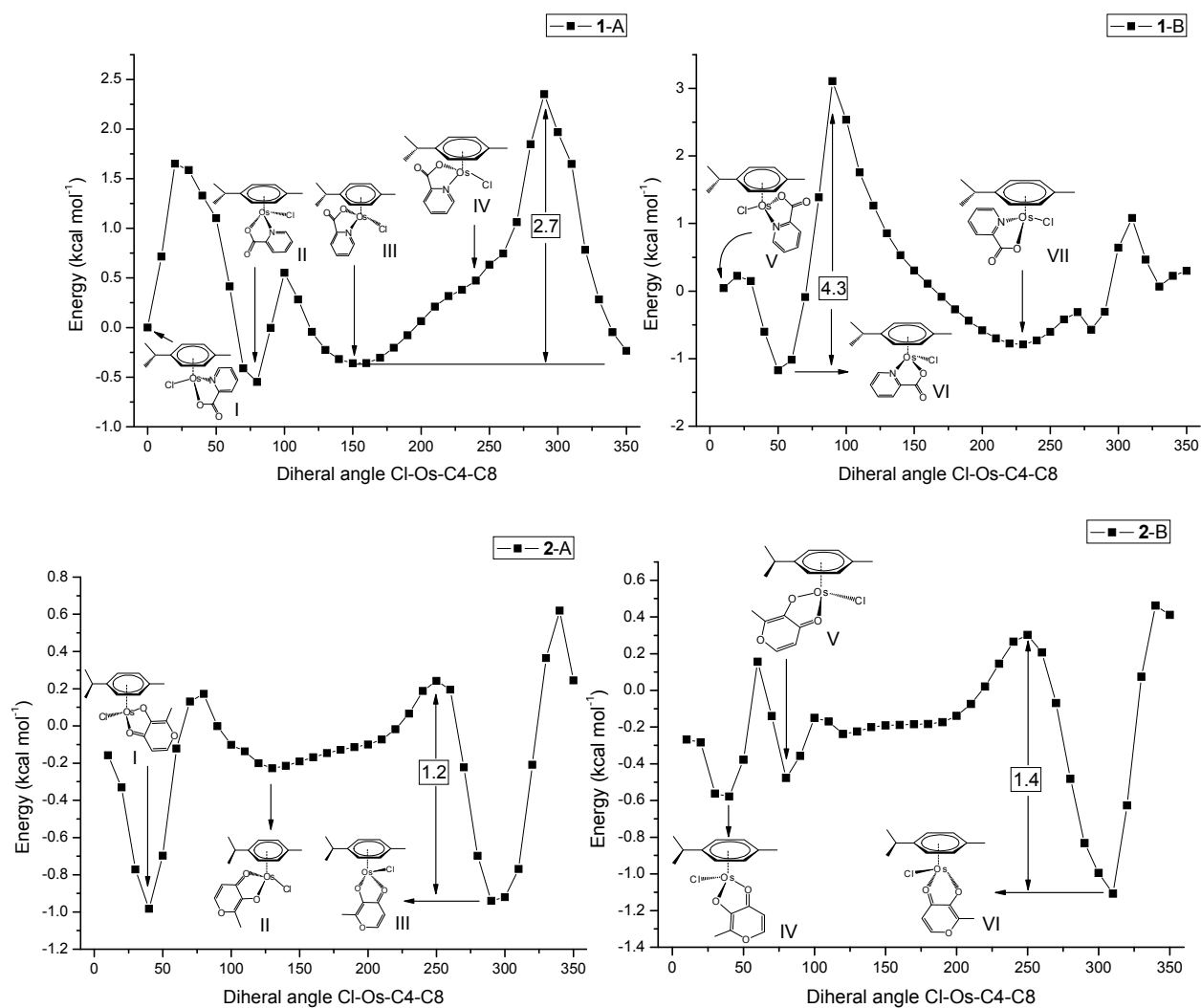


Fig. S1 Rotational energy barrier (kcal mol⁻¹) of *p*-cymene in **1** and **2** at the level of B3LYP/STO-3G (LanL2DZ for Os) level. The rotational profiles were computed in both directions with respect to chelated ligand, labeled as A and B. Please note that freezing the chosen dihedral results in occasional steric clashing between the *i*-Pr substituent of *p*-cymene and the YZ ligand. This causes the discontinuities shown in the figure.

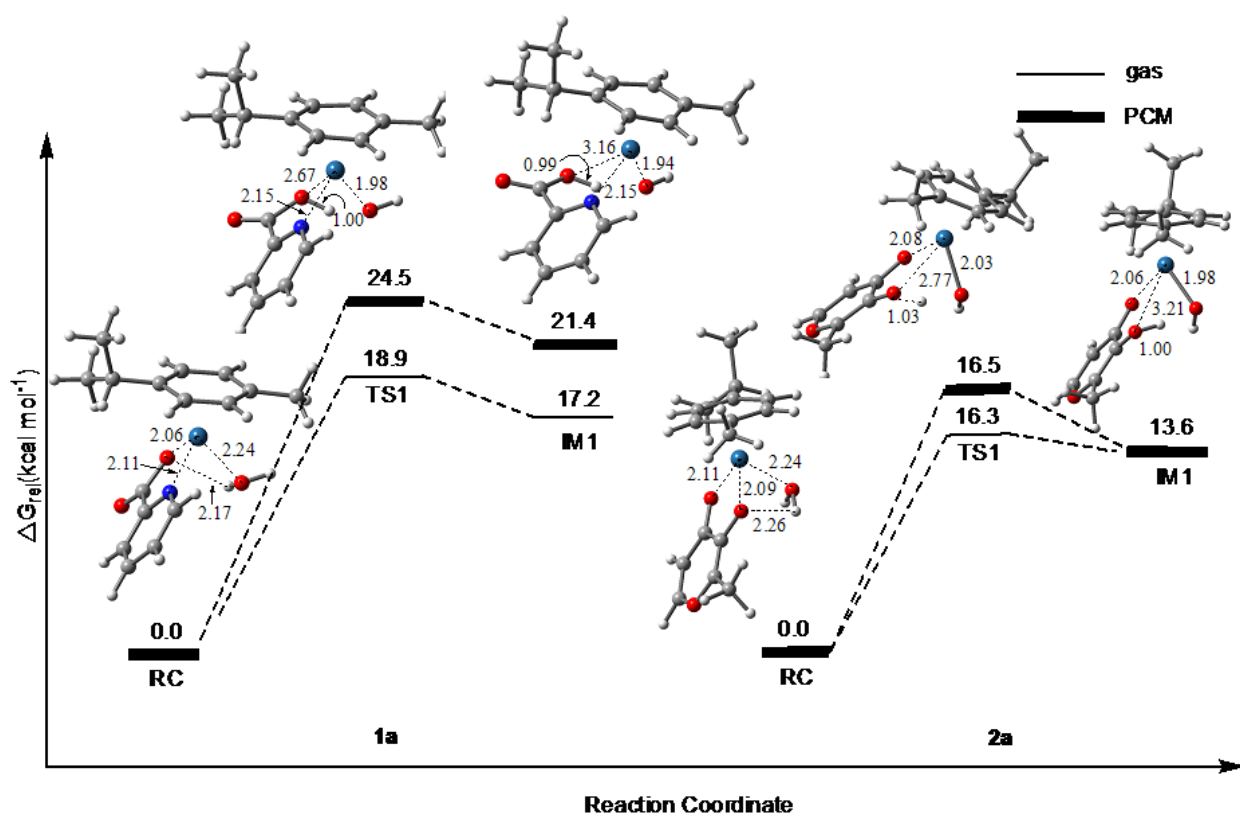


Fig. S2 Free energy profiles (at B3LYP/B3//B3LYP/B1 level) of the open cycle and proton shift of $[(\eta^6-p\text{-cym})\text{Os}(\text{YZ})(\text{H}_2\text{O})]^+$ (**1a** and **2a**) in gas phase and aqueous solution. Bond length values are given in Å.

Table S1 Estimation of activation ΔG_a^{298} , ΔH_a^{298} and ΔrG_r^{298} , ΔrH_r^{298} reaction energies (kcal mol⁻¹) in path A in $[(\eta^6\text{-}p\text{-cym})\text{Os}(\text{YZ})\text{Cl}]$ complex (**1-IV** and **2-I**) with B3LYP and BHandHLYP methods.

		1	2	1	2	1	2	1	2	1	2
		B3LYP						BHandHLYP			
		B1		B2//B1		B3//B1		B1		B2//B1	
ΔG_a^{298}	gas	21.6	22.2	22.3	23.7	22.5	23.9	22.2	24.8	23.6	24.0
ΔrG_r^{298}		7.9	4.2	8.8	5.4	9.6	6.6	7.6	5.2	9.2	4.2
ΔH_a^{298}		19.5	21.4	20.7	23.0	20.9	23.1	21.3	24.3	22.7	23.5
ΔrH_r^{298}		6.5	4.0	7.4	5.2	8.2	6.4	6.5	4.9	8.2	3.9
ΔG_a^{298}	PCM	19.8	18.7	20.5	20.1	20.7	20.2	20.0	20.6	21.7	21.3
ΔrG_r^{298}		3.2	-1.6	4.2	-0.3	5.0	0.7	2.7	-1.5	4.8	0.1
ΔH_a^{298}		16.1	18.0	19.0	19.4	19.1	19.5	19.1	20.0	20.7	20.8
ΔrH_r^{298}		0.8	-1.9	2.8	-0.6	3.6	0.4	1.7	-1.9	3.8	-0.3

Table S2 Estimation of activation ΔG_a^{298} , ΔH_a^{298} and ΔrG_r^{298} , ΔrH_r^{298} reaction energies (kcal mol⁻¹) in path B and C in $[(\eta^6\text{-}p\text{-cym})\text{Os}(\text{YZ})\text{Cl}]$ complex (**1-IV** and **2-I**) with B3LYP method.

		1	2	1	2	1	2	1	2
		TS _B		TS _C		TS _B		TS _C	
		B3LYP							
		B1		B1		B3//B1		B3//B1	
ΔG_a^{298}	gas	29.4	23.5	37.0	30.8	31.6	25.5	42.4	30.6
ΔrG_r^{298}		6.7	7.8	32.7	27.7	10.2	10.1	38.2	29.2
ΔH_a^{298}		27.5	22.1	35.7	31.6	29.8	24.1	41.4	31.5
ΔrH_r^{298}		5.0	7.8	30.9	26.4	8.5	10.0	36.5	28.0
ΔG_a^{298}	PCM	21.9	20.4	29.2	24.9	23.4	22.1	30.9	24.0
ΔrG_r^{298}		3.2	1.5	20.8	18.9	6.3	3.7	22.0	19.8
ΔH_a^{298}		20.0	19.1	27.9	25.7	21.5	20.7	29.8	24.8
ΔrH_r^{298}		1.5	1.4	19.0	17.6	4.6	3.7	20.3	18.5

Table S3 Estimation of activation ΔG_a^{298} , ΔH_a^{298} and ΔrG_r^{298} , ΔrH_r^{298} reaction energies (kcal mol⁻¹)

in dimerization of **1a** and **2a** for the model 1 of first step with B3LYP and BHandHLYP methods.

		1a	2a	1a	2a	1a	2a	1a	2a
		B3LYP						BHandHLYP	
		B1		B2//B1		B3//B1		B1	
ΔG_a^{298}	gas	17.8	16.5	18.6	16.6	18.9	16.5	21.0	18.0
ΔrG_r^{298}		16.6	14.1	17.0	14.2	17.2	13.6	19.8	16.4
ΔH_a^{298}		17.1	15.2	17.9	15.4	18.2	15.3	20.4	17.5
ΔrH_r^{298}		17.2	15.0	17.6	15.1	17.8	14.5	20.5	17.5
ΔG_a^{298}	PCM	21.8	16.5	24.2	16.3	24.5	16.3	28.4	18.3
ΔrG_r^{298}		20.5	14.4	21.3	14.2	21.4	13.6	26.4	16.7
ΔH_a^{298}		21.1	15.2	23.5	15.1	23.8	15.1	27.7	17.8
ΔrH_r^{298}		21.1	15.3	21.8	15.1	22.0	14.5	27.1	17.8

Cartesian coordinates for all of the species involved in
 Figure 1.

1-I

Os	0.18866000	-0.37576700	0.11832500
Cl	0.00177800	0.93716500	2.17616700
C	0.86513200	-2.12274600	-1.09199700
C	1.56701600	-2.11320200	0.17132700
C	2.27884700	-0.97215500	0.59679000
C	2.34166900	0.23097700	-0.20334600
C	1.66296600	0.21267500	-1.44872100
C	0.94026500	-0.95118300	-1.89380700
C	0.03528600	-3.31183200	-1.48920100
C	3.11129600	1.42776500	0.32685900
C	4.61544900	1.24486700	0.03843900
C	2.60390400	2.77936500	-0.18935500
N	-1.48223500	0.79272900	-0.44196400
C	-1.44850700	1.97475400	-1.08569200
C	-2.59964300	2.71704700	-1.32011500
C	-3.82811800	2.23096000	-0.86666100
C	-3.85681200	1.01416000	-0.19274100
C	-2.66676900	0.32230900	0.00531200
C	-2.61957500	-1.00639400	0.72256600
O	-3.65193800	-1.53526000	1.10713700
O	-1.41254000	-1.49178400	0.83250400
H	1.44528100	-2.94964400	0.85051700
H	2.67932900	-0.94877500	1.60383800
H	1.63333700	1.10837400	-2.05775600
H	0.37263600	-0.90304200	-2.81712700
H	2.96231600	1.42265800	1.41323700
H	5.19218100	2.05683900	0.49298200
H	4.81211500	1.25319700	-1.03979500
H	4.99236500	0.29871700	0.44010800
H	3.15592500	3.59014700	0.29561000
H	2.75286000	2.89272000	-1.26996300
H	1.54413000	2.91049300	0.04518900
H	-0.47180100	2.32120000	-1.39971500
H	-2.52480400	3.66421500	-1.84310500
H	-4.74043800	2.79533600	-1.03326900
H	-4.76517600	0.56884800	0.19665600
H	0.67855600	-4.14908100	-1.78388300
H	-0.59071700	-3.63139100	-0.65170000
H	-0.61943600	-3.07131300	-2.33064400

1-II

Os	0.19760200	0.28465600	0.17288500
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Cl	-0.84597300	0.56847500	2.36553500
C	0.89681800	2.38509900	-0.33954200
C	0.78190800	1.55672300	-1.50694600
C	1.50003800	0.32659400	-1.64989500
C	2.27162500	-0.17999000	-0.55742900
C	2.36022300	0.60525700	0.63569100
C	1.66442300	1.84922900	0.73251300
C	0.19965000	3.71312700	-0.22070900
C	2.94483200	-1.53627900	-0.69283100
C	4.28865100	-1.35733500	-1.43091900
C	3.12996500	-2.28709200	0.63304400
N	-1.81445400	0.01958200	-0.42792300
C	-2.65489600	0.98729800	-0.83856700
C	-3.99131400	0.73014400	-1.11960600
C	-4.48360100	-0.56741500	-0.96126100
C	-3.61519800	-1.56129700	-0.52126000
C	-2.28899400	-1.23366600	-0.26081900
C	-1.28862900	-2.25459500	0.22323600
O	-1.61351400	-3.42452200	0.35903400
O	-0.10082700	-1.75223900	0.43086800
H	0.11631800	1.86786400	-2.30727500
H	1.37015600	-0.27461100	-2.54242000
H	2.86341400	0.21484100	1.50916600
H	1.64178500	2.35333400	1.69242800
H	2.28535700	-2.14368000	-1.32439600
H	4.75847100	-2.33216100	-1.59534500
H	4.98106800	-0.74608800	-0.84144100
H	4.15910700	-0.87469900	-2.40509800
H	3.52904000	-3.28569800	0.43007700
H	3.84671600	-1.78296000	1.29129700
H	2.17694400	-2.39991300	1.15391700
H	-2.23566100	1.98214000	-0.92451100
H	-4.63164200	1.54123700	-1.44884800
H	-5.52470900	-0.79224400	-1.17126300
H	-3.91757100	-2.59011100	-0.36250800
H	0.88491400	4.53238000	-0.47015300
H	-0.65095200	3.78146600	-0.90580000
H	-0.16603300	3.87314400	0.79687500

1-III

Os	0.24491800	-0.38513500	-0.18350000
Cl	-1.08558300	-1.83768300	-1.63872400
C	1.60974800	-2.11600000	0.35405200
C	1.27602100	-1.40824900	1.53268300
C	1.46191600	0.01603900	1.61572600
C	2.03464500	0.76380300	0.54541800

C	2.37548200	0.03130000	-0.64929700	C	-0.35701100	3.41420800	1.16239600
C	2.16452800	-1.36225600	-0.74743900	N	1.53488700	0.10531500	-0.59851100
C	1.34652200	-3.58831300	0.20752200	C	1.90389200	0.33613200	-1.87258900
C	2.26726400	2.25882400	0.69603200	C	3.22510900	0.59218700	-2.21961000
C	3.58370100	2.49950600	1.46486500	C	4.20343900	0.59537700	-1.22252400
C	2.25294400	3.03185500	-0.63117300	C	3.82022900	0.33455300	0.08926200
N	-1.65628400	0.05756700	0.62756400	C	2.47969700	0.09009000	0.36662500
C	-2.24931200	-0.58090600	1.65381700	C	1.98707200	-0.20800500	1.76327900
C	-3.54506200	-0.28045000	2.05563500	O	2.76587400	-0.19877600	2.70536700
C	-4.26052900	0.70392500	1.36937200	O	0.70211800	-0.42656800	1.81976500
C	-3.64882600	1.35074500	0.30041400	H	-2.04032600	-1.09525300	-2.36758800
C	-2.34807600	1.00145200	-0.04626100	H	-1.15589900	1.23031400	-2.28006800
C	-1.61765600	1.65469700	-1.19433900	H	-1.75865700	1.31280000	1.99823400
O	-2.14091900	2.56244900	-1.82341600	H	-2.67819900	-0.99105400	1.91509700
O	-0.41937600	1.17174500	-1.38637000	H	-0.22462300	3.02049100	-0.93856700
H	0.80566500	-1.93706700	2.35481400	H	-1.77418200	4.94741800	-0.65142700
H	1.11974900	0.54293500	2.50114000	H	-2.94542700	3.90420700	0.17201200
H	2.69301500	0.57183000	-1.53232400	H	-2.57226600	3.63746200	-1.53773200
H	2.32185800	-1.85747600	-1.69819400	H	0.09782800	4.40199800	1.04106600
H	1.44281500	2.63924700	1.31384900	H	-1.09932100	3.49804700	1.96362800
H	3.73867000	3.57137900	1.62552300	H	0.41857600	2.71656200	1.49026400
H	4.44102100	2.11814900	0.89883000	H	1.11642600	0.29444200	-2.61491700
H	3.58005700	2.00609400	2.44221000	H	3.47663700	0.77523600	-3.25857200
H	2.29118300	4.10687800	-0.42954300	H	5.24275900	0.78876400	-1.46960900
H	3.12903900	2.79099900	-1.24477800	H	4.51617400	0.30499100	0.91988500
H	1.35104300	2.81724500	-1.20936800	H	-3.98962800	-2.66717500	-0.74233700
H	-1.66336000	-1.35093500	2.14025400	H	-2.30499100	-3.23049400	-0.87159000
H	-3.98280500	-0.82011300	2.88831200	H	-3.05334600	-3.04939600	0.71848200
H	-5.27599500	0.95278600	1.66173900				
H	-4.13552300	2.11874400	-0.28983000	1-V			
H	2.29193000	-4.14330700	0.20117000	Os	0.19601500	0.09530900	0.09760700
H	0.73393600	-3.96352800	1.03108800	Cl	0.16149000	-2.00564900	-1.15708300
H	0.81531200	-3.78537900	-0.72741100	C	0.50741900	2.26024000	0.63802500
				C	0.83765000	2.03172700	-0.74646000
1-IV				C	1.79015500	1.05557900	-1.13820600
Os	-0.40148200	-0.42410800	0.06063000	C	2.45701700	0.24128200	-0.15108500
Cl	0.46865400	-2.67684500	-0.31482700	C	2.11467900	0.43203700	1.20770700
C	-2.52602100	-1.19316400	-0.23638500	C	1.12912000	1.41077500	1.59194200
C	-2.06651500	-0.54414500	-1.43538300	C	-0.50469500	3.29895800	1.03850900
C	-1.55186300	0.77950700	-1.37477700	C	3.44171300	-0.81614900	-0.62033100
C	-1.50411100	1.53674500	-0.14774300	C	4.78160900	-0.13605100	-0.97326000
C	-1.91024400	0.85276200	1.02964000	C	3.64487100	-1.97146600	0.36682200
C	-2.43939800	-0.48600900	0.98693600	N	-1.82377800	0.14463500	-0.51117800
C	-2.99473800	-2.62044800	-0.28376400	C	-2.29960200	0.70076300	-1.64163000
C	-0.99741300	2.96867500	-0.15935300	C	-3.63807800	0.60148200	-2.00212400
C	-2.14115100	3.91899400	-0.57160700	C	-4.51516300	-0.10822400	-1.17845600

C	-4.01476400	-0.69750000	-0.02180900	H	-0.46164000	-1.51304400	-2.68144000
C	-2.66507400	-0.55516300	0.28100300	H	-1.22224000	0.83493300	-2.31619100
C	-2.04676900	-1.17224600	1.51363200	H	-2.71997900	-0.22611000	1.58482900
O	-2.74335600	-1.78424600	2.31012100	H	-1.92968900	-2.54788900	1.27071600
O	-0.76581300	-0.94776600	1.61367100	H	-2.07604400	2.54842100	-0.83638600
H	0.31334600	2.59590400	-1.51163300	H	-4.52094900	2.98312500	-0.94269800
H	1.96337900	0.86584400	-2.19062300	H	-4.85491800	1.31443100	-0.45221200
H	2.50652800	-0.23380600	1.96489100	H	-4.07967900	1.63863400	-2.01040500
H	0.81287900	1.45466800	2.62840900	H	-3.10114200	3.46842400	1.16704800
H	3.01482600	-1.24082300	-1.53633500	H	-3.59356500	1.88054800	1.74521000
H	5.47882100	-0.87194700	-1.38600100	H	-1.87163600	2.29215800	1.68807300
H	5.24519700	0.30494400	-0.08363200	H	0.21129200	2.60244500	-0.69844200
H	4.65353500	0.65950800	-1.71460600	H	2.14964400	4.12041200	-1.08416700
H	4.29368500	-2.72736900	-0.08590500	H	4.47704500	3.19018300	-0.89019100
H	4.13285600	-1.64024800	1.29101800	H	4.72634300	0.72749300	-0.30556700
H	2.69331000	-2.44828500	0.61476200	H	-0.68201400	-3.98619000	-1.90471200
H	-1.57753000	1.21511000	-2.26379600	H	0.49656800	-3.53684200	-0.64969100
H	-3.97739600	1.06609400	-2.92149000	H	-1.03172800	-4.31212100	-0.19515500
H	-5.56391400	-0.20448100	-1.44202500				
H	-4.62253700	-1.27495000	0.66542800				
H	-0.02218200	4.27651000	1.15873600	1-VII			
H	-1.28649400	3.40516900	0.28066400	Os	-0.33345600	-0.41524200	-0.16043400
H	-0.98149100	3.03808700	1.98667500	Cl	0.82265400	-2.40265300	-0.99644400
				C	-2.04886000	-1.71663300	0.57426500
				C	-2.39561900	-1.08963600	-0.67865900
1-VI				C	-2.29841500	0.31496000	-0.83080300
Os	-0.16891800	-0.43179200	0.11377100	C	-1.86228100	1.17576600	0.23736300
Cl	0.30154900	0.32019700	2.39086600	C	-1.48649300	0.53051200	1.45420500
C	-1.19656200	-2.23869900	-0.75810700	C	-1.61921700	-0.89071400	1.63971200
C	-1.01747100	-1.26108800	-1.78554800	C	-2.09376200	-3.21274500	0.70571700
C	-1.45649300	0.08401600	-1.56652600	C	-1.78682100	2.67566300	0.00907700
C	-2.19300000	0.48231000	-0.39599300	C	-3.19317400	3.29563500	0.14202600
C	-2.33158900	-0.50912300	0.61424800	C	-0.78145500	3.39734800	0.91605400
C	-1.86226400	-1.85015600	0.44546400	N	1.58787200	0.02447200	0.60482700
C	-0.57084800	-3.60293400	-0.88641500	C	2.05746300	-0.31557000	1.82006400
C	-2.75424400	1.88877400	-0.27542600	C	3.37294600	-0.06886500	2.19364600
C	-4.13289100	1.95941400	-0.96496300	C	4.23798500	0.54018000	1.28110000
C	-2.82666400	2.40882400	1.16787300	C	3.75118000	0.87910600	0.02280800
N	1.38024200	0.93252200	-0.34983400	C	2.42276800	0.60431100	-0.28434700
C	1.22964100	2.23743800	-0.64305600	C	1.81933500	0.94449500	-1.62670000
C	2.31906800	3.07548200	-0.84812600	O	2.48657900	1.51903700	-2.47416000
C	3.61035500	2.55471800	-0.73669800	O	0.56501600	0.59806400	-1.73229200
C	3.76163900	1.20875000	-0.41875800	H	-2.63047900	-1.70728600	-1.53690100
C	2.62705500	0.42712100	-0.22940000	H	-2.44950500	0.74471400	-1.81582400
C	2.70952800	-1.04036800	0.11279800	H	-1.05285600	1.11741000	2.25594600
O	3.79248300	-1.60061600	0.18616500	H	-1.30319600	-1.34484100	2.57223300
O	1.53782700	-1.59696900	0.27392500	H	-1.45082400	2.80975500	-1.02698800

H	-3.16375300	4.36445000	-0.09328200
H	-3.57423100	3.18475800	1.16360300
H	-3.90916400	2.82095400	-0.53634600
H	-0.70306300	4.44750500	0.61973700
H	-1.09432800	3.38165700	1.96654500
H	0.21551700	2.95311900	0.84423200
H	1.35611900	-0.80389100	2.48592200
H	3.70921500	-0.35991400	3.18279700
H	5.27127000	0.73860500	1.54867500
H	4.35633800	1.34709300	-0.74521000
H	-3.13456300	-3.55115000	0.77187500
H	-1.62281700	-3.68387800	-0.16023200
H	-1.56346300	-3.54654000	1.60041800

2-I

C	2.03578700	0.13638100	-1.38227100
C	2.60577900	-0.12399100	-0.09952000
C	2.33198600	0.84285600	0.92632500
C	1.56288600	2.01397400	0.68286200
C	0.12933800	3.45670800	-0.85950000
C	3.39239700	-1.37986200	0.23419100
C	3.00321200	-2.59695800	-0.61627700
C	4.90487100	-1.09388000	0.14355500
C	-2.01043700	-1.11832800	-0.72994000
C	-2.98209000	-2.05936000	-1.17501400
C	-4.28748800	-1.84775300	-0.85478700
O	-4.70052300	-0.78456200	-0.15995400
C	-3.81595500	0.16888500	0.27126500
C	-2.46913200	0.04397000	0.00261500
O	-1.56382500	0.93238300	0.34859800
C	-4.45246000	1.28103800	1.02839800
Os	0.40136100	0.25292800	0.06032900
C	1.02412900	2.26968600	-0.63064900
C	1.30165900	1.33901100	-1.66972200
O	-0.75813800	-1.22706300	-0.95852000
Cl	-0.03886500	-1.16528700	2.00341200
H	2.60644900	0.60653200	1.94853400
H	1.29897500	2.66405400	1.50869000
H	0.85066000	1.47173400	-2.64652700
H	2.09303600	-0.62392900	-2.15230300
H	-0.42961100	3.35571600	-1.79275300
H	0.72468800	4.37581900	-0.91206000
H	-0.58977800	3.55546800	-0.04249800
H	3.14911500	-1.62018800	1.27646500
H	3.51299000	-3.48913100	-0.23952700
H	3.30114300	-2.47552600	-1.66449600

H	1.92538900	-2.77661500	-0.57699900
H	5.48062900	-1.97246900	0.45304200
H	5.19644700	-0.25619900	0.78560600
H	5.19567100	-0.84570700	-0.88381000
H	-2.68284200	-2.93779200	-1.73376000
H	-5.10738700	-2.50551100	-1.11598100
H	-3.67133600	1.95593700	1.37997100
H	-5.15538800	1.84405600	0.40235900
H	-5.00856900	0.90081400	1.89290300

2-II

C	1.83716200	0.84026600	1.23029900
C	1.80646900	1.46340500	-0.05372100
C	2.12006200	0.61365700	-1.17160000
C	2.56446700	-0.73563300	-1.01749900
C	2.95755500	-2.77574700	0.45628100
C	1.39422400	2.90663400	-0.28506400
C	0.46390900	3.46404600	0.80194000
C	2.64442300	3.79366900	-0.45596900
C	-2.06235100	0.11111700	-1.08899600
C	-3.23006100	0.23183300	-1.89532800
C	-4.43860200	0.33399300	-1.27847300
O	-4.57616500	0.35049200	0.05003000
C	-3.48695500	0.26611000	0.87718900
C	-2.21867200	0.14860500	0.34972300
O	-1.12126600	0.10331500	1.07385900
C	-3.82601800	0.30645500	2.32578800
Os	0.57827600	-0.41277400	-0.04213100
C	2.60638700	-1.32471800	0.28257500
C	2.24087400	-0.52434000	1.40941100
O	-0.88058600	-0.00552500	-1.55927800
H	1.95840000	0.99459500	-2.17546800
H	2.73881600	-1.34961900	-1.89255500
H	2.18091900	-0.97639200	2.39191300
H	1.45104700	1.37464500	2.09042400
H	2.45328200	-3.19741000	1.32771400
H	4.04114400	-2.87869600	0.59267700
H	2.65537900	-3.35729000	-0.41637200
H	0.84202700	2.91926800	-1.23442300
H	0.08152100	4.44392300	0.49925400
H	0.99329200	3.60485700	1.75134200
H	-0.38493500	2.79789100	0.97993700
H	2.35583400	4.82443000	-0.68804200
H	3.28759500	3.43240600	-1.26485700
H	3.23965000	3.80942000	0.46401500
H	-3.15797900	0.21534500	-2.97604700

H	-5.39280500	0.40442300	-1.78610100	H	4.46967400	1.51525100	-2.23153000
H	-2.90662400	0.19812800	2.90231300				
H	-4.31012300	1.25186500	2.59919400				
H	-4.51054100	-0.50671300	2.59331100				
Cl	-0.42223300	-2.64333200	-0.11720800				
				2-IV			
				C	-1.82937600	0.22774400	-1.45520400
				C	-2.43231600	0.53995100	-0.19252800
				C	-2.53898100	-0.53781300	0.74955300
				C	-2.08189600	-1.85227800	0.45948100
2-III				C	-0.84561700	-3.47936200	-1.06659600
C	-2.18912600	0.72437700	-0.95542800	C	-2.90303400	1.93409000	0.18785400
C	-1.90251600	1.33592700	0.32172500	C	-2.09014600	3.05890400	-0.47001100
C	-1.90740200	0.49810900	1.47055700	C	-4.40867200	2.08404600	-0.10773900
C	-2.16949900	-0.91197900	1.35446200	C	2.42532700	-0.75846600	0.12259000
C	-2.72088200	-2.99508500	-0.02972000	C	3.75849400	-1.21769300	0.31993900
C	-1.59418500	2.81706700	0.46831500	C	4.78424100	-0.34791500	0.11263000
C	-0.89314500	3.43636700	-0.74976600	O	4.59581100	0.91166400	-0.28892600
C	-2.89207800	3.57755600	0.81175000	C	3.33810100	1.40249200	-0.52135200
C	2.14982200	-0.55619700	0.99144800	C	2.23012700	0.60271900	-0.33243200
C	3.36254100	-0.92694900	1.63935900	O	0.99613300	0.98642800	-0.57171600
C	4.52903700	-0.38668300	1.19379900	C	3.32053400	2.82229600	-0.96721900
O	4.58419000	0.49291400	0.19010600	Os	-0.43908700	-0.38415900	0.10797400
C	3.44757000	0.90898700	-0.45249800	C	-1.44663800	-2.12598100	-0.79869400
C	2.21489700	0.41950800	-0.07583300	C	-1.38003400	-1.08884500	-1.78443800
O	1.07557000	0.79808400	-0.61207400	O	1.38970000	-1.48501600	0.30248000
C	3.70003200	1.88677200	-1.54599600	Cl	0.15997400	0.45520700	2.32508000
Os	-0.54487800	-0.41325000	-0.03338300	H	-2.85901100	-0.31219300	1.76097200
C	-2.49250900	-1.51525900	0.10799900	H	-2.08745400	-2.60705000	1.23659900
C	-2.47751000	-0.66228500	-1.05069200	H	-0.87093700	-1.26650300	-2.72456900
O	1.00266200	-1.01776600	1.31112100	H	-1.60957100	1.03138300	-2.14855700
Cl	0.49129400	-2.07676500	-1.50244700	H	-0.03149200	-3.41154500	-1.79199600
H	-1.60992600	0.90647500	2.43060400	H	-1.60912600	-4.15625800	-1.46851400
H	-2.04145500	-1.54386100	2.22703900	H	-0.44729800	-3.91740500	-0.14846700
H	-2.56806500	-1.11226900	-2.03283900	H	-2.75602500	2.01715900	1.27176300
H	-2.09662100	1.30281600	-1.86565200	H	-2.38375400	4.02379800	-0.04479600
H	-2.16004600	-3.38799800	-0.88205100	H	-2.27296300	3.11573200	-1.54979200
H	-3.78624300	-3.20760000	-0.18003100	H	-1.01818500	2.91982600	-0.30532200
H	-2.38940700	-3.52634100	0.86604900	H	-4.76943400	3.06331700	0.22418100
H	-0.91309900	2.90649700	1.32473800	H	-4.99892900	1.31592800	0.40266300
H	-0.59529100	4.46430000	-0.51808500	H	-4.60640600	1.99989000	-1.18267400
H	-1.55978300	3.48497800	-1.61847300	H	3.94849200	-2.23087700	0.65288900
H	-0.00317600	2.86294100	-1.01844700	H	5.83342000	-0.57666700	0.25397700
H	-2.67881200	4.63938200	0.97397100	H	2.28424100	3.13343000	-1.10293900
H	-3.36520200	3.18298800	1.71660500	H	3.79240800	3.47530800	-0.22391500
H	-3.61661000	3.50240600	-0.00700200	H	3.85924300	2.95234800	-1.91355600
H	3.35664200	-1.64516000	2.45035400				
H	5.51168100	-0.61304200	1.58939300				
H	2.77356100	2.03943500	-2.10103900	2-V			
H	4.04121100	2.85354400	-1.15497900	C	1.86601200	0.74355000	1.35211500

C	1.86510000	1.40004400	0.09137200	C	2.11677600	3.10180500	0.79946500
C	2.21584100	0.62523200	-1.07762000	C	3.69970600	2.75464700	-1.15653700
C	2.53920100	-0.75334500	-0.96781600	C	-1.93612000	1.21531200	0.34093000
C	2.79646700	-2.91272300	0.38012300	C	-2.94278200	2.15130900	0.70999700
C	1.49090300	2.86160100	-0.08599600	C	-4.22884600	1.90325200	0.33985900
C	0.51809500	3.39881700	0.97125700	O	-4.58298500	0.83165800	-0.37350700
C	2.77579400	3.71353300	-0.14890700	C	-3.65475500	-0.08952700	-0.78099800
C	-2.13274400	-0.57488600	0.94624400	C	-2.32439100	0.06663500	-0.44970100
C	-3.34641900	-0.95107900	1.58948900	O	-1.37020100	-0.74961900	-0.83422000
C	-4.51771700	-0.44871500	1.11310900	C	-4.22879800	-1.21447200	-1.56816300
O	-4.57767100	0.40067000	0.08389700	Os	0.46545300	-0.37916800	0.10888400
C	-3.44154500	0.81936600	-0.55780700	C	1.87827200	-2.01553800	-0.39217600
C	-2.20492300	0.35919700	-0.15795300	C	2.37339400	-1.28095800	0.73761200
O	-1.06722500	0.74012900	-0.69703900	O	-0.70133000	1.33895400	0.64792000
C	-3.69705300	1.76911500	-1.67493700	Cl	-0.61443900	-1.36594500	2.07310000
Os	0.57026200	-0.40826800	-0.05235400	H	1.43657700	0.70576200	-2.51035900
C	2.53299200	-1.43424000	0.29693800	H	1.05581700	-1.75485800	-2.38560200
C	2.15030000	-0.66545400	1.43388100	H	2.49194800	-1.79840000	1.68290100
O	-0.97959800	-0.99407500	1.30067900	H	2.84334900	0.64171700	1.61091900
Cl	-0.39531100	-2.16968500	-1.44872500	H	1.27286500	-3.77271500	0.68337300
H	2.13923500	1.07731000	-2.05980800	H	2.55963800	-4.05457900	-0.50989500
H	2.66578700	-1.33509400	-1.87391500	H	0.88501900	-3.81097700	-1.04089700
H	2.00262500	-1.17202800	2.38210100	H	1.54887500	2.72879700	-1.22971800
H	1.53224000	1.26434500	2.24055500	H	2.11886100	4.18504200	0.64034700
H	2.40007400	-3.32767300	1.31037700	H	2.92004000	2.88202500	1.51150100
H	3.87335100	-3.11756500	0.34578900	H	1.16138300	2.81859400	1.24606800
H	2.31515300	-3.43299000	-0.45226100	H	3.78441000	3.84011400	-1.27265400
H	0.98669600	2.92997700	-1.05790700	H	3.83876500	2.29603400	-2.14070200
H	0.23428000	4.42623200	0.72200000	H	4.52011400	2.42085700	-0.51145100
H	0.96899100	3.42372300	1.96977200	H	-2.69307600	3.02804200	1.29514400
H	-0.39034300	2.79311200	1.00777700	H	-5.07903000	2.52834500	0.58374100
H	2.52980900	4.75933200	-0.36013700	H	-3.42655200	-1.90811400	-1.82227200
H	3.45724800	3.36201700	-0.93017500	H	-4.99153600	-1.75058900	-0.99164300
H	3.31320100	3.67953600	0.80537000	H	-4.69970300	-0.85866900	-2.49249200
H	-3.33690900	-1.64285100	2.42300400				
H	-5.50043500	-0.68300600	1.50362500				
H	-2.74978200	1.99240100	-2.16707700				
H	-4.38631000	1.33714900	-2.40934900				
H	-4.14041000	2.70520300	-1.31373300				
2-VI							
C	2.56043300	0.12659100	0.70273600				
C	2.20850500	0.87244300	-0.47388700				
C	1.74980800	0.15983900	-1.62777900				
C	1.55367500	-1.25606000	-1.56003900				
C	1.63560400	-3.49815400	-0.31036400				
C	2.33274800	2.38678400	-0.54191000				

Cartesian coordinates for all of the species involved in
Figure 3.

1-III, IV-R_A

Os	-0.42438400	-0.18987400	-0.14183500
Cl	0.01638200	-2.33149600	-1.26333100
C	-2.65635600	-0.40715300	-0.50284000
C	-2.05282100	0.38516800	-1.54844500
C	-1.28769300	1.53494500	-1.23406600
C	-1.06914400	1.95217600	0.13136200
C	-1.62793300	1.13525300	1.15173200
C	-2.42629200	-0.02114700	0.83627500
C	-3.41542500	-1.66281400	-0.82623300
C	-0.25827800	3.20571400	0.41248300
C	-1.17199100	4.44380800	0.29247200
C	0.47637900	3.19141100	1.75986500
N	1.63326500	0.09962100	-0.52501300
C	2.16241300	0.69748100	-1.60957300
C	3.53524800	0.76605200	-1.81595700
C	4.39529000	0.18630600	-0.88080300
C	3.84442200	-0.44743300	0.22880900
C	2.46187600	-0.47499600	0.37533500
C	1.79638000	-1.15519700	1.54726200
O	2.46484200	-1.68817000	2.41812100
O	0.48972900	-1.07460100	1.51484700
H	-2.12813500	0.05381200	-2.57729400
H	-0.81033500	2.08822500	-2.03702500
H	-1.39497100	1.33409700	2.19038600
H	-2.73084400	-0.69355700	1.62912600
H	0.49956600	3.27323800	-0.38011700
H	-0.58965800	5.36206700	0.41954900
H	-1.94949400	4.42715100	1.06379800
H	-1.66725900	4.48884900	-0.68271200
H	1.12806000	4.06702200	1.83653900
H	-0.22172200	3.23513000	2.60260200
H	1.09282200	2.29541500	1.87475900
H	1.45775600	1.10839700	-2.32195700
H	3.91547600	1.25869900	-2.70418200
H	5.47089000	0.22210000	-1.02285700
H	4.43948300	-0.93332400	0.99359400
H	-4.46187100	-1.41791900	-1.04517700
H	-2.98403700	-2.16139400	-1.69716500
H	-3.37879300	-2.35051200	0.02072000
H	-1.29338600	-3.31933500	0.82329500
O	-1.60678800	-3.04550600	1.69846000
H	-0.87041100	-2.48085200	1.98783300

1-III, IV-TS_A

Os	-0.47785900	-0.25001200	0.17673600
Cl	0.25597600	-3.06487400	-0.40575600
C	-2.57907200	-0.89452000	-0.40843800
C	-1.84578200	-0.52329900	-1.56838600
C	-1.15465400	0.73488600	-1.60807300
C	-1.23891900	1.69272100	-0.53772300
C	-1.96608300	1.27994500	0.62686900
C	-2.64145400	0.02340600	0.68632400
C	-3.19362800	-2.26189800	-0.30116800
C	-0.54288500	3.03805100	-0.66049500
C	-1.41466000	3.98649000	-1.51056700
C	-0.18103600	3.68198300	0.68558300
N	1.56006900	-0.28324500	-0.52701100
C	1.94527500	-0.72245500	-1.74013600
C	3.27337600	-0.67449600	-2.14702700
C	4.24169000	-0.18262300	-1.26884500
C	3.84196600	0.24491800	-0.00698800
C	2.49206000	0.18383300	0.32610600
C	1.98172800	0.60282600	1.67999300
O	2.74424100	1.04259700	2.52772500
O	0.69085900	0.43410100	1.81922300
H	-1.69452100	-1.24931400	-2.35727900
H	-0.51880600	0.95919700	-2.45943100
H	-1.92870900	1.89019300	1.52100400
H	-3.08472700	-0.29632000	1.62054300
H	0.39003200	2.85684800	-1.21105900
H	-0.90357600	4.94399400	-1.65265900
H	-2.37044100	4.18617800	-1.01373200
H	-1.62956100	3.56668100	-2.49833800
H	0.43425300	4.57059400	0.51568300
H	-1.07642800	4.00981100	1.22566200
H	0.37436000	2.99578500	1.32936300
H	1.17058400	-1.14651000	-2.36424600
H	3.53877000	-1.03676700	-3.13408600
H	5.28614200	-0.14493600	-1.56272200
H	4.52971700	0.62436500	0.73983600
H	-4.14554200	-2.27716300	-0.84565800
H	-2.52268200	-3.01256600	-0.72475700
H	-3.38646500	-2.52310500	0.74113300
H	0.10277400	-1.44980800	2.61580200
O	-0.61234300	-1.85914600	2.10575600
H	-0.20954600	-2.57969000	1.56615000

1-III, IV-P_A

Os	-0.30898500	0.26938800	-0.36201200
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Cl	2.10454700	3.09007100	0.81752100	C	-2.18982200	-1.54113100	0.72656000
C	-1.53690000	2.17486000	-0.19676300	C	-1.22274600	-3.66768800	-0.28013100
C	-1.15823900	1.76411800	1.11359500	C	-2.61543000	2.04613000	-0.52849800
C	-1.40036800	0.41896800	1.52077400	C	-1.77682500	2.86553500	-1.50256800
C	-2.09654000	-0.53757200	0.69983500	C	-4.11068100	2.22721300	-0.80617800
C	-2.46860400	-0.08830200	-0.60542000	C	1.91353900	1.25308300	0.02292000
C	-2.20924500	1.24084000	-1.05189700	C	2.87366200	2.27118000	0.23137800
C	-1.18710800	3.55390800	-0.68420300	C	4.17059500	1.98423600	-0.00480000
C	-2.38411200	-1.93576300	1.22205000	O	4.57405600	0.80779400	-0.43930500
C	-3.66043600	-1.91990900	2.08783800	C	3.69858700	-0.19820200	-0.67924000
C	-2.47481800	-3.00030400	0.11896400	C	2.36271000	-0.02098300	-0.47082300
N	1.40555600	-0.64129800	0.47036600	O	1.45398200	-0.92302600	-0.70888100
C	2.04233700	-0.24636900	1.58885000	C	4.33634000	-1.44474500	-1.16006400
C	3.22078000	-0.86075800	2.00309100	Os	-0.41659500	-0.44867200	0.06426500
C	3.76229500	-1.89117800	1.23453300	C	-1.62971000	-2.23048500	-0.37701400
C	3.11485700	-2.26735900	0.05903400	C	-1.41919000	-1.47538700	-1.56695100
C	1.94071500	-1.61692400	-0.29624000	O	0.67377500	1.40053000	0.22672600
C	1.20004800	-1.92864800	-1.57467900	Cl	0.61337700	-0.86015200	2.25302500
O	1.59538900	-2.80501400	-2.32573900	H	-2.83931500	0.34776700	1.55024200
O	0.13275900	-1.18679500	-1.75704500	H	-2.23506900	-2.04019300	1.67853200
H	-0.54586900	2.42341000	1.71778200	H	-0.88861300	-1.93404900	-2.38400700
H	-0.99965300	0.08535200	2.47377200	H	-1.52409700	0.43430700	-2.55452900
H	-2.86620900	-0.80068500	-1.31882600	H	-0.36876700	-3.86960000	-0.91815100
H	-2.45198700	1.52067400	-2.06998600	H	-2.03968500	-4.31858000	-0.58555600
H	-1.54065800	-2.20062500	1.87369400	H	-0.94592000	-3.91854500	0.73796900
H	-3.84097800	-2.91017500	2.51815900	H	-2.40677200	2.39970500	0.47820700
H	-4.53574500	-1.64978700	1.48673700	H	-1.99522500	3.92124500	-1.36756800
H	-3.58278900	-1.20198600	2.91056200	H	-2.00355900	2.62305600	-2.53896000
H	-2.52965200	-3.99646300	0.56815500	H	-0.71705900	2.71333900	-1.33001800
H	-3.37739600	-2.87362700	-0.48949900	H	-4.37519900	3.28003700	-0.75742900
H	-1.60794500	-2.96803400	-0.54654300	H	-4.71992100	1.69493000	-0.08116200
H	1.62362400	0.60476500	2.11043600	H	-4.37164100	1.86214400	-1.79752000
H	3.70897900	-0.51066300	2.90545800	H	2.57770900	3.23908800	0.59304200
H	4.68318900	-2.37951900	1.53818300	H	4.98593200	2.66975300	0.13902700
H	3.48707900	-3.03931100	-0.60460600	H	3.57286000	-2.20283200	-1.27681200
H	-1.95308600	4.26126700	-0.34441200	H	4.83434200	-1.28964900	-2.11511500
H	-0.22007100	3.86971200	-0.28015600	H	5.08064400	-1.79643900	-0.44941400
H	-1.16179400	3.59621300	-1.77700300	H	-0.09130766	0.97123471	3.31846793
H	1.06029900	1.85794200	-2.06189100	O	-0.34720666	1.80391171	2.92074393
O	1.34493800	1.32215300	-1.30961500	H	0.20846786	1.95844620	2.15628492
H	1.70468500	1.99553200	-0.58447700				

2-I-TS_A

2-I-R _A				C	-1.73265300	0.48119200	-1.52208700
C	-1.76205900	-0.10874400	-1.65944300	C	-2.53705900	0.49724800	-0.32519000
C	-2.29308500	0.56932000	-0.52230600	C	-2.61443200	-0.70690000	0.41834800
C	-2.53804200	-0.17256900	0.65976200	C	-1.93673900	-1.90084200	-0.00584500

C	-0.39348400	-3.15689200	-1.59853400	C	3.32652400	-0.92906600	-0.83332300
C	-3.21083800	1.75476500	0.20108200	C	2.89158800	-1.79107400	-2.02600600
C	-2.51703400	3.06160600	-0.21064700	C	4.78007100	-0.43974800	-0.99629100
C	-4.69407800	1.75597200	-0.22293400	C	-2.19880800	-0.87214700	-1.02868900
C	1.89955400	1.57330200	0.03246800	C	-3.17874500	-1.61370900	-1.74872500
C	2.82157200	2.65306200	0.13749900	C	-4.46267000	-1.60205500	-1.30026900
C	4.14874900	2.39943100	-0.04096300	O	-4.84628900	-0.91397600	-0.21980500
O	4.61849300	1.18243100	-0.32017800	C	-3.95303100	-0.17553800	0.50663000
C	3.78180100	0.10847200	-0.45665600	C	-2.62354100	-0.13614500	0.14336800
C	2.41463500	0.26682200	-0.31809500	O	-1.70209400	0.54666100	0.80081600
O	1.54981200	-0.69515600	-0.48316300	C	-4.55915500	0.52178100	1.67399700
C	4.47598100	-1.17366600	-0.75302900	Os	0.22748300	0.32133600	-0.02616000
Os	-0.46452200	-0.28688600	0.03435800	C	0.64523300	2.48607800	0.03553000
C	-1.18980600	-1.93914800	-1.21876300	C	0.80229600	2.03112400	-1.30631300
C	-1.09242700	-0.72429700	-1.97774200	O	-0.96789100	-0.80837900	-1.36720000
O	0.64067700	1.67698400	0.23261000	Cl	2.36946500	-2.06750100	2.63677600
Cl	0.60800200	-2.14324500	2.12908400	H	2.68759100	0.16598500	1.58228400
H	-3.06422500	-0.68933000	1.40445700	H	1.24900300	2.12381600	2.10880600
H	-1.87770700	-2.73936600	0.67594200	H	0.19927600	2.46198500	-2.09722500
H	-0.43451300	-0.68508200	-2.83895800	H	1.64038000	0.49414500	-2.58815900
H	-1.54536200	1.40367000	-2.05813100	H	-1.08305200	3.69499100	-0.40889900
H	0.51280600	-2.87127200	-2.13738700	H	0.19199100	4.52735400	0.50146200
H	-0.99152500	-3.81431300	-2.24079100	H	-0.85476500	3.34544000	1.31179300
H	-0.09548600	-3.70811500	-0.70416500	H	3.27745000	-1.54758000	0.07163800
H	-3.16807400	1.68648800	1.29486700	H	3.50853600	-2.69348700	-2.06979700
H	-2.98187500	3.90321400	0.31255700	H	3.01693800	-1.26893600	-2.98266100
H	-2.62259200	3.25541800	-1.28455000	H	1.84597800	-2.10117800	-1.93511600
H	-1.45233100	3.04569200	0.03583500	H	5.45375100	-1.29448000	-1.11307700
H	-5.20890900	2.62658300	0.19642000	H	5.11144900	0.12870000	-0.12176700
H	-5.21283000	0.85626000	0.12216000	H	4.88835200	0.20029600	-1.88036600
H	-4.78958500	1.80255200	-1.31375800	H	-2.90145100	-2.18442400	-2.62663200
H	2.47713400	3.65302800	0.37345100	H	-5.28771400	-2.13598100	-1.75508200
H	4.94010400	3.13520400	0.03251900	H	-3.79718700	1.13582300	2.15522300
H	3.76284200	-1.99035400	-0.63242000	H	-5.39254500	1.16097200	1.36169300
H	4.86824200	-1.19498700	-1.77791000	H	-4.94856100	-0.19509500	2.40652800
H	5.31806100	-1.32835600	-0.07047500	H	0.90414900	-1.74293200	1.65426000
H	-0.05939800	-0.34451200	2.63838300	O	0.02736000	-1.47351700	1.12420400
O	-0.48026200	0.50607200	2.32418900	H	-0.62816700	-1.27484000	1.81121200
H	0.22060000	1.17269100	2.30513900				

1-III, IV -R_B

2-I-P_A				Os	-0.30770100	0.28352800	-0.28845700
C	1.65437200	0.90921600	-1.58718500	Cl	1.12452600	1.90132700	-1.48574300
C	2.41878600	0.26202700	-0.57440700	C	-1.84447900	1.94004800	0.05117500
C	2.26179400	0.75189700	0.76832400	C	-1.42300000	1.44353300	1.31066400
C	1.40710200	1.84314000	1.07387600	C	-1.43678100	0.03015100	1.55683800
C	-0.33509600	3.57406900	0.37827000	C	-1.97557900	-0.91518300	0.62215800

C	-2.38098000	-0.38165400	-0.64550700	C	-2.42994900	-2.67367700	-1.22671300
C	-2.32165300	1.00830600	-0.93553700	C	-1.08676800	3.01193000	-0.21534200
C	-1.74960700	3.40512800	-0.27280500	C	-2.04020500	3.92882800	-1.01018800
C	-2.06875100	-2.38901100	0.98143200	C	-1.04827400	3.40755000	1.26813600
C	-3.34860200	-2.64409500	1.80496200	N	1.70663400	-0.11954900	-0.59587500
C	-1.99432000	-3.32890300	-0.23082500	C	2.21672500	-0.48311200	-1.79059800
N	1.55745400	-0.28625000	0.53664400	C	3.56882600	-0.34891800	-2.07983900
C	2.13199000	0.24367800	1.63479200	C	4.43017900	0.16399500	-1.10485900
C	3.38561000	-0.17278100	2.07040900	C	3.90158700	0.52396000	0.13061100
C	4.07472200	-1.14902300	1.34799500	C	2.53535300	0.37216200	0.34900800
C	3.48759700	-1.66761000	0.19769400	C	1.87522300	0.73924200	1.65629500
C	2.23004200	-1.21126200	-0.18102900	O	2.53326600	1.21720400	2.56682500
C	1.53596200	-1.70719200	-1.42629000	O	0.58913000	0.50898500	1.66257900
O	2.05370100	-2.56773200	-2.12251300	H	-1.06358700	-0.92780900	-2.88060300
O	0.37323200	-1.14584900	-1.63050800	H	-0.40399200	1.43596100	-2.36543600
H	-0.97005700	2.12177400	2.02385700	H	-2.48389800	1.18326400	1.43820000
H	-1.00883700	-0.34197400	2.48343700	H	-2.99323400	-1.17136200	0.98012000
H	-2.64138200	-1.06289400	-1.44698500	H	-0.07553300	3.14124400	-0.62552600
H	-2.55849400	1.35925700	-1.93232600	H	-1.74365400	4.97577800	-0.89129500
H	-1.20783500	-2.60694200	1.62809500	H	-3.06883900	3.82863900	-0.64658900
H	-3.39678700	-3.69182900	2.11943700	H	-2.03665200	3.69486900	-2.07976600
H	-4.24339300	-2.43074200	1.20954900	H	-0.63824400	4.41718500	1.36805700
H	-3.38527400	-2.01840000	2.70264500	H	-2.05409200	3.42584800	1.70333200
H	-1.91422200	-4.36610900	0.10866400	H	-0.43014100	2.72142200	1.85180800
H	-2.89919700	-3.26240500	-0.84575500	H	1.51808600	-0.90530300	-2.50194200
H	-1.13295900	-3.10119300	-0.86357400	H	3.93690900	-0.65209900	-3.05396500
H	1.59257900	1.04507900	2.12583800	H	5.49086600	0.27304600	-1.30856200
H	3.81292500	0.27778600	2.95970400	H	4.49936400	0.92021400	0.94359600
H	5.05506000	-1.48611300	1.67076300	H	-3.46228700	-2.80565900	-1.57296400
H	3.96236300	-2.41148100	-0.43182100	H	-1.75464500	-3.11261400	-1.96399100
H	-2.72853400	3.87464700	-0.11606600	H	-2.31077200	-3.20650700	-0.27945800
H	-1.01468400	3.89681200	0.36716500	H	0.13290000	-2.89377400	0.51173900
H	-1.45667400	3.55331600	-1.31437200	O	0.69543600	-2.66750500	-0.28634600
H	1.13804700	2.91905500	0.57244400	H	1.58709300	-2.66601900	0.08896600
O	1.16056600	3.31973200	1.46359100				
H	1.85051000	3.99142900	1.40182600				
				1-III, IV-P_B			
				Os	0.17598600	0.09063800	-0.03533800
				Cl	0.16484700	3.72272500	1.95555700
1-III, IV-TS_B				C	0.98380100	1.78875400	-1.33881900
Os	-0.34695800	-0.25530400	-0.01562500	C	0.76453300	0.59603500	-2.09509000
Cl	-0.86795800	-2.46364500	2.12982200	C	1.37553300	-0.65291800	-1.75327900
C	-2.14649200	-1.21137700	-1.02774800	C	2.18136400	-0.75606800	-0.57547000
C	-1.43658900	-0.44895100	-1.98219200	C	2.38481800	0.42089600	0.21258900
C	-1.05051400	0.90125200	-1.67562300	C	1.77473000	1.65458300	-0.15701900
C	-1.46327000	1.55943900	-0.45767100	C	0.37519700	3.11424300	-1.70933500
C	-2.25782900	0.78430800	0.45708500	C	2.77537800	-2.10426800	-0.20060800
C	-2.56977900	-0.56394400	0.19155300				

C	4.09345900	-2.29818900	-0.98103400	C	-3.72834900	-0.19123100	-0.23138300
C	2.98209100	-2.31104700	1.30600300	C	-2.35942800	-0.29888000	-0.32230400
N	-1.85331600	-0.29741400	-0.46954300	O	-1.54246400	0.73948700	-0.37056800
C	-2.64699100	0.43726100	-1.27086300	C	-4.49517500	1.07901900	-0.08839300
C	-3.99487700	0.13997300	-1.43950500	Os	0.46908900	0.21250100	-0.01274100
C	-4.54454100	-0.94593100	-0.75531300	C	1.17387000	2.05575400	-1.00616600
C	-3.72364800	-1.69151700	0.08666200	C	1.41006100	0.94696200	-1.88922200
C	-2.38533300	-1.33683700	0.21015300	O	-0.47603800	-1.68085400	-0.37995500
C	-1.44272200	-2.06840300	1.13613100	Cl	-0.31391700	-0.15125200	2.28677700
O	-1.82417200	-3.03406700	1.77614000	H	2.70063000	0.77518800	1.80564700
O	-0.23652700	-1.55247800	1.16724600	H	1.45898400	2.78427900	1.02368900
H	0.08265300	0.62753100	-2.93998900	H	0.95851100	0.93686900	-2.87442000
H	1.16707900	-1.53783700	-2.34342700	H	2.13410200	-1.08452500	-2.04716100
H	2.92529100	0.36243400	1.14780900	H	-0.39253800	2.92430900	-2.19994800
H	1.80113800	2.49413100	0.53668600	H	0.96039900	4.01511900	-1.84075100
H	2.06139300	-2.86334900	-0.54352600	H	-0.23011400	3.61924300	-0.57596500
H	4.50678600	-3.29055900	-0.77629800	H	3.25045500	-1.50401800	1.52010900
H	4.83933100	-1.55447800	-0.67994300	H	3.37928200	-3.65642300	0.39816700
H	3.94559300	-2.20868800	-2.06203200	H	3.12178000	-2.93821500	-1.18841200
H	3.32239400	-3.33513300	1.48748900	H	1.81060500	-2.92009800	0.00968500
H	3.75048700	-1.64175600	1.70868200	H	5.47642200	-2.16462500	0.59929000
H	2.04889200	-2.16006500	1.85252400	H	5.30495500	-0.40110400	0.62003100
H	-2.18154100	1.28022900	-1.76690400	H	5.12996000	-1.29068000	-0.90106500
H	-4.59841000	0.76050300	-2.09262100	H	-2.21154600	-3.74022200	-0.50861400
H	-5.59415200	-1.19712800	-0.87123200	H	-4.70973100	-3.31421500	-0.37862000
H	-4.07658500	-2.53867700	0.66364600	H	-3.91932300	1.79673200	0.50315700
H	1.09779200	3.71002200	-2.28001000	H	-4.70152900	1.53778000	-1.06394400
H	-0.51228100	2.98731100	-2.33761300	H	-5.45129800	0.88761900	0.40515600
H	0.10669900	3.67178200	-0.80625200	H	-1.40085500	2.45102800	2.10572200
H	-0.44546600	2.06390800	1.78034300	O	-1.71954800	2.94427600	1.33579500
O	-0.76593700	1.06032300	1.62724100	H	-1.73301700	2.24375600	0.65792000
H	-0.55484000	0.56724300	2.43446300				

2-I-R_B

C	2.10040800	-0.20638500	-1.41247100
C	2.65697300	-0.27682900	-0.08706900
C	2.43087900	0.84740400	0.75781900
C	1.71290700	2.00481300	0.31603000
C	0.32371100	3.22203400	-1.43049300
C	3.40839000	-1.49093000	0.43456000
C	2.89167400	-2.82612600	-0.12230300
C	4.91911600	-1.32339800	0.17408700
C	-1.75190900	-1.60739600	-0.37799600
C	-2.61675300	-2.73799000	-0.44073800
C	-3.95965500	-2.53302800	-0.36975600
O	-4.50577600	-1.31783100	-0.26049300

2-I-TS_B

C	1.50921600	0.01067400	-1.68908600
C	2.40988600	-0.30533900	-0.60835900
C	2.60639700	0.68862000	0.38450000
C	1.96466600	1.97187100	0.30680000
C	0.35123200	3.60521600	-0.81535900
C	3.06727000	-1.66647100	-0.44702500
C	2.29847000	-2.81835800	-1.10806200
C	4.51830800	-1.59113400	-0.96531600
C	-1.93802700	-1.36028000	-0.25761000
C	-2.81652400	-2.46880500	-0.45733000
C	-4.15071500	-2.23278600	-0.55981500
O	-4.68178900	-1.00706500	-0.49229200
C	-3.88898600	0.09703100	-0.30410100

C	-2.52464800	-0.03557100	-0.17164200	O	1.65751200	-0.79222000	-0.57209900
O	-1.69583500	0.96826600	0.02626200	C	4.55657000	-1.49663500	-0.61227800
C	-4.65211700	1.37507800	-0.24999100	Os	-0.29750800	-0.15210800	-0.19928200
Os	0.42905600	0.41402700	0.13510000	C	-1.14263600	-1.51019200	-1.72856700
C	1.10139100	2.30225500	-0.77750100	C	-0.99762400	-0.18379100	-2.28185600
C	0.87591300	1.29568000	-1.77880200	O	0.86131200	1.52956300	0.44178300
O	-0.67913500	-1.46096600	-0.15401200	Cl	-1.84369100	-2.33054800	2.88310600
Cl	0.83533200	-1.33856500	2.50408100	H	-2.90854500	-0.68707100	1.10115800
H	3.12929500	0.42184300	1.29498900	H	-1.92322500	-2.60767100	-0.00684500
H	2.03131000	2.64429700	1.15346100	H	-0.37033700	-0.02919600	-3.15242900
H	0.13893800	1.47413800	-2.55482100	H	-1.34116600	1.92770400	-1.98713300
H	1.22763700	-0.75887400	-2.39638500	H	0.56247200	-2.38846900	-2.69981300
H	-0.65894000	3.45824100	-1.20552900	H	-1.00487500	-3.03597800	-3.22793800
H	0.87209600	4.32260100	-1.46049900	H	-0.33374300	-3.50112500	-1.65274200
H	0.27222500	4.03839300	0.18449200	H	-3.03513600	1.68594400	1.37051500
H	3.08626300	-1.86232800	0.63086100	H	-2.60467000	4.03057700	0.87026900
H	2.77414800	-3.76858800	-0.84647300	H	-2.15745100	3.67860100	-0.79497000
H	2.31007900	-2.74382400	-2.20260100	H	-1.12094300	3.11505300	0.53091700
H	1.26261400	-2.84696200	-0.76317200	H	-4.90076300	2.98795300	0.34470300
H	5.02622800	-2.54723400	-0.80236900	H	-5.01453000	1.27227600	-0.08267100
H	5.09219200	-0.81234900	-0.45286900	H	-4.41142400	2.44359100	-1.26765900
H	4.54418600	-1.37686300	-2.04026700	H	2.81168200	3.20498700	1.23294100
H	-2.42393000	-3.47687400	-0.51045300	H	5.24911100	2.49203100	1.11076600
H	-4.90814900	-2.99416500	-0.70134600	H	3.76945200	-2.19826200	-0.89015800
H	-3.94813000	2.20433900	-0.16858600	H	5.19941000	-1.31858200	-1.48261400
H	-5.26219800	1.51064400	-1.15042900	H	5.17542800	-1.94735700	0.17152400
H	-5.32833300	1.40196400	0.61307100	H	-0.48418900	-1.38659000	2.21858200
H	-0.08974600	0.42631800	2.70340500	O	0.24968900	-0.74010600	1.79858700
O	-0.32762100	1.26791200	2.22359500	H	0.23961500	0.04288700	2.36880400
H	-1.27201400	1.22354300	2.00233600				

1-III, IV-R_C

2-I-P_B				Os	-0.39294700	-0.35299400	-0.2272160
C	-1.56818900	0.93506000	-1.61555700	Cl	0.36991800	-2.39914600	-1.33552100
C	-2.34140100	0.78976700	-0.40717400	C	-2.57335400	-0.87499700	-0.59212800
C	-2.47664900	-0.52106700	0.11820900	C	-2.04326300	-0.08656100	-1.68250600
C	-1.89299200	-1.65955700	-0.53261100	C	-1.44283500	1.17348200	-1.44418800
C	-0.43610900	-2.67710000	-2.36203600	C	-1.30292400	1.70238000	-0.10637000
C	-2.97291400	1.97039700	0.31285000	C	-1.78459300	0.90032900	0.96373900
C	-2.15822800	3.26979900	0.22226400	C	-2.42495400	-0.36555200	0.71599700
C	-4.41135100	2.17699200	-0.2043970	C	-3.15169300	-2.23785000	-0.8525020
C	2.12652700	1.30529900	0.40438000	C	-0.65445900	3.06159900	0.09356700
C	3.10521700	2.23703800	0.84478500	C	-1.72155000	4.16446900	-0.06922400
C	4.41805400	1.87740500	0.78825900	C	0.09924500	3.20936300	1.42198100
O	4.81986400	0.69264800	0.32242600	N	1.62586400	0.20461200	-0.51327100
C	3.92780300	-0.23508800	-0.13568100	C	2.12348100	0.85294700	-1.58340800
C	2.57228100	0.03486300	-0.12194500	C	3.48449800	1.09303700	-1.73238300

C	4.36874600	0.63906800	-0.75170700	C	-2.38551800	-0.78859700	0.31822100
C	3.85301000	-0.04313900	0.34603700	C	-2.35120400	0.29156400	1.37288800
C	2.48020100	-0.24615800	0.43271800	O	-3.32617000	0.54057100	2.05052900
C	1.85389500	-0.97432600	1.59507900	O	-1.14845900	0.83722700	1.55374300
O	2.53204800	-1.35392700	2.53692900	H	0.18707000	1.61326000	-2.30965000
O	0.55668800	-1.10447200	1.47888700	H	1.50832900	-0.50174800	-2.39764500
H	-2.04126200	-0.49985600	-2.68427500	H	2.86398400	0.24270800	1.63678000
H	-1.02336800	1.72572300	-2.27939000	H	1.79156700	2.47509600	1.60716100
H	-1.60993100	1.17494800	1.99625800	H	2.50750100	-2.27782000	-1.09557900
H	-2.66710100	-0.97675700	1.57838400	H	4.99465200	-2.39910400	-1.23821200
H	0.07582700	3.18491900	-0.71830000	H	5.12449400	-0.75804000	-0.58680600
H	-1.25939800	5.15510600	-0.00946400	H	4.37535000	-1.02392800	-2.16899700
H	-2.47583700	4.09450500	0.72178400	H	3.64739500	-3.29564500	0.78413300
H	-2.23682300	4.08845300	-1.03214000	H	4.00357700	-1.74091900	1.52774600
H	0.60218400	4.18074500	1.45734900	H	2.32833800	-2.30823400	1.45388300
H	-0.57748000	3.16255300	2.28110600	H	-0.17813500	-2.28246300	-1.60876300
H	0.85563000	2.42874300	1.54257700	H	-2.18150400	-3.63467500	-2.22690300
H	1.40456200	1.16364600	-2.33117900	H	-4.38085500	-3.10476400	-1.13425500
H	3.83811700	1.61947700	-2.61217400	H	-4.45459800	-1.21456400	0.55330200
H	5.43651500	0.80881100	-0.84870300	H	0.74687600	4.33815600	-0.96700700
H	4.46999200	-0.43423800	1.14689500	H	-0.76393000	3.39193900	-0.84374100
H	-4.14047600	-2.14547900	-1.31741200	H	0.08349800	3.93165600	0.63122400
H	-2.50042500	-2.80742100	-1.52095000	H	-0.30328900	-1.96184200	2.55308600
H	-3.25935000	-2.79922700	0.07816600	O	0.34233900	-1.24582900	2.62333900
H	-1.15817000	-1.32780900	4.33555700	H	-0.19270900	-0.45932500	2.82660400
O	-1.33207300	-0.83911400	3.52303700				
H	-0.57289400	-1.04454300	2.94207300				
				1-III, IV-P_C			
				Os	0.38177700	-0.25716100	-0.38286600
				Cl	-2.68640000	-0.98539300	2.03853300
1-III, IV-TS_C				C	0.71728300	-2.18044000	0.69002500
Os	0.29894900	0.30517200	0.22677800	C	0.56661700	-1.11970100	1.63486700
Cl	-2.32698800	1.49167700	-1.74329600	C	1.41081600	0.03604600	1.55438300
C	1.01580600	2.29763700	-0.41354000	C	2.41631400	0.18656300	0.55835700
C	0.91588200	1.39804800	-1.53460400	C	2.52065900	-0.87716000	-0.40357600
C	1.65035200	0.17087600	-1.55771600	C	1.72404400	-2.05034300	-0.32730700
C	2.39379900	-0.27249800	-0.43426500	C	-0.23454400	-3.34075500	0.70996600
C	2.41038400	0.59214100	0.71741200	C	3.33233200	1.39903700	0.54873500
C	1.80447800	1.88312600	0.69913700	C	4.59800600	1.09422700	1.37699400
C	0.21742500	3.56923800	-0.39068100	C	3.70277900	1.89694000	-0.85637700
C	3.11400900	-1.61098700	-0.46756900	N	-1.13180100	1.16184200	-0.03672500
C	4.48194600	-1.43504900	-1.16045900	C	-0.99387500	2.34345200	0.60778400
C	3.27429400	-2.27438300	0.90784400	C	-2.08194900	3.14375000	0.90892300
N	-1.19935300	-1.09578600	-0.25851700	C	-3.36664000	2.71756700	0.53810200
C	-1.14518300	-2.09498100	-1.15783200	C	-3.50990500	1.50039300	-0.10509900
C	-2.26677600	-2.83992400	-1.49443100	C	-2.37463500	0.72575400	-0.34994200
C	-3.48814300	-2.54061700	-0.88296800	C	-2.42809500	-0.52703100	-1.18314700
C	-3.54407600	-1.50669000	0.04410600				

O	-3.45440900	-0.91552900	-1.70002800	H	-3.02051500	0.52840400	1.70992300
O	-1.22401900	-1.05723900	-1.40639200	H	-2.34628500	-1.85120200	1.92481100
H	-0.30598800	-1.12440100	2.29116300	H	-0.88450700	-1.84195100	-2.12390300
H	1.21667800	0.86083100	2.23354700	H	-1.60868300	0.52793000	-2.40993600
H	3.18220800	-0.75860900	-1.25437000	H	-0.41622800	-3.73548400	-0.65913700
H	1.79970400	-2.80147300	-1.10499000	H	-2.08011400	-4.20240900	-0.25534000
H	2.78901800	2.20669100	1.05752300	H	-0.95152200	-3.74165700	1.03413600
H	5.24244100	1.97751900	1.43271100	H	-2.58365100	2.59256800	0.56461300
H	5.17648000	0.28416200	0.91909300	H	-2.15247000	4.07030600	-1.32724400
H	4.34565800	0.79154100	2.39771300	H	-2.09179800	2.72498200	-2.46170200
H	4.25803400	2.83706500	-0.78486400	H	-0.84067500	2.88395200	-1.20398700
H	4.34656500	1.18479700	-1.38379200	H	-4.55117400	3.39727500	-0.74418300
H	2.81450700	2.06814600	-1.47159300	H	-4.88445800	1.80959600	-0.03215100
H	0.01875100	2.63315400	0.86394500	H	-4.49368800	1.94355500	-1.75378500
H	-1.92555900	4.08601400	1.42213200	H	2.37464400	3.54179300	0.79353900
H	-4.23401200	3.32994300	0.76308100	H	4.82681800	3.05605200	0.35126400
H	-4.46737500	1.09701700	-0.41110300	H	4.88109100	-1.60405800	-0.10158300
H	0.15766400	-4.11423200	1.38193500	H	3.62543700	-1.83947200	-1.32689400
H	-1.21013700	-3.01154000	1.08482200	H	5.07927100	-0.87807900	-1.70316300
H	-0.35232600	-3.77273100	-0.28634800	H	1.57731200	-2.40223000	-3.06385500
H	0.00595300	1.49595200	-2.45824600	O	1.41677300	-2.83167100	-2.21472700
O	0.42748000	0.62253800	-2.47148400	H	1.45325800	-2.09871700	-1.56447800
H	-0.26957400	0.00525100	-2.78543900				

2-I-TS_C

2-I-R_C				C	-2.59516300	0.12016700	-0.85398500
C	-1.85307000	0.00335300	-1.49546900	C	-2.15814100	0.99739500	0.18143300
C	-2.40709200	0.71424700	-0.37760100	C	-1.71222400	0.40564900	1.41545600
C	-2.66044000	-0.00313400	0.83718500	C	-1.77542000	-1.01175500	1.62315100
C	-2.29279100	-1.37679100	0.95133200	C	-2.11937100	-3.38387900	0.73222800
C	-1.25694900	-3.52617400	0.00715400	C	-2.04226000	2.50146800	0.01479600
C	-2.75994300	2.19249700	-0.44166100	C	-1.88049900	2.95748300	-1.44034400
C	-1.90397800	3.00825600	-1.41979500	C	-3.25527700	3.17672400	0.68726600
C	-4.26274600	2.34121000	-0.75919100	C	1.91624700	0.49713700	-1.04527900
C	1.78109800	1.51446300	0.23716500	C	2.94512200	1.29569000	-1.60363000
C	2.71083700	2.57506800	0.43906800	C	4.17677000	1.23792500	-1.02987700
C	4.02980100	2.33649400	0.20944100	O	4.45689000	0.43266700	0.00309400
O	4.49064800	1.15869900	-0.22121300	C	3.51955700	-0.38670900	0.54344900
C	3.64426700	0.10816800	-0.46176300	C	2.24653300	-0.39375400	0.02622100
C	2.29162700	0.24870300	-0.24402100	O	1.26771300	-1.17151100	0.49647000
O	1.39989900	-0.69647200	-0.47120600	C	3.97712300	-1.13494500	1.74288200
C	4.34471900	-1.12190700	-0.92835300	Os	-0.5657780	-0.51980000	-0.15528700
Os	-0.5245750	-0.25206200	0.28818700	C	-2.17276500	-1.88800200	0.57946600
C	-1.69657800	-2.09286600	-0.13007200	C	-2.53816500	-1.29366100	-0.68086900
C	-1.46957200	-1.36065600	-1.34639900	O	0.68856000	0.50369900	-1.46273100
O	0.52439200	1.62492700	0.43526200	Cl	1.12531600	2.10084500	1.66062500
Cl	0.52157600	-0.65493600	2.45669400	H	-1.19743700	1.03730700	2.13551300

H	-1.35046800	-1.42566700	2.53113600	H	-3.72063000	-0.69383900	-1.06297300
H	-2.73779700	-1.94092200	-1.52778600	H	-2.59082700	1.42037400	-1.67000000
H	-2.80829700	0.51557600	-1.83868900	H	-3.62169400	-2.79930900	0.33092700
H	-1.78039200	-3.85646300	-0.19318100	H	-4.39433100	-2.01909100	1.72036600
H	-3.11571800	-3.77443200	0.97192900	H	-2.81587400	-2.79913300	1.91007100
H	-1.43987200	-3.67316200	1.53783700	H	0.36653500	2.68556700	0.21765300
H	-1.13128400	2.78272700	0.56174700	H	0.08599700	3.99140200	-1.84204300
H	-1.69325600	4.03530600	-1.46338200	H	-1.55544300	3.40502800	-2.09500800
H	-2.78125300	2.77446300	-2.04007100	H	-0.17885500	2.28464300	-2.23318900
H	-1.03105500	2.45860800	-1.91520600	H	-0.69796300	4.93085100	0.40005500
H	-3.14637700	4.26482300	0.64195400	H	-1.23549600	3.84312300	1.68292100
H	-3.34067000	2.89440600	1.74130500	H	-2.30969300	4.19744200	0.31030200
H	-4.19353500	2.90990100	0.18558200	H	2.88295600	0.85615800	-2.82686700
H	2.74133400	1.97686400	-2.42032200	H	5.09890600	0.53789300	-1.61514100
H	5.03700400	1.82151900	-1.33101800	H	2.80497900	-2.40186900	2.10964900
H	3.29117400	-1.95833100	1.94369600	H	4.52550100	-1.92413800	1.95481400
H	4.99312600	-1.51727200	1.60946700	H	3.31255400	-0.76656400	2.58782600
H	3.96701400	-0.46459800	2.61112300	H	-0.29386200	-2.19387000	-2.21451000
H	0.77218700	-1.98490500	-2.44145000	O	-0.69732900	-2.49703500	-1.38277500
O	0.41310700	-2.60633300	-1.79338200	H	0.05879800	-2.78563400	-0.82506800
H	1.01176100	-2.53507700	-1.03081100				

2-I-P_C

C	-2.40607300	0.98794300	-0.69503800
C	-1.41557300	1.57308600	0.17344600
C	-1.10405700	0.89681300	1.39009500
C	-1.78131000	-0.32140600	1.73838800
C	-3.43171200	-2.20592200	1.22940600
C	-0.65009200	2.83738900	-0.17297400
C	-0.57708900	3.13688600	-1.67573200
C	-1.26771300	4.01904700	0.60415700
C	1.80264000	-0.23922000	-1.27726700
C	2.95515500	0.29794000	-1.90148100
C	4.15019900	0.15298000	-1.26477400
O	4.27194800	-0.49802400	-0.10318100
C	3.20464700	-1.04063200	0.52609100
C	1.96273500	-0.97458900	-0.06784000
O	0.86303200	-1.50783000	0.47261000
C	3.48997500	-1.58490700	1.87658300
Os	-0.85304600	-0.54756600	-0.23940800
C	-2.76164300	-0.90176800	0.88932800
C	-3.05063100	-0.22527900	-0.34963800
O	0.58906700	-0.06632600	-1.71946300
Cl	2.10914100	1.74047900	1.91234500
H	-0.22756400	1.23057900	1.95758700
H	-1.44839800	-0.86918500	2.61372200

Cartesian coordinates for all of the species involved in
 Figure 5.

1-I-R_B				1-I-TS_B			
Os	0.19064300	-0.26121300	-0.07821500	Os	0.15659300	-0.40288200	0.11552200
Cl	-0.03040000	0.37214500	2.28607600	Cl	0.40837300	2.24804700	1.49477800
C	0.90904500	-1.64346800	-1.67735800	C	0.47483000	-2.09134200	-1.19947300
C	1.60816200	-1.93617300	-0.44775400	C	1.34115300	-2.26506000	-0.06194300
C	2.28726400	-0.91805700	0.25101900	C	2.21620900	-1.23500500	0.33712100
C	2.32659500	0.44677200	-0.22268600	C	2.37554100	-0.01693900	-0.43186100
C	1.65118900	0.72222000	-1.44042600	C	1.56658700	0.14009900	-1.57381300
C	0.96132500	-0.31043600	-2.16952200	C	0.58768100	-0.85416200	-1.93143500
C	0.11143700	-2.71508000	-2.36738600	C	-0.52732700	-3.14553700	-1.57792600
C	3.07251100	1.49188700	0.58814800	C	3.38025600	1.01968000	0.04388500
C	4.57167900	1.45218000	0.22734000	C	4.80592000	0.44169000	-0.08881200
C	2.50453100	2.91082400	0.46104500	C	3.27283200	2.37437000	-0.66392600
N	-1.48865300	1.00478600	-0.30917800	N	-1.54816700	0.80478200	-0.38295600
C	-1.46031300	2.31581200	-0.61575000	C	-1.50224000	1.98004800	-1.03788100
C	-2.61620800	3.08639100	-0.66116500	C	-2.65855700	2.67230900	-1.37811400
C	-3.84529300	2.49012700	-0.37118500	C	-3.90186600	2.15314500	-1.01081200
C	-3.86960700	1.13818200	-0.04298600	C	-3.94230400	0.95211900	-0.30989500
C	-2.67521900	0.42645000	-0.01848500	C	-2.74546000	0.30510100	-0.01813200
C	-2.62987000	-1.04000600	0.33406700	C	-2.70067200	-0.98010200	0.76496800
O	-3.65528700	-1.65161500	0.58567200	O	-3.72662800	-1.52308500	1.14396200
O	-1.41915800	-1.54011000	0.30751300	O	-1.48062700	-1.40526200	0.99114400
H	1.46640200	-2.89053900	0.04772000	H	1.19545000	-3.12292000	0.58556400
H	2.67624500	-1.13985000	1.23818200	H	2.71584300	-1.31479000	1.29472200
H	1.60148500	1.74015800	-1.80913700	H	1.59005500	1.07378700	-2.12162100
H	0.39785800	-0.04830800	-3.05871400	H	-0.08472400	-0.66649600	-2.76219600
H	2.96201200	1.19334300	1.63731200	H	3.16439800	1.18853800	1.10545100
H	5.13613000	2.13677100	0.86857400	H	5.53425500	1.14778600	0.32173400
H	4.73296400	1.75450000	-0.81377800	H	5.06313100	0.26585400	-1.13961200
H	4.99106900	0.44899600	0.35396900	H	4.92033400	-0.50534000	0.44785700
H	3.0490630	3.58764200	1.12638100	H	4.00370700	3.06665000	-0.23552000
H	2.6091130	3.30949700	-0.55521800	H	3.49227300	2.29382000	-1.73592300
H	1.4503220	2.93488600	0.75052500	H	2.28210500	2.81054800	-0.51725600
H	-0.4838630	2.74061500	-0.81292500	H	-0.51674400	2.36862200	-1.25389500
H	-2.5441870	4.13885400	-0.91287600	H	-2.57503500	3.61421100	-1.90896900
H	-4.7613380	3.07204500	-0.39583800	H	-4.81679000	2.68228600	-1.25883800
H	-4.7784730	0.60139300	0.20371000	H	-4.86262500	0.48970300	0.02771600
H	0.78187700	-3.42498400	-2.86540400	H	-0.04711000	-3.92661800	-2.17940400
H	-0.4941060	-3.26519300	-1.64269400	H	-0.95790000	-3.60798400	-0.68682800
H	-0.5564500	-2.28926900	-3.12040500	H	-1.34370200	-2.71954700	-2.16730900
H	-0.5671920	-2.85676800	1.55219700	H	-0.54395200	-0.74896000	2.78216000
O	0.19848400	-3.11471300	2.09272300	O	0.35741300	-0.43138000	2.62236500
H	0.34390400	-2.30579500	2.60496500	H	0.32399200	0.55495000	2.66048900

1-I-P_B

Os	0.00000000	0.00000000	0.00000000	C	0.73201900	2.52427800	-0.08888900
Cl	0.00000000	0.00000000	4.01361220	C	0.57485200	1.88896900	-1.36249600
C	0.84220608	0.00000000	-2.05235466	C	1.31371000	0.71762800	-1.73243400
C	0.99004704	-1.32115303	-1.49052593	C	2.18066500	0.08666700	-0.78790300
C	1.62576744	-1.49418465	-0.24013371	C	2.30859400	0.67509300	0.51355100
C	2.21445719	-0.39864758	0.49202477	C	1.58282600	1.85558200	0.84329700
C	2.05097273	0.89148027	-0.07228866	C	-0.00675600	3.78073600	0.28495600
C	1.39097467	1.09839144	-1.33484882	C	2.88660600	-1.20672100	-1.17691400
C	0.06406744	0.19461581	-3.32437214	C	3.85268500	-0.93500900	-2.35062600
C	2.95532609	-0.67823652	1.79309403	C	3.62834100	-1.88868100	-0.02011900
C	4.22651473	-1.49758994	1.48191039	N	-1.87681400	0.03417400	-0.47947400
C	3.30410918	0.57519782	2.60232057	C	-2.77307000	0.99057600	-0.78663800
N	-1.02413860	1.60805749	0.91745582	C	-4.09290000	0.68840900	-1.10022400
C	-0.53318037	2.42440351	1.86835626	C	-4.50930000	-0.64462400	-1.08704300
C	-1.29549647	3.46067065	2.40146465	C	-3.58495000	-1.62865500	-0.75033100
C	-2.60289924	3.64856683	1.95780414	C	-2.28001300	-1.25471400	-0.44869900
C	-3.11737782	2.77939011	0.99668810	C	-1.23131400	-2.26236500	-0.05172700
C	-2.30324401	1.76915256	0.50329706	O	-1.49238100	-3.45371600	-0.01443800
C	-2.79986818	0.75250484	-0.49444676	O	-0.06873100	-1.71962900	0.21771500
O	-3.92449530	0.82490603	-0.96050732	H	-0.14491900	2.29592700	-2.06700800
O	-1.92170195	-0.18995993	-0.75865277	H	1.14877600	0.26431200	-2.70277000
H	0.50757636	-2.16385794	-1.97202270	H	2.84397200	0.15290700	1.29393300
H	1.59982151	-2.47339547	0.22614967	H	1.60002700	2.20197300	1.87091500
H	2.38677418	1.75807083	0.48374436	H	2.10204300	-1.89002700	-1.52566300
H	1.24783157	2.10684014	-1.70589098	H	4.33453400	-1.86846800	-2.65714700
H	2.28804419	-1.28531330	2.41706605	H	4.64035000	-0.23384000	-2.05321500
H	4.73314772	-1.76619042	2.41374471	H	3.34392100	-0.51834200	-3.22532000
H	4.92853676	-0.91851074	0.87089862	H	4.01186500	-2.85633200	-0.35735100
H	4.00104059	-2.42500401	0.94567876	H	4.49043800	-1.29201100	0.30213700
H	3.83227662	0.27956731	3.51303788	H	2.98443500	-2.05697900	0.84602900
H	3.96376520	1.25326332	2.04664837	H	-2.41268500	2.01164800	-0.76223900
H	2.40107503	1.09940906	2.92339610	H	-4.77963200	1.49225100	-1.34194000
H	0.46844511	2.21666053	2.21533742	H	-5.53552700	-0.90513900	-1.32644700
H	-0.86235687	4.08985217	3.17051226	H	-3.82876600	-2.68379900	-0.70236300
H	-3.21433697	4.44847736	2.36368677	H	0.64040900	4.65865100	0.17072500
H	-4.12999955	2.84530540	0.61569335	H	-0.88170000	3.93362300	-0.35409900
H	0.65393165	-0.14819202	-4.18213869	H	-0.34520800	3.73856200	1.32353300
H	-0.86817937	-0.37511036	-3.29298992	O	1.48730900	-1.96996300	2.64304500
H	-0.18513411	1.24700859	-3.47850010	H	0.96163300	-2.27925900	1.88771900
H	-1.81043123	-1.16851546	1.51427452	H	0.93834700	-1.23928800	2.96587700
O	-0.84302082	-1.17223539	1.57377438				
H	-0.56703574	-0.77926965	2.52243620	1-II-TS_A			
				Os	-0.21934100	-0.23006600	0.06799900
1-II-R_A				Cl	1.30438100	-1.80508100	2.06257000
Os	0.12463900	0.35525200	0.12540700	C	-0.50038300	-2.17588100	-1.07821400
Cl	-0.90286800	0.39168900	2.35781800	C	-0.50013000	-0.99867800	-1.91433000

C	-1.42302200	0.08061600	-1.68735300	C	-2.17389100	-1.23264400	0.35802700
C	-2.35428900	0.03783600	-0.58788400	C	-1.14404300	-2.15402100	-0.05113300
C	-2.28421000	-1.07948400	0.27823800	C	0.60788700	-2.97530000	-1.69913500
C	-1.35557800	-2.15513900	0.04374100	C	-3.49192800	0.96681800	0.01468300
C	0.44924000	-3.31936800	-1.30780800	C	-4.79016200	0.77012000	-0.79599500
C	-3.24927500	1.24077500	-0.33970700	C	-3.77307900	0.99954700	1.52200800
C	-4.39849900	1.24572800	-1.36951800	N	1.72890500	0.51526200	-0.30048500
C	-3.78789200	1.33514000	1.09344100	C	2.76689800	-0.28730000	-0.60884600
N	1.85777500	0.22669200	-0.26500200	C	4.03980200	0.23172400	-0.83021400
C	2.82544400	-0.67854800	-0.50470800	C	4.25167500	1.60602700	-0.71876600
C	4.13628600	-0.29658600	-0.76692300	C	3.18281900	2.42286900	-0.35435200
C	4.47059700	1.05897600	-0.76293100	C	1.93805200	1.84354500	-0.14279900
C	3.47385300	1.98915000	-0.48661900	C	0.75175100	2.63659400	0.35478600
C	2.18076000	1.53651000	-0.24356100	O	0.82856600	3.84476700	0.50855100
C	1.06156300	2.47714700	0.11754000	O	-0.29076400	1.88918200	0.62798800
O	1.23942500	3.68566600	0.14461900	H	-0.09988300	-0.55593100	-2.88728700
O	-0.05118500	1.85552100	0.41489800	H	-1.84802500	1.06001800	-2.17026500
H	0.22624100	-0.91494200	-2.71649500	H	-2.63445400	-1.36936900	1.32785500
H	-1.37512400	0.96634700	-2.31208000	H	-0.84128200	-2.95002900	0.62099300
H	-2.83137300	-1.07173700	1.21034800	H	-3.05898300	1.93689400	-0.25873300
H	-1.24018100	-2.91672500	0.80554900	H	-5.50432800	1.56571700	-0.56241400
H	-2.62170800	2.12309400	-0.51698100	H	-5.26163800	-0.18874300	-0.55377100
H	-5.00902700	2.14545700	-1.24539300	H	-4.60409900	0.79060800	-1.87468500
H	-5.04979800	0.37506800	-1.23437600	H	-4.43251400	1.84161200	1.75197600
H	-4.02655700	1.23178300	-2.39910400	H	-4.27919300	0.08999100	1.86483700
H	-4.32254100	2.28133800	1.21992400	H	-2.85095500	1.12755000	2.09500100
H	-4.49847700	0.52945600	1.31243800	H	2.56914800	-1.35193200	-0.61548600
H	-2.98068500	1.29593500	1.82914400	H	4.84993400	-0.44790000	-1.06985600
H	2.53298100	-1.71665200	-0.44247900	H	5.23653400	2.02866200	-0.89238600
H	4.88210800	-1.06119700	-0.95460500	H	3.27305000	3.49375900	-0.21230800
H	5.48948100	1.37826800	-0.95941600	H	0.12033600	-3.81195000	-2.21372400
H	3.65003600	3.05775600	-0.44349200	H	1.31897900	-2.52854800	-2.39992900
H	-0.07744100	-4.15148900	-1.78963400	H	1.15104200	-3.36320600	-0.83131600
H	1.27446600	-3.02995300	-1.96410300	O	0.42795200	-0.43955500	2.02986500
H	0.85847800	-3.67203300	-0.35707400	H	0.95953200	0.29445200	2.37126100
O	-0.64705400	0.33771900	2.49520700	H	1.03596400	-1.30076200	2.00278300
H	-0.23482900	1.21330800	2.45840700				
H	0.04868800	-0.29897700	2.78458000				
				1-V-R_A			
				Os	0.00000000	0.00000000	0.00000000
				Cl	0.00000000	0.00000000	2.45507879
1-II-P_A				C	0.67682451	0.00000000	-2.14537854
Os	-0.26805400	-0.10377200	0.03304000	C	1.80090620	-0.13926783	-1.25419168
Cl	2.02115000	-2.77707700	1.66168200	C	2.06084771	0.80498477	-0.22579184
C	-0.43033400	-1.97926600	-1.26138900	C	1.21189625	1.96012723	-0.05032107
C	-0.70673200	-0.78188700	-2.01634700	C	0.07537590	2.07426884	-0.88145691
C	-1.70650600	0.14227800	-1.61047900	C	-0.20260882	1.08819213	-1.89493292
C	-2.47470700	-0.08008400	-0.40672200				

C	0.41042512	-1.00590721	-3.23185071	C	-4.65925600	0.72471700	-1.06430800
C	1.53175083	2.94231692	1.06508632	C	-3.98888700	0.69112900	1.37966500
C	2.86912847	3.64867974	0.75299147	N	1.74609000	0.55634400	-0.40094500
C	0.42416915	3.96844266	1.33357513	C	1.97992800	1.44628800	-1.38452900
N	-0.31259308	-2.06450601	0.28551247	C	3.26495200	1.88509900	-1.68183500
C	0.64989610	-3.00179994	0.38681856	C	4.34219600	1.41215800	-0.92915900
C	0.35426829	-4.33466908	0.64708759	C	4.09168500	0.51261000	0.10183300
C	-0.97712120	-4.71644044	0.82523975	C	2.78138600	0.10448200	0.33334800
C	-1.96659912	-3.74172559	0.74184499	C	2.42385300	-0.84125700	1.45153700
C	-1.60085610	-2.42713466	0.47449970	O	3.29211300	-1.31399800	2.17024300
C	-2.61805742	-1.31624983	0.39277367	O	1.13760900	-1.05449600	1.55156800
O	-3.80758296	-1.55052103	0.53154391	H	0.10579200	-0.51874500	-2.79541800
O	-2.08236167	-0.14661489	0.14916116	H	-1.72787100	1.03970200	-2.11919300
H	2.43733141	-1.01428894	-1.34423505	H	-2.63946600	-1.51840200	1.24484200
H	2.87764313	0.63281506	0.46432538	H	-0.80328300	-3.04587200	0.58934900
H	-0.66321607	2.83877766	-0.68127387	H	-3.02257800	1.81612500	-0.16584800
H	-1.13415470	1.15528238	-2.44649927	H	-5.41493000	1.48128400	-0.83121800
H	1.66348055	2.33672032	1.97034921	H	-5.14019500	-0.25858700	-1.00836400
H	3.13876191	4.31219262	1.58031058	H	-4.33280500	0.88246800	-2.09698100
H	2.78763214	4.25928701	-0.15333025	H	-4.67870000	1.51089900	1.60196600
H	3.69233707	2.94145596	0.61014229	H	-4.54055200	-0.24479500	1.53048800
H	0.68613573	4.56193574	2.21494278	H	-3.16511800	0.73448600	2.09551800
H	0.31815242	4.66697116	0.49418475	H	1.11052000	1.82636700	-1.90365300
H	-0.54435987	3.49317374	1.51354083	H	3.40806300	2.60124800	-2.48348900
H	1.67036016	-2.65784102	0.27191857	H	5.35290600	1.74852000	-1.13906200
H	1.16287329	-5.05384258	0.71895730	H	4.86651500	0.10978000	0.74381200
H	-1.23215221	-5.75058395	1.03461254	H	0.43975400	-3.75008500	-2.26295700
H	-3.02124738	-3.94926905	0.88232904	H	1.60335100	-2.41739600	-2.20975800
H	0.94985515	-0.73060140	-4.14615090	H	1.29423900	-3.38248400	-0.75467600
H	0.74291273	-2.00589630	-2.93845380	H	-0.56275800	1.53134000	2.09564900
H	-0.65490247	-1.05500299	-3.47055008	O	-0.73462700	0.60092900	2.37466700
H	-1.90059531	1.77504569	2.33482650	H	0.07413700	0.26108900	2.78730800
O	-2.45905091	2.22881244	1.68618539				
H	-2.63270728	1.50971707	1.05602833				
				1-V-P_A			
				Os	0.00000000	0.00000000	0.00000000
				Cl	0.00000000	0.00000000	3.87447943
1-V-TS_A				C	1.83698155	0.00000000	-1.27297368
Os	-0.19366600	-0.26060200	0.08150000	C	2.18713409	0.06721309	0.12122434
Cl	-0.37152300	2.67493100	0.36666400	C	1.70233566	1.09115272	0.98088941
C	-0.28323900	-2.00414500	-1.24974500	C	0.79048406	2.07870546	0.48006921
C	-0.54914300	-0.79238800	-1.97378900	C	0.40493956	2.02076239	-0.89006523
C	-1.61251000	0.09581000	-1.60152700	C	0.90413598	0.97500743	-1.73521012
C	-2.41657500	-0.17663800	-0.45666200	C	2.38124092	-1.07141862	-2.17947108
C	-2.13862100	-1.35408300	0.30120300	C	0.23848821	3.10718147	1.45324373
C	-1.07398300	-2.23295300	-0.07615300	C	1.28342684	4.23095385	1.62721950
C	0.83005900	-2.93769400	-1.63849300	C	-1.13215977	3.67549239	1.06539218
C	-3.48782600	0.82871100	-0.06318900				

N	-0.15991683	-2.01124991	0.63378321	C	2.12665200	3.43215300	-0.43092800
C	0.50693610	-2.56238525	1.66756076	C	3.44384600	2.96830100	-0.41242300
C	0.34539149	-3.90659446	1.99282633	C	3.66708700	1.59803000	-0.32014800
C	-0.53173321	-4.69386294	1.24609487	C	2.57576300	0.73842300	-0.25647100
C	-1.24778792	-4.10367248	0.20576546	C	2.74228300	-0.75604600	-0.14529600
C	-1.04298069	-2.75752465	-0.06860796	O	3.85259600	-1.26139000	-0.12774100
C	-1.83522243	-2.01110500	-1.11858851	O	1.60117300	-1.39942400	-0.09785900
O	-2.64601236	-2.59765265	-1.81734260	H	-0.50089000	-0.88200400	-2.98367200
O	-1.57779562	-0.72615918	-1.14572607	H	-1.36593800	1.32067200	-2.19709000
H	2.79371243	-0.72732061	0.54541439	H	-2.68298400	-0.48352600	1.49093200
H	1.89722455	1.04062357	2.04613299	H	-1.74888700	-2.66278800	0.76224900
H	-0.34557986	2.69640591	-1.27707103	H	-2.24895000	2.70223300	-0.44083200
H	0.49988952	0.87884740	-2.73789672	H	-4.70963000	3.02001800	-0.31926600
H	0.13284867	2.58914467	2.41439694	H	-4.94039800	1.27884800	-0.09339700
H	0.93837982	4.94476688	2.38136716	H	-4.29076600	1.89311000	-1.62157500
H	1.43720254	4.77752233	0.68964001	H	-3.15753900	3.22799700	1.75039000
H	2.25092659	3.83815486	1.95466292	H	-3.55288200	1.54561200	2.08418600
H	-1.49119001	4.33156919	1.86390299	H	-1.85486200	2.03683600	1.98496400
H	-1.08619140	4.27732563	0.15019950	H	0.04769100	2.83274600	-0.35243200
H	-1.86502449	2.87650499	0.92972092	H	1.90155800	4.49141500	-0.49043000
H	1.11737600	-1.89135578	2.26068704	H	4.27538300	3.66428700	-0.46253800
H	0.89330953	-4.31375192	2.83515812	H	4.65659800	1.15649900	-0.28896700
H	-0.66846998	-5.74425327	1.48429011	H	-1.22884300	-3.88803300	-2.13622000
H	-1.97051844	-4.63953946	-0.39891697	H	0.36900000	-3.11720900	-2.22003700
H	3.31313963	-0.73614606	-2.65025913	H	-0.19654800	-3.81879100	-0.68904800
H	2.59990196	-1.98781090	-1.62427812	O	0.55915400	-3.42866200	1.66564700
H	1.67066398	-1.31383069	-2.97415331	H	1.17491400	-2.96611300	1.07213100
H	-1.05805020	0.19374563	2.42581633	H	0.36609800	-2.73542100	2.31357800
O	-1.51971419	0.30927400	1.48181429				
H	-2.24954490	-0.32366534	1.41301155				
				1-VI-TS_B			
				Os	-0.17454000	-0.52332300	0.10109600
				Cl	-0.07722600	1.11359100	2.59683900
1-VI-R_B				C	-1.37093700	-2.24931200	-0.68174400
Os	-0.17607600	-0.30776300	-0.05009300	C	-0.90627400	-1.37078500	-1.72531900
Cl	0.32446600	-0.00254400	2.33381100	C	-1.21753700	0.03218200	-1.69033800
C	-1.14197100	-1.97013200	-1.20102400	C	-2.04523600	0.59854000	-0.64865400
C	-1.04354900	-0.82076000	-2.04751600	C	-2.39842900	-0.25651500	0.41402000
C	-1.54326500	0.43812900	-1.58850000	C	-2.07547300	-1.66266700	0.39391200
C	-2.24741100	0.58877400	-0.34343300	C	-0.95336500	-3.69339200	-0.66708600
C	-2.31701800	-0.57447300	0.47557600	C	-2.44309400	2.06340300	-0.72369600
C	-1.79750200	-1.83913600	0.06207100	C	-3.57406100	2.21376200	-1.76531000
C	-0.50502000	-3.27612100	-1.58454800	C	-2.84647700	2.68226300	0.62081200
C	-2.85753100	1.92509400	0.04428600	N	1.37294200	0.94931100	-0.16956400
C	-4.28307900	2.03524200	-0.53603900	C	1.21057600	2.28213500	-0.07150200
C	-2.84776800	2.19642200	1.55564800	C	2.25198200	3.16726400	-0.32665300
N	1.30282000	1.19021000	-0.28698400	C	3.50905600	2.66752200	-0.67220400
C	1.08358700	2.51630200	-0.36160500				

C	3.68073400	1.28886000	-0.74142700	C	2.64206000	-1.36843100	0.01135300
C	2.59110200	0.46254000	-0.48431800	O	3.67509600	-2.01578100	0.01050700
C	2.71321000	-1.03805000	-0.48012900	O	1.48913200	-1.77084600	0.50310600
O	3.76602200	-1.58621000	-0.76857900	H	-0.56417900	-2.34202800	-2.17784600
O	1.60977200	-1.63974500	-0.11106300	H	-1.14440700	0.05299800	-2.52185800
H	-0.26158200	-1.76106300	-2.50546800	H	-2.73294500	0.27829900	1.47909000
H	-0.82043900	0.68100500	-2.46475300	H	-2.16711800	-2.11397300	1.84627500
H	-2.83832700	0.15612800	1.31189100	H	-1.81741600	2.22533500	-1.51354900
H	-2.27158900	-2.25346500	1.28004400	H	-4.17984000	2.65662500	-2.13389000
H	-1.57290400	2.61187500	-1.10935200	H	-4.69201200	1.18134500	-1.29975200
H	-3.83642200	3.26963500	-1.88526500	H	-3.66636300	1.07314200	-2.73987600
H	-4.47261900	1.67775900	-1.44126400	H	-3.15171000	3.63191600	-0.01825200
H	-3.28330700	1.82332100	-2.74586100	H	-3.73599500	2.23758900	0.88260200
H	-3.00591500	3.75814800	0.49721400	H	-2.01056900	2.69758700	0.95840400
H	-3.78934000	2.25772500	0.98425000	H	0.30525400	2.38083500	-0.78395900
H	-2.08252600	2.52334900	1.38760400	H	2.24756200	3.66918700	-1.64923900
H	0.23700800	2.62183000	0.25159100	H	4.49249700	2.54938400	-1.78175700
H	2.07386800	4.23320800	-0.23668400	H	4.66980600	0.14291700	-0.98025700
H	4.33720000	3.34112900	-0.86989500	H	-1.52829800	-4.55523700	-0.52006500
H	4.62664500	0.81660200	-0.98031800	H	0.11279100	-3.96532900	-0.17260600
H	-1.56350700	-4.26863000	-1.37312800	H	-1.06091800	-4.13584700	1.13994400
H	0.09658300	-3.78934700	-0.95650300	O	0.36162100	0.15455500	2.11371800
H	-1.07570300	-4.12530100	0.32821800	H	1.25175700	-0.15788700	2.33840300
O	0.37806200	-1.73300700	2.21239000	H	0.38158400	1.21884000	2.13793600
H	1.29757800	-1.93674500	1.98529300				
H	0.38711000	-0.89562300	2.73565600				
1-VI-P_B				1-VII-R_B			
Os	-0.18820400	-0.59671200	0.19203300	Os	-0.18997700	0.39989100	0.07458300
Cl	0.39522800	2.98874800	2.02830300	Cl	0.92996500	1.30722800	2.05868600
C	-1.40321500	-2.44829600	-0.15583600	C	-1.17253100	2.33187000	-0.54110500
C	-1.10905400	-1.80461600	-1.41023100	C	-1.92801000	1.70641600	0.51279800
C	-1.44743700	-0.43582700	-1.60081400	C	-2.39017000	0.37508900	0.42072000
C	-2.14238800	0.33797900	-0.60236400	C	-2.10103400	-0.42326000	-0.74873600
C	-2.36039800	-0.30186000	0.64358900	C	-1.38059200	0.18314600	-1.81451000
C	-2.03032700	-1.68338900	0.86173800	C	-0.89434000	1.53071800	-1.68457000
C	-0.94287600	-3.85854500	0.09041900	C	-0.66082700	3.73838800	-0.39493300
C	-2.61269900	1.74766100	-0.92481300	C	-2.56166400	-1.87079400	-0.76831200
C	-3.85965700	1.65454000	-1.83216300	C	-4.07542500	-1.92030300	-1.06359600
C	-2.88628800	2.62080200	0.30536300	C	-1.77845500	-2.77111700	-1.73098700
N	1.38057400	0.63130000	-0.51814500	N	1.79490700	0.01423700	-0.55056400
C	1.27564100	1.91891400	-0.89497700	C	2.56437300	0.83258700	-1.29308800
C	2.37677900	2.63173800	-1.36309000	C	3.89246600	0.53765600	-1.57763800
C	3.62171300	2.00957500	-1.42294100	C	4.45412700	-0.63601300	-1.07040300
C	3.73317400	0.68831700	-0.99144800	C	3.66126200	-1.47138900	-0.28956700
C	2.59570000	0.03363600	-0.53995600	C	2.33899000	-1.11584100	-0.04700300
				C	1.42672500	-1.96864000	0.79962200
				O	1.82297400	-3.01769100	1.28080200

O	0.21910000	-1.47329100	0.91547900	H	2.19795900	1.63075700	1.63702400
H	-2.03193700	2.22889900	1.45724000	H	0.44482100	1.22341000	-2.30276600
H	-2.78943400	-0.10295400	1.30915700	H	1.48688000	-1.03607600	-2.53142800
H	-1.09948000	-0.39778800	-2.68358800	H	0.50575700	3.18940400	0.86827900
H	-0.26591500	1.93759100	-2.47124700	H	1.52911700	5.14022800	-0.30365600
H	-2.39984200	-2.25044500	0.24721300	H	2.21419400	4.06363300	-1.53239100
H	-4.43711700	-2.95145700	-1.00286400	H	2.77224800	3.96211500	0.14510800
H	-4.29248800	-1.54473400	-2.07007800	H	-0.86132400	4.37863700	-0.76901600
H	-4.64659000	-1.32079100	-0.34822700	H	-0.24873100	3.40067200	-2.10047500
H	-2.10304200	-3.80859800	-1.60891400	H	-1.26300600	2.65967900	-0.84525500
H	-1.95096000	-2.50013200	-2.77921800	H	-1.22417400	-1.19898000	-2.29163500
H	-0.70526100	-2.73157700	-1.52762600	H	-3.60719600	-1.07264200	-3.01653600
H	2.09460200	1.74205900	-1.64699100	H	-5.30519900	-0.09742100	-1.44101500
H	4.47295400	1.22697700	-2.18101000	H	-4.48782100	0.73475100	0.81847000
H	5.49029500	-0.88621400	-1.27558600	H	4.02914700	-2.34348000	-1.16895300
H	4.02222000	-2.39332600	0.15175500	H	3.13916500	-2.80640300	0.29603100
H	-1.46537900	4.46298900	-0.56811000	H	2.37581500	-3.01395500	-1.27981500
H	-0.26257400	3.89752800	0.61082200	H	-0.07161300	-1.38174500	2.66904700
H	0.13697600	3.94544500	-1.11382400	O	0.63044100	-1.81677300	2.16222500
H	-0.96567700	-1.48186600	2.52186800	H	0.20657400	-2.54171700	1.64470400
O	-1.55360500	-0.99862000	3.12701600				
H	-1.01398200	-0.22014100	3.32869300				
				1-VII-P_B			
				Os	0.00000000	0.00000000	0.00000000
				Cl	0.00000000	0.00000000	3.87848483
1-VII-TS_B				C	2.19693052	0.00000000	0.57332432
Os	0.48401700	-0.25117300	0.18870900	C	2.04550296	0.52425928	-0.75115716
Cl	-0.31681100	-3.06677300	-0.29995700	C	1.32136300	-0.21196890	-1.73344783
C	2.49127500	-0.97298100	-0.61754600	C	0.76401248	-1.50604796	-1.47070206
C	2.69174200	-0.18512400	0.56909000	C	0.90825980	-1.98876410	-0.12752460
C	2.12882000	1.11109900	0.68672600	C	1.63620941	-1.27517940	0.87570627
C	1.33876800	1.69334300	-0.36234200	C	2.85819712	0.80922796	1.65370746
C	1.11228700	0.87307500	-1.52422700	C	0.06494190	-2.27237576	-2.58198244
C	1.72656500	-0.42180000	-1.67179300	C	1.11504985	-2.99012973	-3.45546617
C	3.03771000	-2.37011900	-0.69963500	C	-1.00147001	-3.26062411	-2.09035497
C	0.78117500	3.09597700	-0.18957600	N	-1.86866952	-0.69051351	0.71185336
C	1.89328400	4.12425900	-0.48640800	C	-2.05334185	-1.54423805	1.73824856
C	-0.47034000	3.39013900	-1.02723300	C	-3.33080299	-1.94570107	2.12050758
N	-1.56221400	-0.27350800	-0.47549000	C	-4.44092466	-1.44705206	1.43908394
C	-1.97956900	-0.74356000	-1.66609900	C	-4.24150512	-0.53829436	0.40076803
C	-3.31487500	-0.68370300	-2.04741200	C	-2.94235829	-0.17720488	0.06751867
C	-4.25579100	-0.14505400	-1.16693300	C	-2.63441344	0.85225141	-0.99616102
C	-3.82262800	0.31699400	0.07163300	O	-3.53247997	1.36052503	-1.64763995
C	-2.46767300	0.24017800	0.38019600	O	-1.35683718	1.13223527	-1.09448205
C	-1.92142600	0.69200200	1.70969400	H	2.39062527	1.52611272	-0.97540374
O	-2.65582800	1.17788500	2.55654100	H	1.11082945	0.26101338	-2.68772559
O	-0.63363700	0.48903700	1.83242700	H	0.39846785	-2.90104104	0.16163312
H	3.15963700	-0.64155100	1.43173300				

H	1.64727285	-1.62807848	1.89989300	H	3.80049800	-3.16948100	0.15689700
H	-0.43782292	-1.52173784	-3.20537956	H	2.52850800	-3.35594500	-1.07129700
H	0.63074829	-3.49498532	-4.29743730	H	1.18745500	3.10770400	-0.89581500
H	1.65521103	-3.74579803	-2.87422717	H	0.44386600	4.37370600	1.03300200
H	1.85070834	-2.28817398	-3.86025496	H	1.24036500	3.28498300	2.16505600
H	-1.53211530	-3.68819751	-2.94617258	H	-0.14949800	2.70775800	1.22662500
H	-0.55772170	-4.09626657	-1.53731642	H	2.81568700	4.75664400	0.03064900
H	-1.73907484	-2.77408611	-1.44609822	H	3.66281300	3.40903500	-0.74771700
H	-1.16660004	-1.85052123	2.27924408	H	3.55788600	3.48726400	1.01807500
H	-3.43952435	-2.62775944	2.95619915	H	-3.05897300	0.74239600	-3.15438800
H	-5.44417624	-1.74946190	1.72325129	H	-5.30414300	0.87363000	-1.98136100
H	-5.05220225	-0.08700619	-0.15972734	H	-3.09181800	-0.39052600	2.60988000
H	3.90249335	0.48960812	1.75472478	H	-3.76129600	1.24982300	2.64854600
H	2.84835109	1.87395986	1.41053921	H	-4.81347800	-0.11338600	2.22797200
H	2.35016694	0.65856233	2.61091698	O	-0.82182300	-1.60451400	2.97654500
H	-1.15205610	1.96479236	1.39759450	H	-0.88864400	-2.32307400	2.33035500
O	-0.29180327	1.52717847	1.47968894	H	-0.89071700	-0.82931400	2.39242100
H	-0.23679415	1.05903727	2.42293197				
2-II-R_A				2-II-TS_A			
C	1.92220900	0.57913400	1.23144000	C	1.53988200	1.46417800	1.12136500
C	1.97151300	1.39709900	0.05587200	C	1.26834400	1.86991500	-0.23114700
C	2.23752700	0.70890600	-1.17449500	C	1.79264400	1.03389300	-1.26878700
C	2.55605900	-0.68583500	-1.22594400	C	2.60755600	-0.11335000	-0.98501900
C	2.75185100	-2.95359100	-0.08145600	C	3.64902000	-1.74795700	0.65895500
C	1.68737000	2.88922400	0.05740300	C	0.40711400	3.06985000	-0.58796000
C	0.74664500	3.33335300	1.18773600	C	-0.58260100	3.47560000	0.51346000
C	3.01063800	3.68053200	0.08858900	C	1.31317000	4.25347300	-0.98573600
C	-1.99330700	0.43112000	-1.27059800	C	-2.05710400	-0.33304800	-1.03312200
C	-3.14518700	0.66291000	-2.07755200	C	-3.19627000	-0.47888500	-1.88241300
C	-4.36010300	0.73289500	-1.46949800	C	-4.43448700	-0.42693200	-1.32602200
O	-4.52281500	0.61224000	-0.14772800	O	-4.63883000	-0.23041100	-0.01851200
C	-3.45019400	0.42885900	0.68307100	C	-3.58463600	-0.07744300	0.84603500
C	-2.17992800	0.37506200	0.15983400	C	-2.28817700	-0.13618700	0.38578000
O	-1.08564700	0.27580100	0.89811400	O	-1.22139500	-0.00466900	1.15030800
C	-3.80144200	0.28624700	2.12442100	C	-4.00120500	0.13797900	2.25977700
Os	0.58760500	-0.34076500	-0.22068300	Os	0.69579700	-0.23163200	0.09252800
C	2.52406100	-1.46876700	-0.03463800	C	2.90771200	-0.47415500	0.36099200
C	2.20317100	-0.82281000	1.20314100	C	2.36602200	0.32751900	1.41260400
O	-0.81180600	0.27864000	-1.73211000	O	-0.85859900	-0.35756200	-1.44377600
Cl	-0.62555400	-2.47431100	-0.38383300	Cl	0.68196400	-2.97483900	-1.09779600
H	2.13515200	1.25271200	-2.10878500	H	1.47241100	1.20331900	-2.29154000
H	2.69950400	-1.17074400	-2.18394000	H	2.86790700	-0.79219800	-1.78693800
H	2.03630900	-1.41216500	2.09645000	H	2.46828200	-0.00345400	2.43889100
H	1.56246500	1.00513500	2.16082400	H	1.04847600	1.97171200	1.94245700
H	2.11594300	-3.46805300	0.64106700	H	3.45531100	-2.08255900	1.68030300
				H	4.72732900	-1.58479000	0.54442900

H	3.33001600	-2.53602200	-0.02792000	H	1.66117600	2.74640500	-1.60732800
H	-0.17294800	2.77883900	-1.47324500	H	0.60434600	4.71892200	-0.64340800
H	-1.27102200	4.23621100	0.13212600	H	0.78492800	4.10965000	0.99879600
H	-0.06556900	3.91276200	1.37540000	H	-0.30074000	3.28088900	-0.14138300
H	-1.16598500	2.61941200	0.86252600	H	3.15409700	4.61046000	-0.89080000
H	0.70597600	5.10803300	-1.30173500	H	3.99586700	3.05705700	-0.76274500
H	1.98228000	3.98955400	-1.81057000	H	3.37325800	3.84932000	0.69311500
H	1.93130100	4.57407600	-0.13973100	H	-3.18202300	1.87148000	-2.39789400
H	-3.06934500	-0.64761300	-2.94474500	H	-5.49481600	1.23084900	-1.55827800
H	-5.36558100	-0.54025900	-1.86789500	H	-3.28173700	-1.56814200	2.37429700
H	-3.11312800	0.31943800	2.86665300	H	-4.75907900	-0.59779400	2.59246700
H	-4.67576400	0.99752100	2.34681200	H	-4.78854000	-2.02437900	1.54518900
H	-4.52886600	-0.73638500	2.65951300	O	-0.31723700	-1.64989100	-1.21315500
O	0.34120900	-2.05154000	1.59103300	H	0.37188000	-2.44335400	-1.34775100
H	0.32093200	-2.71625400	0.84693100	H	-0.42092800	-1.27657900	-2.10096000
H	-0.57699000	-1.80831400	1.79364400				

2-II-P_A

C	1.42541800	1.31934200	1.45528200
C	1.89557200	1.56067500	0.12254800
C	2.47581000	0.47249900	-0.60949900
C	2.51851900	-0.83306400	-0.05270000
C	2.05704500	-2.50045700	1.82927400
C	1.81416400	2.92896000	-0.53630300
C	0.65344000	3.80384700	-0.04504500
C	3.16735700	3.65068700	-0.36448700
C	-2.19986400	0.73884100	-0.81122600
C	-3.31953400	1.25008300	-1.52109200
C	-4.56934100	0.92046800	-1.08971400
O	-4.78089300	0.15265100	-0.01839200
C	-3.74564200	-0.34722500	0.71857600
C	-2.43916000	-0.07074200	0.36135600
O	-1.39388700	-0.48811700	1.03716900
C	-4.17066200	-1.18160200	1.87482800
Os	0.42042600	-0.09259600	0.08769400
C	2.03495800	-1.10262600	1.27149800
C	1.48085100	-0.00419200	1.99565900
O	-0.97854300	0.96298300	-1.14881800
Cl	1.64170700	-3.66285400	-1.69557500
H	2.77932000	0.62182300	-1.63934100
H	2.78207600	-1.68101300	-0.68342000
H	0.99241700	-0.19822600	2.94538500
H	0.94373600	2.10580600	2.02111900
H	1.25564400	-2.64468300	2.55912000
H	3.01366300	-2.68552800	2.33316600
H	1.94494900	-3.23110500	1.02251400

2-III-R_A

C	2.45878900	0.42702400	0.70445900
C	2.09695200	0.98072500	-0.55931000
C	1.82655000	0.07747500	-1.64757900
C	1.87728400	-1.33074900	-1.43875100
C	2.28231600	-3.39412000	0.03487200
C	1.95481700	2.47775400	-0.79761400
C	1.92521400	3.32790200	0.47962900
C	3.08622600	2.94756900	-1.73767800
C	-2.19795000	-1.04401800	-0.66971100
C	-3.44861200	-1.65254200	-0.97973100
C	-4.57245400	-0.88868100	-0.92997900
O	-4.55280700	0.41194000	-0.62025000
C	-3.37995800	1.05846800	-0.34078700
C	-2.18848900	0.36796600	-0.37689700
O	-1.00829600	0.93200400	-0.16676500
C	-3.54084000	2.50084200	0.00027100
Os	0.54011900	-0.48918500	0.06363900
C	2.25645800	-1.90397400	-0.17411400
C	2.51836200	-0.99426500	0.88681700
O	-1.08609200	-1.67505600	-0.64899300
H	1.48332300	0.46709700	-2.59897100
H	1.54029100	-1.99173100	-2.23114000
H	2.65682300	-1.38281500	1.88943900
H	2.57389700	1.07151200	1.56496500
H	2.07317700	-3.64488100	1.07750700
H	3.26709400	-3.80125900	-0.22517600
H	1.53454400	-3.89090400	-0.58912800
H	0.99811800	2.61408200	-1.31793500
H	1.76009900	4.37593100	0.21000300

H	2.88387300	3.28187600	1.00990800	H	1.85485300	2.30719700	1.98380200
H	1.12501400	3.03421700	1.16552500	H	3.46185200	4.22047400	-0.85908200
H	2.96364900	4.01011600	-1.96973100	H	3.17593800	2.99717000	-2.10736800
H	3.09531100	2.39502000	-2.68249900	H	4.37473500	2.70319400	-0.83779900
H	4.06575500	2.81851300	-1.26379100	H	-3.89871600	-2.11112100	-1.02445700
H	-3.50409100	-2.70752300	-1.21894200	H	-5.81766500	-0.45941900	-0.84584300
H	-5.57764000	-1.24450100	-1.11910300	H	-2.39731200	3.38239600	0.48447600
H	-3.14576300	3.14138200	-0.79787900	H	-3.89230000	3.63523600	-0.45000400
H	-4.59734900	2.73655200	0.14374500	H	-3.98607600	3.20426800	1.26221100
H	-2.98292500	2.73302400	0.91447700	Cl	-0.09359800	-2.45894500	2.02273000
Cl	-0.49105100	-0.90531500	2.25686200	O	0.26223300	0.37745400	2.30004000
O	-0.95531100	2.46631700	2.18640400	H	0.03703400	-0.54802200	2.59732000
H	-0.89199100	1.70954100	2.78787100	H	-0.57342800	0.84695700	2.14636500
H	-0.93031400	2.01726600	1.32106200				

2-III-TS_A

C	2.65098500	-0.00658000	0.35508500
C	2.16820900	1.03876300	-0.47709800
C	1.41932000	0.65435800	-1.64810000
C	1.21141600	-0.72779700	-1.97984300
C	1.39059600	-3.21697600	-1.39963800
C	2.30910900	2.51526000	-0.14434800
C	2.58685100	2.79898300	1.33814100
C	3.39304900	3.14367200	-1.04436800
C	-2.42452200	-0.59959200	-0.45826700
C	-3.73858100	-1.07513200	-0.75197700
C	-4.78059800	-0.20802100	-0.65967100
O	-4.63207600	1.07636900	-0.31698900
C	-3.39399200	1.59221000	-0.02796800
C	-2.27405300	0.79198900	-0.07598900
O	-1.05323100	1.20364500	0.20031300
C	-3.42108500	3.03584600	0.33739100
Os	0.49355800	-0.33700700	0.01281900
C	1.72780700	-1.77483600	-1.13769200
C	2.43189400	-1.39152100	0.03279300
O	-1.38089800	-1.31774900	-0.51551400
H	0.93370400	1.42188800	-2.24165100
H	0.56984900	-0.98592700	-2.81509300
H	2.67040200	-2.14376300	0.77391300
H	3.06948200	0.23162800	1.32390400
H	1.21564900	-3.73945100	-0.45656700
H	2.21331800	-3.70484900	-1.93579300
H	0.48535800	-3.30014000	-2.00569800
H	1.34510500	2.97554400	-0.39806600
H	2.54427800	3.87742200	1.52007100
H	3.58804800	2.46244500	1.63121000

2-III-P_A

C	2.44115200	0.25163000	0.14226900
C	1.86599900	1.19308300	-0.75129500
C	1.25528600	0.68254600	-1.96029900
C	1.20259000	-0.71095800	-2.21712100
C	1.65793800	-3.14230300	-1.55150400
C	1.83481400	2.68609500	-0.46969500
C	1.61376000	3.02960400	1.01030800
C	3.11901800	3.33830900	-1.02068800
C	-2.50434600	-0.90187400	-0.24787000
C	-3.79133600	-1.50481900	-0.27042200
C	-4.87822300	-0.73033600	0.00332100
O	-4.78234400	0.57283400	0.27691800
C	-3.57560300	1.21311200	0.29082700
C	-2.41216900	0.51559600	0.02427900
O	-1.22117200	1.06595900	-0.00990100
C	-3.66261200	2.66213800	0.61765700
Os	0.33111700	-0.32280300	-0.24087400
C	1.77980900	-1.66394500	-1.29818700
C	2.39928400	-1.15885700	-0.12798000
O	-1.41218900	-1.54614800	-0.45905900
H	0.73672100	1.36611300	-2.62375100
H	0.63928500	-1.07184900	-3.07162400
H	2.72777700	-1.82395500	0.66416200
H	2.79340800	0.54619300	1.12436500
H	1.74999200	-3.70606300	-0.62031600
H	2.45152600	-3.47564100	-2.23092900
H	0.69542000	-3.38596200	-2.00982100
H	0.98146900	3.08751600	-1.03136000
H	1.52022300	4.11425500	1.12593600
H	2.44976100	2.70568600	1.63801700
H	0.70098900	2.56048400	1.38623100

H	3.07615500	4.42528500	-0.89794900	H	-2.46547837	-1.41011424	3.39265613
H	3.25835100	3.12353400	-2.08555200	H	-0.75240037	-1.84699337	3.30005444
H	4.00185200	2.97308800	-0.48497500	H	-1.80204725	-2.07436384	1.89076073
H	-3.90294100	-2.56131000	-0.48315000	H	1.30402199	5.48815323	-2.23882752
H	-5.90278500	-1.07929600	0.03415300	H	0.00023310	7.49170665	-1.38880550
H	-2.65404500	3.07487400	0.65540000	H	-1.23182248	4.94926079	3.04102936
H	-4.24332200	3.20691100	-0.13614700	H	-1.59976586	6.62674980	2.56042516
H	-4.14792800	2.81822700	1.58765600	H	-2.66822098	5.30184097	2.06636848
Cl	2.25212300	-1.14832700	3.26255300	O	-0.01882253	2.78136232	4.05894122
O	-0.15759500	-0.71651100	1.81537500	H	0.93549481	2.94586309	4.05271698
H	0.72398800	-0.82616500	2.40231800	H	-0.23529731	2.91118834	3.11777559
H	-0.59263000	-1.58055700	1.87207300	2-IV-TS_A			
2-IV-R_A				C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	0.00000000	C	0.00000000	0.00000000	1.44114489
C	0.00000000	0.00000000	1.43494255	C	1.26711273	0.00000000	2.08673715
C	1.25878740	0.00000000	2.11647686	C	2.49890534	-0.03433785	1.34930597
C	2.48558125	0.02436528	1.38080230	C	3.78437050	0.04292648	-0.84414838
C	3.80191349	0.11612283	-0.81209924	C	-1.26971597	0.08617955	2.27248908
C	-1.27440509	0.01989084	2.26438343	C	-2.44262376	0.76975489	1.55469955
C	-2.48233085	0.64248979	1.55131818	C	-1.65992086	-1.32334315	2.76269860
C	-1.58710958	-1.41477165	2.73941911	C	1.25541557	3.85137933	-1.37730759
C	0.68131261	4.25291836	-0.54612365	C	1.59075912	4.79222082	-2.39853074
C	0.71427496	5.44201489	-1.33141943	C	0.70377912	5.77794930	-2.69335706
C	0.02513313	6.52927260	-0.89272174	O	-0.47785430	5.90304913	-2.07913534
O	-0.69597643	6.52951747	0.23325387	C	-0.85919637	5.02626063	-1.09474751
C	-0.79544692	5.40638596	1.01034353	C	-0.02574121	3.99941482	-0.71124935
C	-0.15211400	4.25084550	0.63297811	O	-0.30935273	3.12240069	0.23096530
O	-0.25085719	3.10623705	1.28938325	C	-2.20146870	5.32648304	-0.52292267
C	-1.62114858	5.58231768	2.23876756	Os	1.25861450	1.63197503	0.60944622
Os	1.23252927	1.71241826	0.72770579	C	2.49834125	-0.06739636	-0.07197506
C	2.51090784	0.04025082	-0.04254152	C	1.22885526	-0.05059897	-0.74494738
C	1.23749939	0.07023462	-0.70866661	O	2.00512270	2.89436159	-1.02108944
O	1.33302009	3.19143917	-0.82697710	Cl	3.66312735	3.14002607	1.53894410
Cl	2.73828703	3.25258265	1.91051015	H	1.30937829	0.16986739	3.15665955
H	1.27695805	0.10728645	3.19400401	H	3.43081272	0.13391532	1.87337436
H	3.41452456	0.16228388	1.92252087	H	1.19991974	0.03717238	-1.82531549
H	1.21546764	0.21608614	-1.78424361	H	-0.93151919	0.12215551	-0.53893469
H	-0.93079870	0.06915916	-0.54734504	H	3.61629415	0.52402698	-1.81030321
H	3.67629395	0.69306024	-1.73231414	H	4.20494196	-0.95443532	-1.01940821
H	4.14600751	-0.88893984	-1.08548742	H	4.50737367	0.64393148	-0.28831268
H	4.58351989	0.59452196	-0.21702465	H	-1.01525560	0.69413216	3.14943017
H	-1.05023716	0.63315932	3.14535205	H	-3.26438340	0.92590331	2.26073522
H	-3.32191886	0.71218272	2.25007479	H	-2.83419768	0.14925531	0.73997095
H	-2.81895048	0.03226079	0.70473914	H	-2.14571052	1.73778671	1.14259774
H	-2.24811028	1.64827634	1.19451967	H	-2.54060627	-1.26924155	3.41086950
				H	-0.84976941	-1.79267310	3.32949226

H	-1.90391762	-1.97798889	1.91830177	H	1.41757486	7.22344982	-2.35640426
H	2.54305117	4.72856346	-2.91059455	H	-2.40712550	4.54368755	0.17225230
H	0.85698226	6.55139349	-3.43615975	H	-2.24550395	6.31521808	0.18292200
H	-2.45515554	4.56121763	0.21153007	H	-2.69859178	5.48300675	-1.31134999
H	-2.21491059	6.30587789	-0.02958343	O	1.69319016	3.11731179	2.19288130
H	-2.97103657	5.34057504	-1.30329490	H	2.17723584	2.64138439	3.01526219
O	0.96472295	3.03499275	2.50763648	H	2.36339056	3.72856417	1.85049061
H	1.90640201	3.36444255	2.45810063				
H	0.40587657	3.68623472	2.05301437				
2-IV-P_A				2-V-R_A			
C	0.00000000	0.00000000	0.00000000	C	1.86592500	0.78570000	1.32144400
C	0.00000000	0.00000000	1.44243073	C	1.74187600	1.63297700	0.18770900
C	1.26921893	0.00000000	2.08837792	C	2.06444200	1.06367500	-1.10314800
C	2.49765505	-0.00217100	1.35605516	C	2.51318600	-0.27605200	-1.22790400
C	3.75771203	0.14626750	-0.85497918	C	3.04635100	-2.57363000	-0.21524100
C	-1.27563343	0.01109294	2.26956340	C	1.24211900	3.06536100	0.25557400
C	-2.43880190	0.76640247	1.60975061	C	0.37542500	3.37150000	1.48354300
C	-1.67540598	-1.43616474	2.62180288	C	2.43745500	4.03602400	0.16249600
C	1.54183989	4.17913427	-0.81525664	C	-2.11194100	-0.47654600	0.88569300
C	2.02473452	5.29702318	-1.54815121	C	-3.29686200	-0.87129500	1.56351300
C	1.16361033	6.31657387	-1.82208551	C	-4.49483500	-0.43261000	1.08671500
O	-0.11546062	6.29921450	-1.43998200	O	-4.59833900	0.36780900	0.02358000
C	-0.64233910	5.24460698	-0.74983169	C	-3.49187700	0.79804500	-0.65553600
C	0.14948774	4.15858513	-0.42350801	C	-2.22963800	0.40439100	-0.25528400
O	-0.28514416	3.09895106	0.21601997	O	-1.12018000	0.80104500	-0.83377200
C	-2.08155084	5.40717496	-0.40825352	C	-3.79945200	1.68078900	-1.81347200
Os	1.22014194	1.69837173	0.66269505	Os	0.58358100	-0.23996600	-0.16410400
C	2.48199765	0.03103581	-0.06580831	C	2.64701700	-1.13140600	-0.07668900
C	1.20847678	-0.00297269	-0.74451904	C	2.29113100	-0.58381500	1.18412200
O	2.27461310	3.17898352	-0.47648986	O	-0.93212700	-0.83469800	1.24020800
Cl	3.10942861	1.78792080	4.26724475	Cl	-0.32989300	-2.11221600	-1.47273600
H	1.34104406	0.15096645	3.16235494	H	1.87574700	1.64440900	-1.99966400
H	3.41883145	0.12958405	1.91224295	H	2.63964600	-0.70146300	-2.21677500
H	1.17360918	0.07594307	-1.82547646	H	2.23968900	-1.24546300	2.04131200
H	-0.93643754	0.11212196	-0.53359516	H	1.53179400	1.13003400	2.29232200
H	3.62058972	0.77999333	-1.73496545	H	2.58547200	-3.16691500	0.57744500
H	4.07736914	-0.84639465	-1.19379617	H	4.13695800	-2.67178200	-0.15175100
H	4.55740344	0.57228578	-0.24515625	H	2.71844300	-2.97347200	-1.17783400
H	-1.02737878	0.52941524	3.20379856	H	0.61454200	3.20967600	-0.63310900
H	-3.26958566	0.85383429	2.31690583	H	-0.02821100	4.38594000	1.40784900
H	-2.82219002	0.23436169	0.73079649	H	0.95253500	3.32309300	2.41389900
H	-2.13556118	1.77014988	1.30094494	H	-0.46577900	2.67710200	1.55964800
H	-2.56201668	-1.44078097	3.26417549	H	2.08625100	5.07250000	0.12817600
H	-0.87164390	-1.95769466	3.15048607	H	3.03718900	3.85299100	-0.73471700
H	-1.91307709	-2.00872163	1.71766574	H	3.09494200	3.93094300	1.03272700
H	3.05918387	5.34338771	-1.86691502	H	-3.24892200	-1.52600100	2.42530700
				H	-5.46227900	-0.68428200	1.50309900

H	-2.87041200	1.90582100	-2.33833700	H	4.49280300	-1.01369600	2.52753900
H	-4.49115500	1.19065400	-2.50771900	H	4.06069100	0.67333600	2.84989300
H	-4.26301500	2.62094800	-1.49046500	H	0.48807700	-1.91063000	-2.04117000
H	-0.11914300	-2.59882400	1.78842400	O	-0.33964000	-2.13754600	-1.59447100
O	0.36177700	-3.41923000	1.59997800	H	-0.11193200	-2.73479400	-0.82475800
H	0.20077000	-3.50889200	0.64746200	2-V-P_A			
2-V-TS_A			C	1.86630100	0.78665700	1.32034200	
C	-1.90536100	1.27206900	-0.98942500	C	1.74203000	1.63311400	0.18603100
C	-1.49300100	1.72336600	0.31594600	C	2.06456700	1.06299800	-1.10445000
C	-1.72490100	0.82562300	1.40594900	C	2.51338900	-0.27672600	-1.22832800
C	-2.35430600	-0.44608200	1.21187600	C	3.04631300	-2.57371100	-0.21423600
C	-3.41245200	-2.21630800	-0.28082100	C	1.24400700	3.06609300	0.25355900
C	-0.77335500	3.03807800	0.56286500	C	0.37082200	3.37164200	1.47711400
C	-0.03917700	3.58990700	-0.66722400	C	2.44156300	4.03482700	0.16889700
C	-1.76997800	4.07403700	1.12250100	C	-2.11165900	-0.47534600	0.88583200
C	2.15934500	0.15561300	-1.12719800	C	-3.29630700	-0.87000800	1.56409800
C	3.38080200	0.27969100	-1.85133600	C	-4.49443400	-0.43148500	1.08751100
C	4.55711600	0.21248700	-1.16745900	O	-4.59821600	0.36888500	0.02441800
O	4.61493600	0.04593300	0.15545700	C	-3.49196400	0.79902800	-0.65521200
C	3.47818300	-0.05317800	0.91073800	C	-2.22970100	0.40407100	-0.25636000
C	2.23549600	0.03477800	0.31354900	O	-1.12039100	0.79884800	-0.83646800
O	1.10906000	0.01717800	0.97584800	C	-3.80066900	1.67988500	-1.81425600
C	3.72385400	-0.25186700	2.36460300	Os	0.58358000	-0.23992700	-0.16420200
Os	-0.66153900	-0.25503500	-0.13025900	C	2.64714400	-1.13134400	-0.07655500
C	-2.83440100	-0.84260700	-0.08362000	C	2.29139100	-0.58297900	1.18393100
C	-2.61863200	0.03771000	-1.17346700	O	-0.93163900	-0.83246900	1.24081800
O	0.99980900	0.14212200	-1.66415900	Cl	-0.32986400	-2.11497400	-1.46936400
Cl	-0.03832300	-2.92354500	1.13798500	H	1.87572900	1.64320500	-2.00127700
H	-1.27779500	1.04371600	2.37034200	H	2.63981800	-0.70284400	-2.21689800
H	-2.36978700	-1.16187000	2.02369600	H	2.24010600	-1.24407500	2.04155000
H	-2.83483500	-0.30058800	-2.17980000	H	1.53229500	1.13173400	2.29101300
H	-1.63569200	1.84889400	-1.86562500	H	2.58597300	-3.16645800	0.57919000
H	-3.37274800	-2.51237800	-1.33114200	H	4.13696700	-2.67178700	-0.15150000
H	-4.45898800	-2.22938600	0.04683400	H	2.71766600	-2.97434300	-1.17624300
H	-2.84966400	-2.94640300	0.30719500	H	0.62185600	3.21312000	-0.63847800
H	-0.02352900	2.83382900	1.33775000	H	-0.03103800	4.38673100	1.40058600
H	0.56761300	4.45400300	-0.37941300	H	0.94261000	3.32128000	2.41063800
H	-0.74075500	3.93109600	-1.43700800	H	-0.47162000	2.67818600	1.54755600
H	0.61959500	2.84025900	-1.11357000	H	2.09243600	5.07200800	0.13466300
H	-1.25391700	5.01020900	1.35946900	H	3.04583400	3.85231400	-0.72537600
H	-2.25505500	3.71439700	2.03521700	H	3.09403000	3.92680800	1.04252100
H	-2.55396500	4.29756000	0.39029900	H	-3.24810400	-1.52426100	2.42621400
H	3.37455700	0.40427000	-2.92781000	H	-5.46171900	-0.68263400	1.50458900
H	5.54221000	0.27420400	-1.61347600	H	-2.86507600	1.96460300	-2.29669200
H	2.79283800	-0.57447300	2.83323000	H	-4.43170500	1.16168800	-2.54553100
				H	-4.33232100	2.58541300	-1.49859800

H	-0.11900600	-2.59781300	1.79306000
O	0.35956200	-3.41830100	1.59927800
H	0.19960000	-3.49989700	0.64571900

2-VI-R_A

C	-2.58020000	0.29009700	0.62000900
C	-2.37177000	-0.31951300	-0.64787300
C	-1.71328900	0.45082800	-1.67686500
C	-1.24783300	1.76450100	-1.41139200
C	-0.88282000	3.75453700	0.16853200
C	-2.80657600	-1.74248500	-0.97002500
C	-3.15589300	-2.59544600	0.25612300
C	-3.99085300	-1.69426800	-1.95983500
C	1.89279000	-1.27019100	-0.37622700
C	2.81027200	-2.34935600	-0.48572600
C	4.13605000	-2.06500600	-0.61541900
O	4.60404200	-0.81600500	-0.66321600
C	3.76755300	0.26204400	-0.58155300
C	2.40484900	0.07963700	-0.44341500
O	1.53793200	1.06331700	-0.39092200
C	4.46493500	1.57513100	-0.64568500
Os	-0.40300900	0.44137400	0.11008300
C	-1.43104500	2.38345100	-0.12069900
C	-2.09352000	1.61376100	0.87697200
O	0.62417600	-1.42198400	-0.23862200
Cl	0.52196500	0.21087800	2.37697300
H	-1.48406400	-0.01449400	-2.62904100
H	-0.64389100	2.27293900	-2.15582300
H	-2.13234300	1.99305800	1.89189200
H	-2.98709300	-0.28769200	1.43841000
H	-0.69396600	3.88028500	1.23720900
H	-1.59390900	4.52711000	-0.14865000
H	0.05852500	3.91799200	-0.36277300
H	-1.95680000	-2.21467700	-1.48074800
H	-3.39745100	-3.61238000	-0.06966600
H	-4.04268500	-2.20693000	0.77084100
H	-2.32690600	-2.66205800	0.96812600
H	-4.27392600	-2.70944600	-2.25533600
H	-3.74936800	-1.13359900	-2.86853900
H	-4.86521900	-1.22349700	-1.49678700
H	2.46608300	-3.37552900	-0.43994200
H	4.92815600	-2.80007300	-0.68437700
H	3.73606400	2.36740800	-0.47156000
H	5.25088100	1.63943100	0.11497300
H	4.93466400	1.73372800	-1.62411600
O	-0.32668000	-2.97407600	2.02867900

2-VI-TS_A

C	-2.63851000	0.56903600	0.32582200
C	-2.45776400	-0.55914400	-0.51078300
C	-1.60136600	-0.40207700	-1.66206000
C	-0.99648400	0.86275300	-1.97795000
C	-0.44636100	3.28780700	-1.35887600
C	-3.03698300	-1.93169700	-0.20691500
C	-3.40500100	-2.14535900	1.26760500
C	-4.24844000	-2.19008800	-1.12696000
C	1.89992900	-1.60196800	-0.00663300
C	2.81027700	-2.69436100	0.07319100
C	4.14121300	-2.45003100	-0.08802000
O	4.62647200	-1.23054900	-0.32785500
C	3.80211400	-0.14392100	-0.43922700
C	2.43264100	-0.29145600	-0.31486200
O	1.57953000	0.68568600	-0.45794500
C	4.51286200	1.13818900	-0.69393900
Os	-0.44252800	0.27731300	0.00949300
C	-1.19411900	2.00444600	-1.12518500
C	-1.99488800	1.82215500	0.03693900
O	0.63903300	-1.69872800	0.18121600
Cl	0.56180100	2.10267900	2.14958200
H	-1.35627600	-1.27257100	-2.26188700
H	-0.29016900	0.92723500	-2.79824500
H	-2.01048900	2.60111600	0.78861200
H	-3.13453600	0.45548000	1.28042500
H	-0.20626400	3.76296700	-0.40531300
H	-1.05268900	3.97511400	-1.96096200
H	0.49099100	3.09609400	-1.88642300
H	-2.25450900	-2.65712500	-0.46542200
H	-3.68703200	-3.19073100	1.42809800
H	-4.26543700	-1.53203000	1.55918800
H	-2.56849200	-1.90393100	1.92855600
H	-4.63449900	-3.20262300	-0.97084200
H	-3.98601700	-2.08827600	-2.18498300
H	-5.05811500	-1.48402800	-0.91190200
H	2.45355200	-3.69712300	0.27682900
H	4.92401600	-3.19634200	-0.03075000
H	3.80627600	1.95911200	-0.56416200
H	5.34623100	1.26811200	0.00443200
H	4.92079100	1.18005800	-1.71199500
O	-0.47039900	-0.57284200	2.30048500
H	0.24844900	-1.21909700	2.27058900

H -0.07610700 0.28302700 2.63167600

2-VI-P_A

C 2.47684400 -0.40040000 -0.02749000
C 2.24843200 0.86186400 -0.63540700
C 1.41090200 0.88282100 -1.81109900
C 0.84202700 -0.30053700 -2.34984700
C 0.37403100 -2.80929600 -2.20373900
C 2.80645000 2.16309300 -0.08314800
C 2.88693800 2.19941300 1.44965800
C 4.17850700 2.44895800 -0.72696600
C -2.15081700 1.35683200 0.28255100
C -3.12663500 2.34381200 0.60396200
C -4.43660300 1.97897000 0.63309000
O -4.84877400 0.73648900 0.36118000
C -3.96049500 -0.25188700 0.03639000
C -2.60787700 0.01316900 -0.00496300
O -1.69056700 -0.89148300 -0.29834800
C -4.59930600 -1.56950100 -0.23218300
Os 0.27772100 -0.12822400 -0.22638000
C 1.06752900 -1.57190000 -1.70340600
C 1.90570800 -1.60651300 -0.55632400
O -0.89613100 1.59180000 0.22377900
Cl 2.02674300 -2.14087300 2.83803900
H 1.13145900 1.84125900 -2.23729600
H 0.15653800 -0.23641300 -3.18759100
H 2.01014200 -2.50979800 0.03482800
H 2.96417500 -0.48132600 0.93840200
H 0.31857100 -3.56848700 -1.42064000
H 0.92578400 -3.23084800 -3.05232300
H -0.64217900 -2.57975000 -2.53439600
H 2.11444700 2.95554300 -0.39783700
H 3.20057400 3.19501300 1.77903900
H 3.61562800 1.48203000 1.83988100
H 1.91746900 1.97583900 1.90307000
H 4.56025900 3.42017000 -0.39582700
H 4.11799200 2.46422000 -1.82038500
H 4.90873000 1.68435600 -0.44052900
H -2.82752200 3.35931600 0.83351600
H -5.26227300 2.63601400 0.87651500
H -3.83053000 -2.28113800 -0.53517900
H -5.10461300 -1.95533400 0.66106800
H -5.34903000 -1.48934600 -1.02736500
O -0.09343000 -0.53076900 1.83694300
H -0.85381900 -1.13381400 1.85825800
H 0.70418100 -1.08933700 2.26809200

Cartesian coordinates for all of the species involved in
Scheme 2.

1a-RC

Os	0.36744400	-0.48481400	-0.15274600
C	2.37015000	-1.42861100	0.36058600
C	1.83018300	-0.84718200	1.54417900
C	1.38791900	0.50798700	1.52369400
C	1.52250600	1.35082000	0.37094800
C	2.08881600	0.74100800	-0.79733500
C	2.52004000	-0.61222300	-0.80814200
C	2.76327500	-2.88108900	0.33200600
C	1.10289900	2.81099700	0.43356600
C	2.22690800	3.62826500	1.10683800
C	0.72226000	3.41206700	-0.92713100
N	-1.57967200	-0.24309500	0.63571800
C	-1.96095100	-0.47703100	1.90746700
C	-3.27212800	-0.27818800	2.32569400
C	-4.22119300	0.17569900	1.40709000
C	-3.82625500	0.40418300	0.09040300
C	-2.50035600	0.18157800	-0.26031600
C	-2.00308300	0.35436700	-1.67392600
O	-2.73645100	0.72944700	-2.56330900
O	-0.72635500	0.02092200	-1.82474000
H	1.68159500	-1.45694500	2.42751600
H	0.88336400	0.90645900	2.39867500
H	2.09771400	1.29258800	-1.73006800
H	2.88959500	-1.04840700	-1.72880700
H	0.21950200	2.85306500	1.08427900
H	1.91814000	4.67227600	1.21052800
H	3.14121500	3.60709100	0.50442300
H	2.46891900	3.24792300	2.10415400
H	0.31124200	4.41438000	-0.78063100
H	1.59545700	3.51961400	-1.57971200
H	-0.02629100	2.81241200	-1.45259400
H	-1.19466800	-0.83461900	2.58452800
H	-3.53784600	-0.48058900	3.35722000
H	-5.24907100	0.34150200	1.71303400
H	-4.50732400	0.74582700	-0.68104800
H	3.80665400	-2.98084500	0.65288900
H	2.15057300	-3.47900900	1.01188600
H	2.69798600	-3.29929800	-0.67658300
H	-0.83200300	-2.14399400	-1.76860600
O	-0.53300000	-2.40640200	-0.87715200
H	0.07774600	-3.14949500	-0.98455500

1a-TS1

Os	0.48030700	-0.56820400	-0.12390400
C	2.65499700	-1.07905900	0.20257900
C	1.98427100	-0.66352600	1.41202100
C	1.40793900	0.64729600	1.52691200
C	1.34368100	1.53292000	0.42338700
C	1.82421300	1.01934400	-0.82058800
C	2.54582200	-0.22281300	-0.91630000
C	3.32649600	-2.42064700	0.11989600
C	0.72086900	2.91209900	0.57523100
C	1.78995400	3.87050500	1.14723700
C	0.10857300	3.48120800	-0.71198700
N	-1.55860700	-0.45921900	0.56179200
C	-1.87062000	-0.80263100	1.82843800
C	-3.17401600	-0.76683000	2.31244700
C	-4.19990600	-0.34028600	1.47036200
C	-3.88150700	0.02532000	0.16441400
C	-2.56049100	-0.06842700	-0.26510100
C	-2.21430600	0.34051600	-1.67340300
O	-2.81439700	1.21330400	-2.24394000
O	-1.14229500	-0.28658300	-2.22324400
H	1.96931600	-1.33051200	2.26733100
H	0.91819700	0.92283500	2.45537900
H	1.65456600	1.58289900	-1.73012500
H	2.90800200	-0.54972600	-1.88469800
H	-0.07823600	2.81828700	1.32212300
H	1.34939500	4.85584100	1.32311100
H	2.62106900	3.99409500	0.44502200
H	2.19772300	3.50794900	2.09566400
H	-0.38759500	4.42933000	-0.48865700
H	0.87309000	3.69387400	-1.46669500
H	-0.63704700	2.81498700	-1.15487000
H	-1.04591500	-1.11472800	2.45696300
H	-3.36921700	-1.06568600	3.33620800
H	-5.22469700	-0.29113900	1.82336000
H	-4.62871800	0.38135700	-0.53527600
H	4.34678200	-2.33914000	0.51220600
H	2.80090400	-3.16819300	0.72016400
H	3.39506700	-2.77616400	-0.91092100
H	-1.03286600	-1.23580800	-1.91585800
O	-0.22848700	-2.25576200	-0.87694700
H	0.42270300	-2.88995000	-1.20647600

1a-IM1

Os	0.54749600	-0.58959500	-0.11012600
C	2.78096900	-0.88306400	0.14398800

C	2.12526100	-0.50588300	1.37722000	C	2.26662300	0.78467900	-0.5899540
C	1.44832000	0.74419500	1.51664300	C	2.52599800	-0.57905100	-0.87517900
C	1.23471300	1.58920500	0.40219600	C	2.37129300	-3.05864200	-0.25800700
C	1.70659500	1.10727100	-0.86066500	C	1.43570100	2.65667500	1.0163340
C	2.54608800	-0.05683200	-0.97494600	C	2.60546200	3.15846800	1.8905210
C	3.58496100	-2.14959700	0.05766200	C	1.21603500	3.57443300	-0.19495400
C	0.49267400	2.90679000	0.5695530	N	-1.59752800	-0.10264300	0.46210100
C	1.48125900	3.94221300	1.1548970	C	-2.06686300	-0.67306100	1.59103300
C	-0.16486700	3.44637300	-0.70770900	C	-3.35226600	-0.41035900	2.05495500
N	-1.49594300	-0.56171600	0.54721800	C	-4.17798200	0.45766900	1.33752800
C	-1.72931100	-0.95954500	1.82159800	C	-3.69668000	1.02137800	0.15677200
C	-2.99995600	-1.00565000	2.37648900	C	-2.40480400	0.71638700	-0.25248800
C	-4.08824800	-0.59847000	1.60549300	C	-1.82896900	1.22673900	-1.55111900
C	-3.85487700	-0.16900000	0.30367000	O	-2.46073200	1.96210100	-2.2790220
C	-2.55798500	-0.18636100	-0.21192900	O	-0.61710400	0.74759100	-1.8092670
C	-2.38124800	0.31706100	-1.63386100	H	1.29078900	-1.98441800	2.0146600
O	-2.98482100	1.30084900	-1.99107900	H	0.82229300	0.42442800	2.49162400
O	-1.56500100	-0.35986100	-2.44470300	H	2.42545000	1.51812400	-1.3716880
H	2.19861300	-1.16795500	2.2338440	H	2.91117600	-0.85587300	-1.84985600
H	0.98642000	0.98908800	2.4671910	H	0.52506100	2.67727200	1.62961800
H	1.45262000	1.64948300	-1.76362300	H	2.41994800	4.18918400	2.20567500
H	2.90415500	-0.35602600	-1.95415300	H	3.54715500	3.14304900	1.33159100
H	-0.29371100	2.73568200	1.31597500	H	2.73429500	2.54843500	2.78994600
H	0.95967200	4.88465300	1.34303000	H	0.91425500	4.56731600	0.14894400
H	2.29763200	4.14390700	0.45358800	H	2.13621700	3.70602300	-0.77465800
H	1.91929600	3.60357100	2.09860100	H	0.43971800	3.19688700	-0.86611900
H	-0.71596700	4.35965300	-0.46860300	H	-1.40401400	-1.36921900	2.08979600
H	0.57964400	3.71586100	-1.46450800	H	-3.69442300	-0.88708700	2.96681200
H	-0.87623600	2.74541200	-1.15150000	H	-5.18063600	0.68090900	1.68771200
H	-0.85893900	-1.24687300	2.39824800	H	-4.28559800	1.68688900	-0.46452500
H	-3.12228500	-1.34782600	3.39790900	H	3.31095800	-3.41221300	0.18183400
H	-5.09427400	-0.60924000	2.01185600	H	1.55346500	-3.65613600	0.15350400
H	-4.65491900	0.18542400	-0.33524500	H	2.44242200	-3.22029600	-1.33800600
H	4.59999400	-1.95990600	0.42563900	H	-1.00065400	-1.28436900	-2.29393200
H	3.15163100	-2.94067100	0.67554200	O	-0.65776900	-1.87503200	-1.59310500
H	3.66577200	-2.50880800	-0.97076000	H	-0.01906900	-2.46457800	-2.02108500
H	-1.20815600	-1.18620600	-2.03451400	O	-0.75424500	-3.57505400	1.03519400
O	-0.11357000	-2.13321100	-1.08699700	H	-1.13471600	-4.42512700	1.29212300
H	0.53194800	-2.64243200	-1.59899100	H	-1.22067100	-3.31982400	0.22804100
1a-RC•H₂O				1a-TS1•H₂O			
Os	0.35810300	-0.30632600	-0.3162600	Os	0.24025000	-0.34674300	-0.44286600
C	2.18189200	-1.60294800	0.0732130	C	0.54053600	-2.47370000	-0.05286800
C	1.61935200	-1.21976100	1.3215970	C	0.33469300	-1.81537500	1.20944600
C	1.35194800	0.15784600	1.5821340	C	1.14094200	-0.72397300	1.61895600
C	1.67863600	1.20006100	0.6540480	C	2.14734000	-0.20320000	0.75714600
				C	2.40907500	-0.90350900	-0.47780400

C	1.64455800	-2.02267400	-0.86368100	C	1.58800000	-2.19871500	-0.72505000
C	-0.30499300	-3.64333000	-0.47345400	C	-0.39711900	-3.74992400	-0.27876300
C	2.96961900	0.99861100	1.19622400	C	2.85390400	0.97781800	1.12899400
C	4.10591300	0.49594000	2.11608200	C	3.94252500	0.56523400	2.14590100
C	3.52561300	1.85310900	0.04817900	C	3.46744900	1.72186700	-0.06534700
N	-1.58887000	0.64016800	0.12172400	N	-1.51278400	0.73337500	0.01657800
C	-2.63997200	-0.07865400	0.56701800	C	-2.63005700	0.05570500	0.37810200
C	-3.83815200	0.51774300	0.94968800	C	-3.80541100	0.69407700	0.74903200
C	-3.96200200	1.90385600	0.89478200	C	-3.84127800	2.08659500	0.78382500
C	-2.87572600	2.64940100	0.44046000	C	-2.69050600	2.78647200	0.43554900
C	-1.71747100	1.98931400	0.04116700	C	-1.55044000	2.09158700	0.03011400
C	-0.54480900	2.79739900	-0.44383400	C	-0.33174000	2.92803200	-0.31586800
O	-0.33874200	3.91896600	-0.06116500	O	-0.02141700	3.85113600	0.39910600
O	0.29872800	2.14936200	-1.29144100	O	0.33788400	2.62723100	-1.43160100
H	-0.51490700	-2.11090600	1.81583800	H	-0.62149900	-2.10784900	1.92110500
H	0.89553800	-0.19052600	2.53029300	H	0.75069500	-0.11661700	2.49455000
H	3.14082400	-0.50250100	-1.16857000	H	3.10808300	-0.71552800	-1.09904900
H	1.80911600	-2.47510400	-1.83603100	H	1.77304900	-2.73114000	-1.65176800
H	2.30282200	1.62988800	1.79699300	H	2.16036800	1.66329800	1.63170300
H	4.68001900	1.34740700	2.49202300	H	4.49421100	1.45128100	2.47207600
H	4.79437500	-0.15760700	1.56982400	H	4.65949500	-0.12941600	1.69521000
H	3.72090100	-0.05958200	2.97654400	H	3.51675200	0.08695700	3.03320600
H	4.01870500	2.73542300	0.46485300	H	3.94715500	2.63678000	0.29162500
H	4.28182300	1.31359900	-0.53296500	H	4.24399500	1.12949700	-0.56189300
H	2.73849300	2.19723200	-0.62684200	H	2.71223700	2.01366500	-0.79936400
H	-2.52748600	-1.15439600	0.61859900	H	-2.57871200	-1.02628400	0.38110400
H	-4.64826900	-0.11729700	1.28959600	H	-4.66370100	0.08837800	1.01600500
H	-4.88024600	2.39548400	1.19902900	H	-4.73974600	2.61642100	1.08319900
H	-2.89761600	3.73150800	0.38469000	H	-2.64567200	3.86844600	0.47018000
H	0.18612400	-4.57171400	-0.15651100	H	0.05790800	-4.66519500	0.12031600
H	-1.29563400	-3.60744700	-0.01314100	H	-1.40310600	-3.65684300	0.13836300
H	-0.41723500	-3.68109500	-1.56003700	H	-0.46670000	-3.85907900	-1.36394100
H	-0.16549700	1.50960100	-1.92378800	H	-0.03127800	1.84008500	-1.90595000
O	-0.54798200	-0.01745100	-2.24615400	O	-0.23687300	0.16866600	-2.25958800
H	-0.13567600	-0.48310100	-2.98565900	H	0.31876200	-0.15049100	-2.98591500
O	-3.43700800	-3.14291800	1.00180200	O	-3.56416600	-2.96842900	0.94615000
H	-3.64500000	-3.67435200	1.78120500	H	-3.83940800	-3.35499000	1.78760100
H	-3.98901500	-3.51263100	0.30042000	H	-4.11958800	-3.40333700	0.28603100

1a-IM1•H₂O

Os	0.20310200	-0.45983000	-0.47144000
C	0.46567200	-2.57776100	0.09654700
C	0.23836400	-1.85295800	1.31209300
C	1.02141700	-0.72447900	1.63807900
C	2.05118400	-0.26102700	0.76181000
C	2.35086500	-1.05809700	-0.40394000

1a-IM1a•H₂O

Os	0.20310200	-0.45983000	-0.47144000
C	0.46567200	-2.57776100	0.09654700
C	0.23836400	-1.85295800	1.31209300
C	1.02141700	-0.72447900	1.63807900
C	2.05118400	-0.26102700	0.76181000
C	2.35086500	-1.05809700	-0.40394000

C	1.58800000	-2.19871500	-0.72505000	C	2.71650000	0.37659700	-0.56502600
C	-0.3971190	-3.74992400	-0.27876300	C	3.72301900	-1.74934400	0.40855500
C	2.85390400	0.97781800	1.12899400	C	-0.00485700	2.85311700	0.77260900
C	3.94252500	0.56523400	2.14590100	C	0.54165600	3.74394000	1.91186800
C	3.46744900	1.72186700	-0.06534700	C	-0.19391400	3.67298000	-0.51001000
N	-1.51278400	0.73337500	0.01657800	N	-1.40146300	-0.90691500	0.28067700
C	-2.63005700	0.05570500	0.37810200	C	-1.53204200	-1.94785200	1.14898900
C	-3.80541100	0.69407700	0.74903200	C	-2.75120300	-2.41650300	1.60910600
C	-3.84127800	2.08659500	0.78382500	C	-3.91775600	-1.77257600	1.19333200
C	-2.69050600	2.78647200	0.43554900	C	-3.79489100	-0.67290700	0.35670100
C	-1.55044000	2.09158700	0.03011400	C	-2.53504400	-0.26381400	-0.09976500
C	-0.33174000	2.92803200	-0.31586800	C	-2.53647600	1.01690900	-0.92930700
O	-0.02141700	3.85113600	0.39910600	O	-3.22416100	1.93188000	-0.52748700
O	0.33788400	2.62723100	-1.43160100	O	-1.84475500	1.06417100	-2.04986200
H	-0.62149900	-2.10784900	1.92110500	H	1.91526900	-1.15883600	2.40660700
H	0.75069500	-0.11661700	2.49455000	H	0.28062300	0.71029200	2.47782700
H	3.10808300	-0.71552800	-1.09904900	H	1.68168200	2.11842200	-1.35404400
H	1.77304900	-2.73114000	-1.65176800	H	3.33023900	0.24610600	-1.44894600
H	2.1603680	1.66329800	1.63170300	H	-0.98634700	2.47545200	1.08363900
H	4.4942110	1.45128100	2.47207600	H	-0.13497700	4.58760500	2.07195400
H	4.6594950	-0.12941600	1.69521000	H	1.52767700	4.14666600	1.65737400
H	3.5167520	0.08695700	3.03320600	H	0.63001700	3.20208800	2.85858100
H	3.9471550	2.63678000	0.29162500	H	-0.93339900	4.45671900	-0.32960000
H	4.24399500	1.12949700	-0.56189300	H	0.73755000	4.16788000	-0.80796400
H	2.71223700	2.01366500	-0.79936400	H	-0.56146500	3.06798000	-1.34202300
H	-2.57871200	-1.02628400	0.38110400	H	-0.60735600	-2.39132800	1.50056600
H	-4.66370100	0.08837800	1.01600500	H	-2.77570900	-3.25874200	2.29167200
H	-4.73974600	2.61642100	1.08319900	H	-4.89269800	-2.10509300	1.53414700
H	-2.64567200	3.86844600	0.47018000	H	-4.65691000	-0.09502200	0.04637500
H	0.05790800	-4.66519500	0.12031600	H	3.29401800	-2.63591400	0.88047900
H	-1.40310600	-3.65684300	0.13836300	H	3.97402500	-1.99292700	-0.62560600
H	-0.46670000	-3.85907900	-1.36394100	H	4.65234700	-1.50235200	0.93521100
H	-0.03127800	1.84008500	-1.90595000	H	-1.23088600	0.26820500	-2.18540200
O	-0.23687300	0.16866600	-2.25958800	O	-0.02446300	-0.68303300	-2.19935500
H	0.31876200	-0.15049100	-2.98591500	H	0.57121500	-0.27766000	-2.84482200
O	-3.56416600	-2.96842900	0.94615000	H	0.37867500	-2.33795100	-1.74252300
H	-3.83940800	-3.35499000	1.78760100	O	0.70843500	-2.60680400	-0.84356800
H	-4.11958800	-3.40333700	0.28603100	H	0.03007400	-3.18653600	-0.46419100

1a-IM1•H₂O

Os	0.65866900	-0.44078100	-0.24573100
C	2.78870900	-0.57559500	0.48844900
C	1.91195900	-0.41559700	1.61722500
C	0.99218500	0.65909100	1.66016000
C	0.91831400	1.65122800	0.61779400
C	1.77506000	1.45582300	-0.50174000

1a-TS2

Os	0.95257900	-0.32990500	-0.41606400
C	2.86791900	-0.81499700	0.65717800
C	1.85119500	-0.77140000	1.64899000
C	0.95770900	0.32453800	1.71324700
C	1.10683800	1.48960600	0.87689900
C	2.15968300	1.47579900	-0.07697700

C	2.99310700	0.31632800	-0.22549100	C	2.91921900	-1.01436200	0.73182800
C	3.75092200	-2.01960900	0.48801600	C	1.88260200	-3.03497500	1.90906700
C	0.14359600	2.65374600	1.03298600	C	1.65031100	2.60877500	0.15479100
C	0.68723400	3.59136100	2.13482300	C	2.29412600	3.52109000	1.22330900
C	-0.14604000	3.41957800	-0.26524500	C	2.24861200	2.86470300	-1.23531400
N	-1.92336800	-1.00686700	0.08723100	N	-3.23359000	-0.48142700	-0.59342600
C	-1.89712200	-1.90243800	1.09705200	C	-4.18162700	-1.42523200	-0.47876100
C	-2.97378700	-2.14624200	1.94469200	C	-5.35453200	-1.22727600	0.24931000
C	-4.14748200	-1.41835100	1.75350600	C	-5.53823400	-0.01338600	0.91150500
C	-4.18759200	-0.48110300	0.72594300	C	-4.54928800	0.96607600	0.81552400
C	-3.06474100	-0.30468300	-0.08896000	C	-3.42600500	0.69553200	0.03728400
C	-3.18937800	0.74854700	-1.17736500	C	-2.34370700	1.73034300	-0.11077000
O	-4.16157000	1.46715900	-1.20932400	O	-2.07852900	2.53252400	0.75459100
O	-2.20970300	0.86225100	-2.07707300	O	-1.65331500	1.69495500	-1.26911800
H	1.66623000	-1.64860700	2.25860200	H	-0.06986600	-1.15221600	2.42072900
H	0.10642300	0.27239600	2.38253400	H	-0.16439700	1.20237800	1.62783800
H	2.26058400	2.29134000	-0.78292100	H	3.68609800	0.72177200	-0.31595100
H	3.72457400	0.28402400	-1.02595700	H	3.72276600	-1.65996200	0.39302700
H	-0.80244300	2.22770800	1.39061300	H	0.58068200	2.84109300	0.11273600
H	-0.03099500	4.39408300	2.32263600	H	2.16130700	4.56891000	0.93987100
H	1.63303100	4.05003400	1.82832100	H	3.36876900	3.32975500	1.31428200
H	0.85562100	3.06174400	3.07751400	H	1.83726400	3.37928900	2.20724800
H	-0.90314000	4.18439900	-0.07378300	H	2.02890900	3.89053400	-1.54282300
H	0.74085400	3.93972300	-0.64294700	H	3.33878800	2.75589600	-1.24411000
H	-0.53584200	2.76271600	-1.04848600	H	1.82253600	2.19190600	-1.98614200
H	-0.96860600	-2.45220400	1.22898100	H	-3.98804400	-2.36737700	-0.98380600
H	-2.88787000	-2.89068800	2.72886100	H	-6.09875300	-2.01436800	0.29983800
H	-5.01152800	-1.57668900	2.39097100	H	-6.43575200	0.16767500	1.49422000
H	-5.06222500	0.12611000	0.52637400	H	-4.63274400	1.92419500	1.31539200
H	3.25124500	-2.93289200	0.81807200	H	0.87609300	-3.42820800	2.06793900
H	4.05926200	-2.14648300	-0.55253800	H	2.37721000	-3.64435300	1.14880400
H	4.65716200	-1.89115900	1.09152200	H	2.44238500	-3.14601500	2.84531900
H	-1.45868800	0.23994500	-1.96940200	H	-2.04119200	1.03589400	-1.86630900
O	0.27424000	-0.10334700	-2.22737500	O	1.28929000	-0.90057600	-2.28010500
H	0.54890500	0.68044300	-2.72527600	H	2.13761200	-0.68826600	-2.69351800
H	0.47600700	-2.32875100	-2.03157700	H	-0.61113400	-1.55327300	-2.05766100
O	0.33596400	-2.37433000	-1.06761000	O	-0.76679800	-1.47855600	-1.09663800
H	-0.63481600	-2.30427200	-0.96660100	H	-1.67489000	-1.06837000	-0.92491400

1a-IM2•picH

Os	1.07856100	-0.67853600	-0.38553800
C	1.84981100	-1.58441600	1.51331900
C	0.78045900	-0.73026900	1.89691200
C	0.72020100	0.60539000	1.43629300
C	1.76324200	1.16936900	0.62384400
C	2.89741600	0.34614100	0.32403200

Cartesian coordinates for all of the species involved in
Scheme 3.

2a-RC

C	1.86265400	-0.10278200	-1.37723600
C	2.58410100	-0.25501800	-0.15246500
C	2.47623400	0.82049000	0.77825300
C	1.76740300	2.02765600	0.48343100
C	0.24255300	3.38837300	-1.04066700
C	3.39062100	-1.49793900	0.18621700
C	2.80078800	-2.79455700	-0.38864300
C	4.85255400	-1.29839600	-0.26644200
C	-1.93015800	-1.36836900	-0.20101100
C	-2.83279400	-2.41454300	-0.52363900
C	-4.16175000	-2.11908700	-0.58556500
O	-4.63536200	-0.89021300	-0.35365900
C	-3.81959500	0.15041900	-0.03892000
C	-2.45778800	-0.05584500	0.05277700
O	-1.58703800	0.89998300	0.37202400
C	-4.53195900	1.43593500	0.19032900
Os	0.39827000	0.27500200	0.21661800
C	1.07209000	2.17039900	-0.74975800
C	1.11672400	1.07712900	-1.68371500
O	-0.64791000	-1.52316900	-0.11788300
H	2.89417500	0.69440500	1.77187500
H	1.67966700	2.79595600	1.24248000
H	0.54883700	1.12978800	-2.60522800
H	1.79031300	-0.94453700	-2.05616500
H	-0.65870900	3.12632500	-1.59910100
H	0.82761000	4.08980300	-1.64663200
H	-0.05395800	3.89749800	-0.12140600
H	3.38625500	-1.58176900	1.28078100
H	3.34520100	-3.65473800	0.01059000
H	2.89734300	-2.83638400	-1.47908500
H	1.74287800	-2.90714300	-0.13311100
H	5.45661000	-2.16278000	0.02424700
H	5.29940000	-0.40697900	0.18414500
H	4.91567200	-1.19588100	-1.35519600
H	-2.47739000	-3.41902200	-0.71911300
H	-4.95087100	-2.82148600	-0.82219800
H	-3.80302200	2.23171600	0.34540300
H	-5.16437300	1.68558500	-0.66787100
H	-5.18183900	1.37319000	1.07072700
O	-0.13450100	-0.23896100	2.33465500
H	-0.98180200	0.23012400	2.44197900
H	-0.33210500	-1.18816500	2.39117200

2a-TS1

C	2.05250000	0.21430200	1.39136300
C	2.64212600	0.31074300	0.08286200
C	2.59577000	-0.85825700	-0.75927500
C	1.89666600	-2.01911000	-0.35951600
C	0.37727800	-3.24497200	1.28499400
C	3.36737900	1.55620700	-0.39819000
C	2.76107400	2.87252100	0.10912800
C	4.85971900	1.44057800	-0.01788200
C	-2.07794800	1.17766700	0.23803700
C	-2.88234200	2.28624900	0.64949700
C	-4.23037500	2.14792600	0.68641400
O	-4.84796500	1.00682900	0.33971100
C	-4.14781900	-0.06803300	-0.09601600
C	-2.77683000	-0.01535300	-0.17103600
O	-2.06641900	-1.09705700	-0.58253700
C	-5.00282600	-1.23262900	-0.45129500
Os	0.54962600	-0.25882800	-0.20068300
C	1.20994000	-2.05308300	0.90296300
C	1.35923400	-0.94430800	1.80127700
O	-0.79754200	1.25132800	0.27213200
H	2.98190200	-0.79434700	-1.77091200
H	1.76109400	-2.83341300	-1.06226100
H	0.82182400	-0.94441200	2.74238200
H	2.01506500	1.09523800	2.02066100
H	-0.41915500	-2.96948400	1.97953400
H	1.01635800	-3.98766500	1.77769000
H	-0.07229000	-3.71424500	0.40732000
H	3.29582400	1.55203500	-1.49305600
H	3.25503100	3.71479700	-0.38282500
H	2.90740700	3.00278400	1.18676500
H	1.68953700	2.93625100	-0.10413100
H	5.41205100	2.29653000	-0.41591500
H	5.31339700	0.53000800	-0.42075500
H	4.98883400	1.43270300	1.06956900
H	-2.41243900	3.21484000	0.94982200
H	-4.93371900	2.91168200	0.99340300
H	-4.38307600	-2.05703400	-0.80103300
H	-5.58127500	-1.55768800	0.42012500
H	-5.71587500	-0.95467500	-1.23463600
O	-0.24996800	-0.21867600	-2.06290500
H	-1.49566700	-0.83966200	-1.39787000
H	-0.54249300	0.67458100	-2.30311700

2a-IM1

C	1.92501500	0.31406200	1.44951900	C	-2.34681500	0.57429500	0.88765400
C	2.64426600	0.50902800	0.24135600	C	-2.72627600	-0.74822900	0.56262900
C	2.78350600	-0.61992100	-0.64879800	C	-2.89369200	-2.69202300	-1.08932200
C	2.22883300	-1.88880000	-0.34592400	C	-1.38075500	2.86981600	0.31313800
C	0.68483400	-3.33365900	1.09021000	C	-0.29844800	3.50233100	-0.57131000
C	3.26850500	1.83919200	-0.14478900	C	-2.64111500	3.75975800	0.37116800
C	2.50403400	3.06310700	0.37849600	C	2.06732600	0.34666900	0.82773500
C	4.74323200	1.85420000	0.31372200	C	3.19646200	0.88076200	1.49886900
C	-2.11409000	1.10215100	-0.07400200	C	4.39368000	0.88953200	0.84524600
C	-2.80111600	2.35496300	0.00987700	O	4.53232400	0.41742800	-0.39589400
C	-4.14041000	2.38117100	0.21413200	C	3.48726400	-0.10247200	-1.09195800
O	-4.86567200	1.25924700	0.32789700	C	2.23475800	-0.16113000	-0.50689800
C	-4.29040700	0.03985800	0.21702000	O	1.17185800	-0.66695400	-1.11369900
C	-2.93142600	-0.08704200	0.01921000	C	3.83715100	-0.58244000	-2.45541600
O	-2.40359300	-1.33072500	-0.02348600	Os	-0.59896200	-0.43067300	-0.03313600
C	-5.25318100	-1.08680500	0.35434900	C	-2.55482200	-1.26232500	-0.77194500
Os	0.63315400	-0.33339700	-0.33135700	C	-1.98959800	-0.39676800	-1.74451300
C	1.40122700	-2.04288100	0.80801000	O	0.87937900	0.29012200	1.34483400
C	1.26417800	-0.91455900	1.70093300	H	-2.40152800	0.90047300	1.92066800
O	-0.83490200	1.10334400	-0.19707100	H	-3.06366200	-1.41390100	1.34930600
H	3.27666200	-0.47302600	-1.60404500	H	-1.75997000	-0.78299200	-2.73123200
H	2.28692100	-2.68943500	-1.07422200	H	-1.10562300	1.54875100	-2.16293700
H	0.59883600	-0.99816300	2.55313600	H	-2.35496900	-3.04023500	-1.97328800
H	1.72267700	1.15809600	2.09638300	H	-3.96796000	-2.78180200	-1.28724500
H	-0.27701200	-3.15463800	1.57648200	H	-2.64729800	-3.34961000	-0.25224100
H	1.29641800	-3.94858200	1.76128000	H	-0.97683100	2.78591200	1.33042400
H	0.51215100	-3.90098800	0.17313000	H	0.01318100	4.45856100	-0.14234100
H	3.25724500	1.87926100	-1.24163300	H	-0.66638100	3.71017600	-1.58170400
H	2.93183800	3.97315000	-0.05057800	H	0.58731900	2.86433000	-0.65051400
H	2.57992300	3.15784500	1.46712200	H	-2.37888800	4.75671600	0.73691200
H	1.44455900	3.02399300	0.10666300	H	-3.40264000	3.34641300	1.03947100
H	5.22696800	2.77659300	-0.01989700	H	-3.08732600	3.87149700	-0.62257000
H	5.30662500	1.01112100	-0.09762700	H	3.11512400	1.28024900	2.50282100
H	4.81537800	1.81081500	1.40549600	H	5.32538800	1.26881100	1.24536400
H	-2.23688400	3.27642700	-0.06594400	H	2.92294200	-0.82808900	-2.99671600
H	-4.74818500	3.27215500	0.30764200	H	4.39236400	0.18428600	-3.00484000
H	-4.78177100	-2.01963500	0.04797800	H	4.46852200	-1.47762200	-2.40837500
H	-5.57945700	-1.18517300	1.39641300	O	0.07191300	-2.38368800	0.70949400
H	-6.14241400	-0.89969200	-0.25456800	H	0.90197800	-2.58647900	0.24985400
O	-0.45105500	-1.02448600	-1.83135100	H	0.24854000	-2.31525400	1.69549500
H	-1.72630000	-1.39274200	-0.75104400	O	0.33575900	-1.72950800	3.20212100
H	-0.94406600	-0.30266900	-2.25689200	H	0.89981900	-2.04671200	3.91792100
				H	0.59024900	-0.81130000	3.00593400
2a-RC•H₂O				2a-TS1•H₂O			
C	-1.61139400	0.95255800	-1.41393200	C	-1.40663000	0.31070000	-1.56687200
C	-1.78391300	1.46463100	-0.10059200				

C	-2.41665800	0.50191800	-0.58115600	C	-1.27758800	0.46818400	-1.51907800
C	-2.74932600	-0.62842800	0.24182300	C	-2.41757100	0.62159500	-0.69264900
C	-2.15722000	-1.91274700	0.03718800	C	-2.86702500	-0.55529800	-0.00407000
C	-0.41960300	-3.40632400	-1.09765500	C	-2.28058800	-1.83987700	-0.20178200
C	-3.07584300	1.84293900	-0.31178100	C	-0.45037000	-3.30932700	-1.21321900
C	-2.21201000	3.05235100	-0.69494500	C	-3.10109900	1.95577100	-0.44373100
C	-4.44551500	1.87876700	-1.02429700	C	-2.15837900	3.16257500	-0.55308900
C	2.00962600	1.27184600	0.17968800	C	-4.31168600	2.09995600	-1.39000000
C	2.80632000	2.44585100	0.11297800	C	2.09851300	1.02942800	0.39173100
C	4.11927600	2.33459700	-0.23326900	C	2.76631200	2.29385100	0.43298200
O	4.68033300	1.15759300	-0.51504000	C	4.03793600	2.41695400	-0.02343500
C	3.97378900	-0.00247600	-0.46487400	O	4.71537400	1.37205600	-0.51272800
C	2.63094500	-0.00376400	-0.11262800	C	4.16330900	0.13808900	-0.55011700
O	1.90068200	-1.08991700	-0.04719700	C	2.86698900	-0.08594100	-0.11992900
C	4.77604300	-1.20907400	-0.80476100	O	2.38611400	-1.33069900	-0.22398000
Os	-0.58442700	-0.39121900	0.33383800	C	5.06467400	-0.90997700	-1.10335000
C	-1.15033800	-2.10118200	-0.95730300	Os	-0.71803300	-0.42506100	0.44387900
C	-0.76181100	-0.96352800	-1.73520100	C	-1.14652900	-1.98629000	-1.06892100
O	0.75760400	1.31527800	0.49360900	C	-0.63990800	-0.81107100	-1.70008700
H	-3.42376100	-0.48679700	1.07946200	O	0.88326700	0.95463700	0.81370800
H	-2.37517800	-2.71624200	0.73104400	H	-3.64757400	-0.45208300	0.74339700
H	0.08160100	-1.04945600	-2.40984700	H	-2.63171200	-2.68811600	0.37386500
H	-1.01996700	1.16365000	-2.11016400	H	0.27600500	-0.87540000	-2.27541600
H	0.63625500	-3.23435900	-1.31823900	H	-0.81077700	1.34376900	-1.95365300
H	-0.85766900	-3.98172900	-1.92130700	H	0.59706200	-3.17398300	-1.49003700
H	-0.49474200	-4.00359600	-0.18664600	H	-0.94257500	-3.89649100	-1.99695600
H	-3.25537800	1.88549100	0.76981200	H	-0.49186700	-3.87672600	-0.28092800
H	-2.69077200	3.97031000	-0.34320600	H	-3.48165300	1.92099000	0.58534100
H	-2.10187300	3.14562800	-1.78085900	H	-2.67587400	4.06726200	-0.22268900
H	-1.21480100	2.99199200	-0.24921500	H	-1.83789000	3.33734800	-1.58598100
H	-4.96403200	2.81179300	-0.78561500	H	-1.26607900	3.03243000	0.06802400
H	-5.08781800	1.04822000	-0.71605500	H	-4.85213200	3.02577900	-1.17201100
H	-4.32414200	1.82915800	-2.11141800	H	-5.01332600	1.26729400	-1.28094400
H	2.37582700	3.41659700	0.32846700	H	-3.98926600	2.13564200	-2.43604000
H	4.82000200	3.15557700	-0.31774200	H	2.23637600	3.15869000	0.81368200
H	4.12365500	-2.08217700	-0.81024500	H	4.61786500	3.33070900	-0.04586400
H	5.24475400	-1.10014600	-1.78868900	H	4.78424000	-1.88537400	-0.70416000
H	5.57803900	-1.36849900	-0.07485900	H	4.97975200	-0.95842700	-2.19600700
O	0.49671600	-1.67535200	1.85103700	H	6.10469500	-0.68546100	-0.85582900
H	1.32502200	-1.59830800	1.24880700	O	0.51982200	-1.69946100	1.46334200
H	0.71356800	-1.23774300	2.68549900	H	1.67013900	-1.53242200	0.48323100
O	-0.92110600	0.87011100	2.37343300	H	0.88196300	-1.27877200	2.25759100
H	-0.89460300	0.55149900	3.28577900	O	-1.08359200	0.45360300	2.48270200
H	-0.21761000	1.53143900	2.25523600	H	-1.05255600	-0.20623400	3.19226200
				H	-0.33411800	1.06140000	2.61243300

2a-IM1•H₂O

2a-TS2

C	1.25510700	0.48365500	1.48842300
C	2.16335300	1.23722000	0.68358600
C	3.10775000	0.49809300	-0.06909600
C	3.15541900	-0.93067300	-0.00489800
C	2.42220900	-3.17653600	0.99520500
C	2.07048900	2.74676600	0.53224800
C	0.64560800	3.30294800	0.67583000
C	3.03519100	3.41674600	1.53408500
C	-2.80099400	0.57196700	-0.72375100
C	-3.81801900	1.52930000	-1.05255600
C	-5.02866300	1.46276500	-0.44494800
O	-5.32862500	0.52333000	0.46134700
C	-4.42336300	-0.42831600	0.81339900
C	-3.16671200	-0.42891100	0.26196700
O	-2.27241600	-1.35610100	0.66509300
C	-4.93849000	-1.39534000	1.82182900
Os	1.09472600	-0.46950300	-0.47373400
C	2.33570700	-1.67945800	0.91738700
C	1.37001500	-0.94340600	1.65070600
O	-1.64468200	0.56136100	-1.23594600
H	3.71481200	1.00730500	-0.80961400
H	3.82745000	-1.46562000	-0.66759200
H	0.63601400	-1.46842100	2.25196400
H	0.43214900	0.98991300	1.97756700
H	1.46700700	-3.61338900	1.29331100
H	3.17757500	-3.46122500	1.73673400
H	2.71359900	-3.60585500	0.03365900
H	2.41991500	2.97722600	-0.48180300
H	0.64154700	4.36542300	0.41786500
H	0.27934700	3.22415900	1.70523800
H	-0.06110200	2.79015200	0.01596200
H	3.02470700	4.50162700	1.39515400
H	4.06410000	3.06929300	1.40126200
H	2.73702500	3.20674900	2.56688700
H	-3.61202800	2.30484500	-1.78046600
H	-5.85812900	2.13678500	-0.61974700
H	-4.23466500	-2.21918700	1.93713400
H	-5.07380300	-0.90799000	2.79424400
H	-5.91166100	-1.78688100	1.50999000
O	-0.12647800	-1.86117000	-1.08613100
H	-1.55256500	-1.47812200	0.00371700
H	-0.61182100	-1.56558100	-1.87411800
O	0.61035000	0.64160800	-2.30025400
H	0.73257500	0.18061800	-3.14236500
H	-0.36408700	0.82723600	-2.17055500

2a-IM2•malH

C	2.03523700	1.07162600	1.10231600
C	2.17405400	1.43828100	-0.28883300
C	2.88584500	0.54409200	-1.13648700
C	3.34871100	-0.70282200	-0.65222400
C	3.68301500	-2.40550300	1.22664900
C	1.62591800	2.74267300	-0.84234200
C	0.34502100	3.23719700	-0.15340400
C	2.73988000	3.81135300	-0.77833100
C	-3.40767400	-0.99766500	-0.57445000
C	-4.72155300	-1.39262600	-0.99507900
C	-5.80532000	-0.67658200	-0.60985800
O	-5.70684800	0.39990900	0.18331200
C	-4.50459000	0.80694000	0.66035100
C	-3.34862400	0.15122100	0.30807100
O	-2.17106600	0.63000900	0.77411300
C	-4.59264700	2.00124400	1.54585400
Os	1.20364400	-0.57098200	-0.04693100
C	3.20822700	-1.06641200	0.73502600
C	2.59734400	-0.12726800	1.61830600
O	-2.37768200	-1.64322100	-0.95149500
H	2.94270900	0.75464100	-2.19900500
H	3.75645000	-1.42888000	-1.34664400
H	2.40890100	-0.40569900	2.64867200
H	1.44318800	1.69597400	1.76024100
H	3.11387900	-2.73546500	2.09803700
H	4.73811300	-2.33032500	1.51571700
H	3.60166800	-3.16679700	0.44709500
H	1.39486100	2.56059000	-1.89988600
H	-0.04829200	4.09949500	-0.69901800
H	0.54019300	3.57358300	0.87057700
H	-0.43524800	2.47077800	-0.12051000
H	2.38553700	4.74449800	-1.22553100
H	3.63838000	3.49709900	-1.31766100
H	3.02218100	4.02210700	0.25862800
H	-4.83056700	-2.25501900	-1.64144000
H	-6.83105100	-0.88285800	-0.88884700
H	-3.64625700	2.14688700	2.06537500
H	-4.81412100	2.90138900	0.96058400
H	-5.39869400	1.87336000	2.27427400
O	-0.25942100	-1.31440600	1.02597200
H	-1.52021100	-0.09425400	0.94986700
H	-0.85385600	-1.87981000	0.49942900
O	-0.06614900	-1.11103900	-1.60124600
H	0.07007500	-0.82050900	-2.51024300

H	-1.08254100	-1.25065300	-1.37161800	H	1.10445700	0.79986100	2.30021600
				H	-1.26666800	1.52871400	2.13188000
2a-IM2				H	-1.00119500	1.52027800	-2.20224400
C	0.88300300	0.77488500	-1.17341000	H	1.28137200	0.57545700	-2.03312400
C	1.41387200	0.62756600	0.14474600	H	-3.20887800	1.73272600	-1.06613500
C	0.58771400	1.05118300	1.24731400	H	-2.82224100	3.15251400	-0.07328100
C	-0.68602200	1.63798700	1.04354300	H	-3.32727100	1.63815400	0.69659900
C	-2.62193900	2.29648400	-0.48603600	H	2.95093800	-0.21872200	1.29953800
C	2.78196200	0.03224200	0.42030600	H	4.08872800	-1.49967200	-0.45352300
C	3.24840800	-0.98886200	-0.62656800	H	3.02869800	-0.85044700	-1.70353900
C	3.79564000	1.18977200	0.57647200	H	2.35814600	-1.90363200	-0.44757500
Os	-0.51702800	-0.44041700	-0.01224600	H	4.85955000	0.87335700	0.12802800
C	-1.24422700	1.73930200	-0.25301800	H	3.68206100	2.08601300	0.66240300
C	-0.44795000	1.26294300	-1.35244500	H	3.74845300	1.60440700	-1.03968000
H	0.94256400	0.88654200	2.25866100	O	-1.56625300	-1.56949100	-1.14586800
H	-1.29478500	1.89210000	1.90454600	H	-1.63088600	-2.42157500	-0.67719000
H	-0.88260100	1.25075100	-2.34681000	O	-0.57046000	-2.10512800	1.06199400
H	1.43018200	0.39865100	-2.02829600	H	-0.11936200	-2.05059900	1.91353300
H	-3.11546700	1.80781100	-1.32960400				
H	-2.54775400	3.36509400	-0.71944500	2a-IM4			
H	-3.25395100	2.19382700	0.39925900	Os	-1.68229100	0.19066500	-0.05366700
H	2.70592400	-0.48092300	1.38779200	C	-3.83795900	-0.25570100	0.35797600
H	4.17136800	-1.46307500	-0.28279300	C	-3.34760400	0.68149000	1.31162200
H	3.47363900	-0.51354100	-1.58716400	H	-3.39098500	0.45778800	2.36935700
H	2.50305300	-1.77225800	-0.79192300	C	-2.72363300	1.90514800	0.88150800
H	4.77484600	0.78337200	0.84380300	H	-2.28988500	2.55754500	1.63232400
H	3.49809000	1.89466800	1.35869700	C	-2.61521900	2.26107300	-0.49035100
H	3.90577700	1.74465800	-0.36075600	C	-2.01094100	3.56838200	-0.92813600
O	-0.27038500	-2.11190700	-0.87518400	H	-1.50565500	3.47484000	-1.89390800
H	-0.81103500	-2.81185900	-0.46684700	H	-1.29852300	3.95118400	-0.19130600
O	-1.94337800	-1.67689400	1.17233300	H	-2.79438100	4.32601700	-1.04451500
H	-2.87780700	-1.57022500	0.93659300	C	-3.01620500	1.26862100	-1.43171100
H	-1.88058500	-1.56448100	2.13233200	H	-2.80730100	1.42733500	-2.48489200
				C	-3.63706400	0.03786100	-1.03070900
2a-IM3				H	-3.92323700	-0.68801000	-1.78311000
C	0.76971700	0.87809600	-1.12711300	C	-4.50089900	-1.56495200	0.75504000
C	1.40495300	0.65489200	0.15516200	H	-4.20708600	-2.30676400	-0.00079600
C	0.68127800	1.01603900	1.32510400	C	-4.08245200	-2.09598300	2.13398600
C	-0.67626700	1.41509400	1.22938400	H	-4.50586300	-3.09214900	2.28940400
C	-2.74928800	2.05931100	-0.13039200	H	-4.45613300	-1.45941500	2.94285000
C	2.82019800	0.10912600	0.25980800	H	-2.99489600	-2.16931200	2.23334100
C	3.08333000	-1.10855100	-0.64047200	C	-6.03331400	-1.39698800	0.66729100
C	3.83610700	1.23691800	-0.01104100	H	-6.52816200	-2.34774200	0.88565100
Os	-0.53447500	-0.43627100	0.03393800	H	-6.34873200	-1.07165000	-0.32834700
C	-1.30934900	1.62690100	-0.05491500	H	-6.38651600	-0.65774100	1.39381000
C	-0.52936600	1.44329700	-1.22955500	O	-1.01207900	-1.66758700	0.24679700

O	-0.01265200	0.15333300	-1.47956300	H	-2.80212400	1.36345500	-2.58850500
H	-0.14550000	-0.61448700	-2.05120600	C	-3.61164500	0.02072700	-1.08099300
H	-1.74048300	-2.28695400	0.38242100	H	-3.89531300	-0.73432000	-1.80519300
H	6.14828900	-0.55874700	2.01780100	C	-4.47574300	-1.51232100	0.77076200
C	6.12403300	0.33870300	1.39040100	H	-4.20470200	-2.27715000	0.02946600
C	4.68261700	0.87272600	1.24677700	C	-4.02193800	-2.00657200	2.15218600
H	6.76092700	1.09494700	1.85845500	H	-4.44370800	-2.99669400	2.34582000
H	6.56099600	0.08456700	0.41985900	H	-4.37227200	-1.34776700	2.95365600
C	3.84227600	-0.15485000	0.50732700	H	-2.93211300	-2.08010300	2.22163900
H	4.71706400	1.76486600	0.60814100	C	-6.00877300	-1.33784100	0.71720400
C	4.10888400	1.29179600	2.60694000	H	-6.50258500	-2.27938800	0.97436400
C	3.00259100	-1.09526700	1.15658000	H	-6.34801700	-1.03845600	-0.27880100
C	3.84942200	-0.18031200	-0.93247500	H	-6.33971300	-0.57690800	1.43170300
H	4.70094000	2.11315900	3.01950100	O	-0.97621300	-1.63298700	0.19873600
H	4.14598600	0.47479600	3.33579700	O	0.10047700	0.20151500	-1.43167800
H	3.07228500	1.63358700	2.52130900	H	0.00035200	-0.27346600	-2.26581000
H	2.87617300	-1.04266800	2.23162900	H	-1.67809300	-2.28749700	0.30714700
C	2.21477600	-2.04588300	0.41765900	H	6.27302700	0.29865100	1.64380800
C	3.12622000	-1.14725100	-1.67843400	C	5.95092200	1.11518200	0.98881400
H	4.38657900	0.59761900	-1.46525600	C	4.41569800	1.28038600	1.02010000
H	1.49855700	-2.67148500	0.93534400	H	6.43114400	2.03480600	1.33515800
C	2.27516300	-2.08907100	-1.00562800	H	6.31823300	0.90508800	-0.02039200
H	3.13208300	-1.10399400	-2.76136400	C	3.77432900	0.03002400	0.44390400
C	1.39860600	-3.04062100	-1.77354700	H	4.14206100	2.10196900	0.34762000
H	1.26093500	-2.71125900	-2.80768300	C	3.92668300	1.64623600	2.42723500
H	0.42250200	-3.12170700	-1.28864100	C	3.20925800	-1.00115700	1.23904200
H	1.86290700	-4.03269900	-1.80312700	C	3.69415000	-0.11955500	-0.98738200
Os	1.72492900	-0.05334400	-0.32480700	H	4.35260300	2.60838200	2.72349400
O	0.22740200	0.62560500	0.97038300	H	4.24194000	0.91157500	3.17649600
O	1.49596100	2.14159200	-0.71026300	H	2.83673200	1.74025600	2.46535000
H	0.22505900	0.13459600	1.80276500	H	3.15289900	-0.88103200	2.31355800
H	0.92804800	2.33619100	0.06098800	C	2.51792500	-2.09275200	0.63179400
H	0.87870400	2.09428600	-1.46407900	C	3.13686300	-1.27819300	-1.59550500
2a-TS3				H	4.03565700	0.69584000	-1.61547900
Os	-1.66907400	0.20583900	-0.10816400	H	1.96419900	-2.78619700	1.25455500
C	-3.81490700	-0.22023900	0.31994600	C	2.49180900	-2.26736800	-0.79825300
C	-3.32482000	0.75861800	1.23034100	H	3.05592500	-1.32663400	-2.67571500
H	-3.36133100	0.57344200	2.29618700	C	1.75913400	-3.42956200	-1.40849600
C	-2.70568000	1.96927900	0.75518900	H	1.54202100	-3.25379100	-2.46482800
H	-2.27521300	2.65324500	1.47914800	H	0.81734600	-3.60627700	-0.88407700
C	-2.59829200	2.26901600	-0.62917400	H	2.37462500	-4.33369400	-1.33674400
C	-1.97692700	3.55004200	-1.11920900	Os	1.65389200	-0.30442000	-0.22525700
H	-1.68806400	3.46969500	-2.17031800	O	0.24730200	0.60310700	0.94958700
H	-1.08844500	3.82154100	-0.54303200	O	1.39694600	2.73351400	-0.51420100
H	-2.69849100	4.37057600	-1.03736400	H	0.24481400	0.37564800	1.88796100
C	-3.00326300	1.24052500	-1.52909000	H	0.90116600	2.33802800	0.22106300

H	0.94244100	2.38131000	-1.29201600	H	5.94859600	1.17624000	1.40485100
				C	5.40717700	1.88760900	0.77151500
2a-PC				C	3.88113500	1.69090400	0.89021400
Os	-1.54780400	0.33727900	-0.16543900	H	5.67926500	2.89735300	1.09207000
C	-3.57708900	-0.48678400	0.31650900	H	5.75500000	1.75706300	-0.25775400
C	-3.26920000	0.55945400	1.22724000	C	3.50944800	0.31161800	0.36558200
H	-3.25106300	0.36016200	2.29149000	H	3.37848500	2.41549600	0.23862300
C	-2.86471100	1.85403100	0.75343600	C	3.40274400	1.96081200	2.32331700
H	-2.53368000	2.59646200	1.47215600	C	3.19040200	-0.79991700	1.22139700
C	-2.79564400	2.16288300	-0.63155400	C	3.41690400	0.08626800	-1.03453400
C	-2.34464800	3.51630100	-1.11428400	H	3.60084200	3.00401700	2.58294800
H	-2.15356600	3.50233700	-2.19021700	H	3.92916800	1.34084500	3.05795900
H	-1.42382500	3.82732800	-0.61148400	H	2.32700000	1.79112500	2.42826800
H	-3.12530800	4.26084000	-0.92407300	H	3.14102700	-0.64635900	2.29250600
C	-3.10560600	1.09660200	-1.54394000	C	2.82381300	-2.06815700	0.70272400
H	-2.96833500	1.26331400	-2.60742300	C	3.07157800	-1.19936600	-1.57499900
C	-3.49267200	-0.19160800	-1.09187700	H	3.55039000	0.92365500	-1.71101500
H	-3.66896800	-0.98082800	-1.81421000	H	2.52484700	-2.85862200	1.38156200
C	-3.98721400	-1.87819700	0.76817800	C	2.76029800	-2.28920100	-0.71872800
H	-3.73141800	-2.55988000	-0.05381900	H	2.96602000	-1.31700800	-2.64793800
C	-3.25708000	-2.37087000	2.02570000	C	2.34611800	-3.62794400	-1.26610800
H	-3.53979800	-3.40711400	2.23190400	H	1.93233900	-3.53944000	-2.27382100
H	-3.52631500	-1.78595700	2.91169400	H	1.60598300	-4.10897400	-0.62091800
H	-2.17192000	-2.33054300	1.89327900	H	3.21790100	-4.29008400	-1.31991500
C	-5.51995800	-1.91502600	0.94816700	Os	1.48224100	-0.53573100	-0.16958900
H	-5.84499600	-2.93106300	1.18992500	O	0.18364900	0.64650700	1.04940100
H	-6.04302400	-1.60035800	0.03990800	O	0.89126900	3.17241600	-0.17311900
H	-5.83395400	-1.25695500	1.76515700	H	0.07923900	0.28957200	1.94094200
O	-0.42567400	-1.45340900	-0.06117700	H	0.70324900	2.59697000	0.58440800
O	0.18424800	0.64813600	-1.36883300	H	0.74103900	2.55240400	-0.90434400
H	0.10326400	0.37418000	-2.29002300				
H	-0.62740900	-2.13950400	-0.70844600				