

Supplementary Information

**Stereodivergent Synthesis of Enantioenriched Azepino[3,4,5-*cd*]-Indoles via
Cooperative Cu/Ir-Catalyzed Asymmetric Allylic Alkylation and
Intramolecular Friedel-Crafts Reaction**

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Computational Methods

All quantum mechanical computations were carried out in the Gaussian 09 program with the M06-L functional. Geometries were optimized by using M06-L and a mixed SDD(Fe, Cu, Zn, Ir)-6-31G(d) basis set¹ and were verified by harmonic vibrational frequency calculations to be energy minima or transition states (no or one imaginary frequency, respectively). Single-point energies were evaluated with M06-L and the def2-TZVP basis set² for all atoms, in which the solvation effects were considered using the SMD model³ with DCE and DCM solvent. The GoodVibes package was utilized for computing thermodynamic quantities at 1 mol/L. Molecular visualizations were carried out in CYLview and PyMOL.⁴ Steric contour and non-covalent interaction (NCI) plots were produced in Multiwfn. The independent gradient model (IGM) was employed for visualizing intermolecular NCIs between allyl-iridium and copper azomethine ylide species.⁵ Grimme's dftd code was utilized to estimate dispersion energies using DFT-D3(BJ) parameters for Hartree-Fock theory.⁶

- (1) (a) D. Andrae, U. Häussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta.* 1990, **77**, 123-141.
- (b) L. E. Roy, P. J. Hay, R. L. Martin, *J. Chem. Theory Comput.* 2008, **4**, 1029-1031.
- (2) F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297-3305.
- (3) A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* 2009, **113**, 6378-6396.
- (4) (a) C. Y. Legault, *CYLview, 1.0b*; Université de Sherbrooke: Quebec, Montreal, Canada, 2009. (b) W. L. Delano, *The PyMOL molecular graphics system*; Delano Scientific: 2002.
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- (6) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* 2011, **32**, 1456-1465.

Supplementary Computational Results

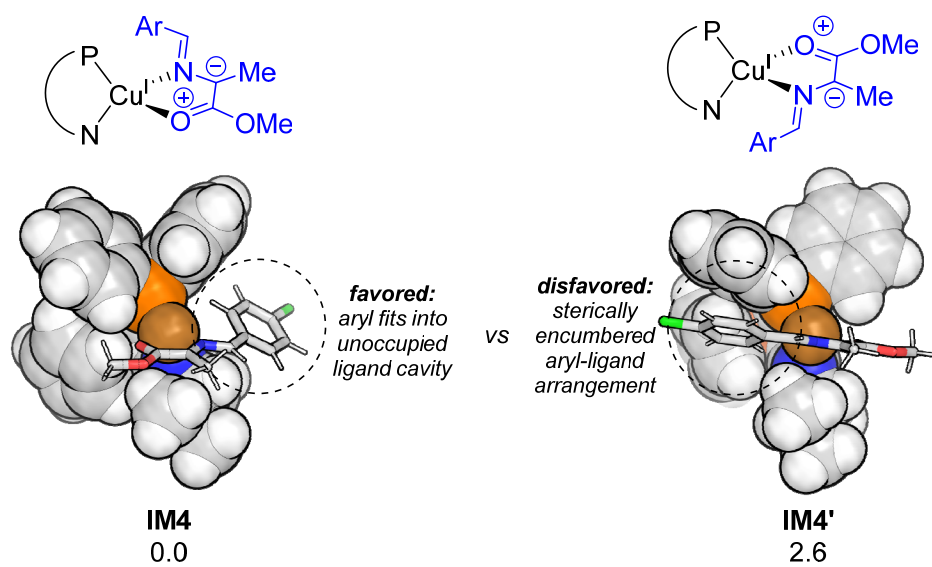


Fig. S1 Diastereomers of Cu-AMY species (ligand: (*S,S*)-L1). Relative free energies are given in kcal/mol.

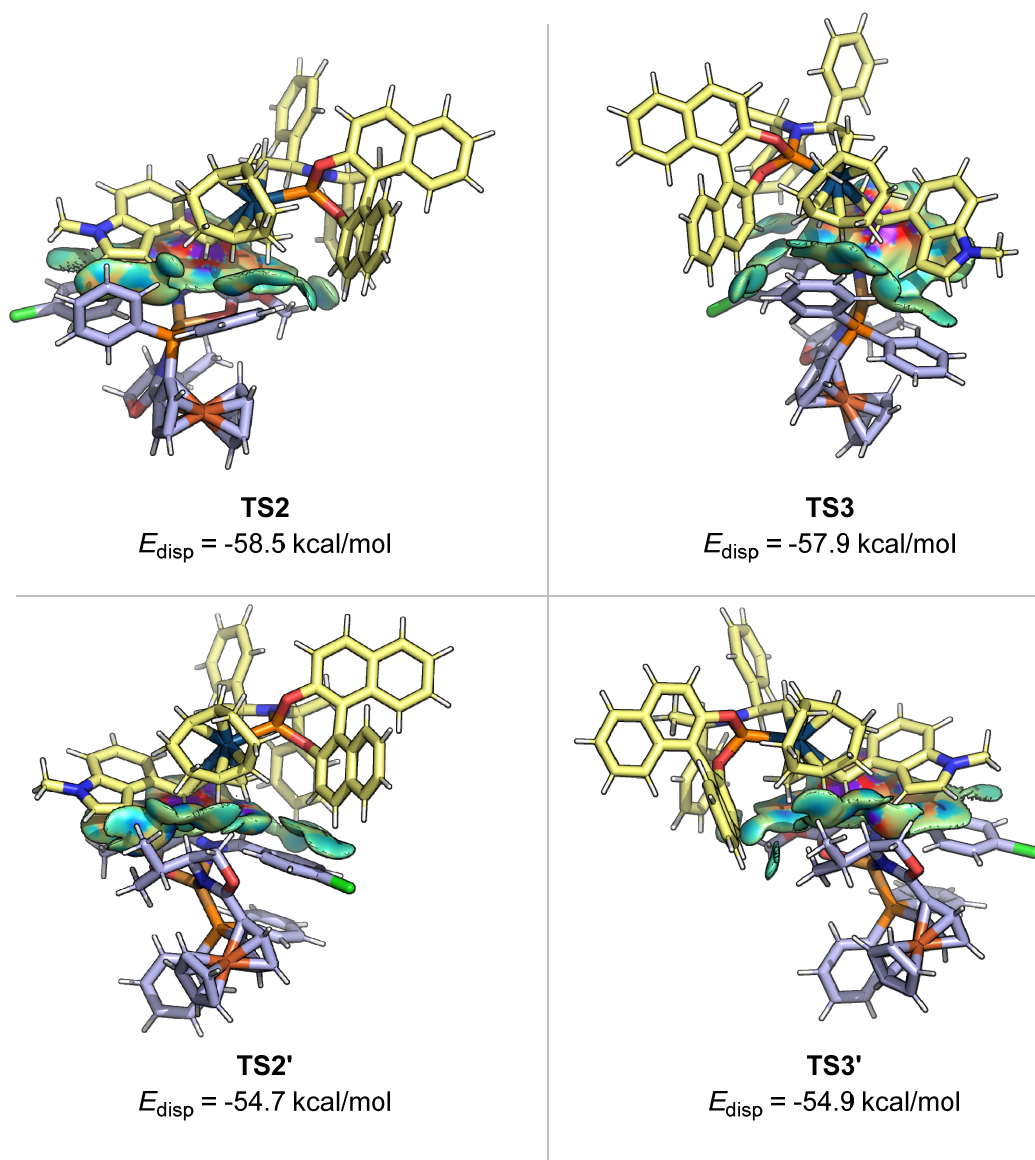


Fig. S2 Non-covalent interaction plots for bond-forming transition states in Cu/Ir dual catalysis. Dispersion interaction energies are provided alongside.

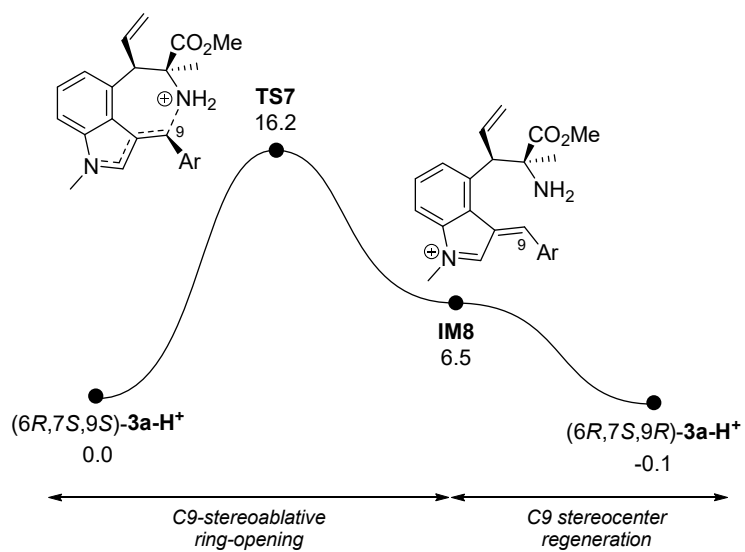


Fig. S3 Free-energy profile for the TFA-promoted C9-epimerization of (6R,7S,9S)-**3a** (kcal/mol).

Electronic Energies, Enthalpies and Free Energies of Optimized Structures

	E_{gas} (a.u.)	E_{DCE} (a.u.)	H_{DCE} (a.u.)	G_{DCE} (a.u.)	ν_{imag} (cm^{-1})
2a	-822.835283	-823.157936	-822.871871	-822.934821	
$^{-}\text{OCO}_2\text{Me}$	-303.701032	-303.917754	-303.857811	-303.888852	
IM1	-2352.170326	-2352.938258	-2352.154749	-2352.266783	
IM2a	-3175.049332	-3176.122615	-3175.049232	-3175.195855	
IM2b	-3175.030447	-3176.109773	-3175.037358	-3175.18638	
TS1a	-3175.011647	-3176.101278	-3175.030509	-3175.179049	-154.01
TS1b	-3175.007779	-3176.096823	-3175.025758	-3175.174282	-170.08
IM3a	-2871.192734	-2872.186196	-2871.176668	-2871.311268	
IM3b	-2871.185382	-2872.179776	-2871.17038	-2871.306668	
IM4	-2967.547282	-5551.157434	-5550.415977	-5550.538326	
IM4'	-2967.538643	-5551.15148	-5550.410095	-5550.534242	
TS2	-5838.777487	-8423.354292	-8421.601883	-8421.831105	-341.69
TS2'	-5838.769827	-8423.347516	-8421.595799	-8421.823669	-344.49
TS3	-5838.776810	-8423.354241	-8421.60234	-8421.832724	-327.84
TS3'	-5838.768257	-8423.345466	-8421.593456	-8421.822427	-324.94
$\text{Zn}(\text{OTf})_2$	-2149.942748	-3702.750861	-3702.674013	-3702.738374	
^{-}OTf	-961.447160	-961.828725	-961.793161	-961.830549	
IM5	-1610.261600	-1610.722229	-1610.282117	-1610.36147	
IM6	-1610.256951	-1610.719838	-1610.280322	-1610.362051	
TS4	-2798.602034	-4351.625821	-4351.144631	-4351.247034	-264.28
TS4'	-2798.621165	-4351.637428	-4351.156034	-4351.256732	-213.73
TS5	-2798.625269	-4351.641454	-4351.160003	-4351.261702	-181.27
TS5'	-2798.593802	-4351.622007	-4351.1406	-4351.242732	-277.78
(6<i>S</i>,7<i>S</i>,9<i>R</i>)-3a	-1610.256045	-1610.725308	-1610.282722	-1610.362064	
(6<i>S</i>,7<i>S</i>,9<i>S</i>)-3a	-1610.255654	-1610.723917	-1610.281764	-1610.360066	
(6<i>R</i>,7<i>S</i>,9<i>S</i>)-3a	-1610.258951	-1610.727453	-1610.285031	-1610.363924	
(6<i>R</i>,7<i>S</i>,9<i>R</i>)-3a	-1610.254040	-1610.722868	-1610.279997	-1610.357554	

	E_{low} (a.u.)	$E_{\text{DCM,high}}$ (a.u.)	$H_{\text{DCM,high}}$ (a.u.)	$G_{\text{DCM,high}}$ (a.u.)	ν_{imag} (cm^{-1})
(6<i>S</i>,7<i>S</i>,9<i>R</i>)-3a-H⁺	-1610.649720	-1611.177946	-1610.720707	-1610.799924	
(6<i>S</i>,7<i>S</i>,9<i>S</i>)-3a-H⁺	-1610.655455	-1611.182585	-1610.725232	-1610.804146	
(6<i>R</i>,7<i>S</i>,9<i>S</i>)-3a-H⁺	-1610.656875	-1611.183643	-1610.726107	-1610.803521	
(6<i>R</i>,7<i>S</i>,9<i>R</i>)-3a-H⁺	-1610.654655	-1611.181322	-1610.724193	-1610.803646	
TS6	-1610.644690	-1611.154845	-1610.701173	-1610.781756	-53.75
TS7	-1610.637868	-1611.152762	-1610.698957	-1610.777696	-45.08
IM7	-1610.649281	-1611.162430	-1610.707567	-1610.788087	
IM8	-1610.653378	-1611.166037	-1610.711714	-1610.793108	

Cartesian Coordinates of Optimized Structures

2a

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-2.52069700	-0.09362900	-0.83597800
H	-2.95656500	0.25718300	-1.78214800
H	-2.41542000	-1.18370300	-0.91243000
C	-1.23528600	0.56953900	-0.52206200
H	-1.28690800	1.64355300	-0.33465100
C	-0.06091300	-0.07978300	-0.49644100
H	-0.08224100	-1.16062000	-0.66334200
O	-3.45899300	0.22073000	0.22138100
C	-4.70577300	-0.19803100	-0.02243700
O	-5.08902900	-0.79431900	-1.00421600
O	-5.46115000	0.16273400	1.02650000
C	-6.82880000	-0.22591200	0.90429900
H	-7.29320400	0.25282400	0.03617500
H	-7.30826100	0.10744400	1.82558200
H	-6.91613500	-1.31145100	0.79644500
C	1.25888300	0.49148900	-0.27063500
C	2.37414100	-0.36301000	-0.10230200
C	1.49421300	1.86906200	-0.21130000
C	3.65838400	0.20153100	0.12275200
C	2.54257500	-1.78057500	-0.09730400
C	2.76870100	2.39884200	0.01436100
H	0.66260000	2.55663900	-0.35739700
C	3.87594200	1.57574500	0.18569600
C	3.87287000	-2.02350000	0.11883300
H	1.78092400	-2.53870700	-0.23048600
H	2.89554100	3.47918100	0.04919100
H	4.86815400	1.99093600	0.35561700
H	4.41299900	-2.96052100	0.19292500
N	4.55676400	-0.83450500	0.25412200
C	5.96874800	-0.68368300	0.48701700
H	6.15906200	-0.14120500	1.42191000
H	6.45061000	-0.13884100	-0.33493800
H	6.42694400	-1.67284800	0.56237400

⁻OCO₂Me

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
O	-1.68463600	-0.62501300	-0.00010200
C	-0.66730300	0.07497400	0.00010200
O	-0.45388400	1.29874000	0.00001300

O	0.55476500	-0.76524100	0.00012900
C	1.73630300	-0.03499100	-0.00008400
H	2.57336300	-0.75537100	-0.00052900
H	1.84103600	0.62401800	-0.88134500
H	1.84164900	0.62357700	0.88145100

IM1

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Ir	-1.60521600	-1.76923200	0.54933100
O	0.77666400	0.12101600	-1.19956300
O	0.80632300	0.23115500	1.35659800
C	1.93107900	-0.64375100	-1.17621700
C	2.01632600	-1.71859600	-2.08223000
H	1.18959100	-1.88047700	-2.77030700
C	3.13073600	-2.51823900	-2.08913600
H	3.20762800	-3.34980200	-2.78878500
C	4.18569400	-2.29282800	-1.17301300
C	5.30854800	-3.15265200	-1.11276600
H	5.35213500	-3.99632500	-1.80157800
C	6.31366700	-2.94298200	-0.19932100
H	7.16814000	-3.61595700	-0.15972600
C	6.22917200	-1.85916400	0.69835000
H	7.01371100	-1.70767900	1.43749700
C	5.15992700	-0.99512400	0.65461000
H	5.10211500	-0.16864600	1.35957900
C	4.11291800	-1.17229200	-0.28410100
C	2.98026700	-0.29661600	-0.34006400
C	2.90289200	0.94538000	0.45614000
C	3.89703300	1.97202700	0.35163000
C	4.96746300	1.90692700	-0.57562100
H	5.04155700	1.04741400	-1.23729700
C	5.89759000	2.91617400	-0.66207300
H	6.70368300	2.84252000	-1.38988900
C	5.81235200	4.04694000	0.17491800
H	6.55718400	4.83686400	0.09960000
C	4.77679000	4.15307300	1.07151900
H	4.68598500	5.02974900	1.71294000
C	3.79346700	3.13969600	1.17660200
C	2.69662400	3.26457400	2.06277400
H	2.63093900	4.14874600	2.69609100
C	1.71482000	2.30804100	2.10446200
H	0.85157200	2.40262300	2.75899400

C	1.81324100	1.16629300	1.28276000	H	-0.31540400	-5.40363500	1.71113400
P	-0.27281600	-0.03075300	0.09058300	H	-0.47163100	-4.01008300	2.76726000
N	-1.21401400	1.32712300	-0.13668100	C	-0.24490500	-3.47544900	0.73274800
C	-2.79259400	-0.12458800	1.15364700	H	0.76234300	-3.09675500	0.93336300
H	-2.50390200	0.06785200	2.20286800	C	-0.69521900	-3.42762400	-0.60148700
H	-3.86802600	-0.35926100	1.18136600	H	-0.01159700	-2.99082200	-1.32792900
C	-2.61886800	1.16706200	0.34984900	C	-1.73336200	-4.36114500	-1.19090800
H	-3.25895100	1.11357900	-0.54651200	H	-1.47338500	-4.57605800	-2.23533900
C	-3.02762800	2.38147200	1.15271300	H	-1.70139800	-5.33187500	-0.67989400
C	-2.28598000	2.75155800	2.27983100	C	-3.15073300	-3.77197300	-1.14623400
H	-1.40872200	2.15879400	2.54540300	H	-3.90311500	-4.57580300	-1.21989900
C	-2.65453200	3.85054700	3.04461100	H	-3.30475800	-3.13487300	-2.02749000
H	-2.06626000	4.12745300	3.91854400				
C	-3.78022600	4.59779600	2.69551300				
H	-4.07199300	5.45897700	3.29416200				
C	-4.52634500	4.23763900	1.57767000				
H	-5.40449300	4.81770300	1.29777100				
C	-4.14750400	3.13800300	0.80796000				
H	-4.72181500	2.86347300	-0.07834800				
C	-1.02841300	2.55081900	-0.95036400				
H	-1.44600300	3.35928000	-0.33017400				
C	-1.86613800	2.48636100	-2.21425000				
C	-2.63516900	3.58983000	-2.58735100				
H	-2.64921200	4.46932300	-1.94094800				
C	-3.38835100	3.57159800	-3.75850300				
H	-3.98645600	4.43913300	-4.03288900				
C	-3.38467700	2.43994400	-4.56906100				
H	-3.97743900	2.41870400	-5.48199000				
C	-2.62471900	1.33061200	-4.20117200				
H	-2.62235300	0.44047800	-4.82863400				
C	-1.87065000	1.35291100	-3.03210400				
H	-1.28717900	0.47983000	-2.73745500				
C	0.40196000	2.96405500	-1.26784300				
H	1.01510000	3.02130800	-0.36348200				
H	0.88856600	2.29818200	-1.98334400				
H	0.36582400	3.96614500	-1.71103300				
C	-3.40847100	-2.92972400	0.07247300				
H	-4.20923700	-2.19630000	-0.04040500				
C	-3.00904200	-3.25414000	1.37868500				
H	-3.51044200	-2.71666500	2.18722200				
C	-2.31338000	-4.53954800	1.77319300				
H	-2.65632100	-4.83800400	2.77184400				
H	-2.62417500	-5.35167400	1.10371400				
C	-0.78128000	-4.40664200	1.79070000				

IM2a

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Ir	-1.14336700	-0.55771800	1.18563700
O	1.81930100	-0.37914700	-0.80130100
O	1.81743100	0.82691000	1.43968800
C	2.81909700	-1.20991600	-0.32479300
C	2.71452300	-2.58267300	-0.62818800
H	1.87617400	-2.93018700	-1.23216800
C	3.68082100	-3.44657600	-0.17910000
H	3.61620100	-4.50848000	-0.41322200
C	4.76113200	-2.98222900	0.60849400
C	5.72179000	-3.87529500	1.14104300
H	5.62167100	-4.93681100	0.91473300
C	6.74679200	-3.42322400	1.93637100
H	7.47382800	-4.12233400	2.34496300
C	6.84466800	-2.04950700	2.23663000
H	7.64147700	-1.69434000	2.88778600
C	5.93759300	-1.15248500	1.72162900
H	6.01986800	-0.09764900	1.97262400
C	4.87860500	-1.58034200	0.88216000
C	3.90915600	-0.67159600	0.34442500
C	4.02365700	0.79352000	0.52213200
C	5.17346900	1.53738300	0.09956100
C	6.24522000	0.94711900	-0.61637500
H	6.19914900	-0.11203100	-0.85889000
C	7.33023800	1.69229900	-1.01696200
H	8.13576500	1.21312500	-1.57039200
C	7.40578100	3.06885500	-0.72345500
H	8.27248300	3.64606000	-1.03955700
C	6.37487800	3.67871600	-0.05016500
H	6.40981200	4.74573000	0.16976000

C	5.23761600	2.94550400	0.36486100	H	-0.19891300	0.99468800	3.20247800
C	4.15787300	3.58054500	1.02484800	C	0.42591400	-1.02253200	3.84485400
H	4.22551100	4.64671600	1.23987200	H	1.25668400	-0.46246100	4.29133700
C	3.03426600	2.87205700	1.36664700	H	-0.07419100	-1.52491800	4.68562800
H	2.18285700	3.33770100	1.85914100	C	0.99699800	-2.05297400	2.86409400
C	2.97126300	1.49348100	1.08732100	H	1.31428600	-2.96656700	3.39601100
P	0.74692500	0.34481600	0.24565500	H	1.90740500	-1.64306300	2.40582500
N	0.33968000	1.67141200	-0.69667200	C	0.03929500	-2.42066000	1.75756500
C	-1.58373700	1.51861100	0.86372500	H	0.50623500	-2.82496100	0.85614100
H	-1.18936600	2.08933500	1.72140500	C	-1.32161700	-2.68624700	1.95268700
H	-2.67340500	1.65165200	0.86744800	H	-1.81514300	-3.26631900	1.17155800
C	-1.04065600	2.13221600	-0.42397400	C	-1.98581800	-2.77351400	3.31668600
H	-1.67854600	1.78204600	-1.24849800	H	-2.76362900	-3.54751600	3.26923300
C	-1.14285800	3.64042600	-0.38577600	H	-1.25552600	-3.14913500	4.04662300
C	-0.05253900	4.46325300	-0.09375400	C	-2.60562200	-1.45448500	3.79318300
H	0.92734000	4.00850400	0.05543000	H	-2.56141200	-1.39046200	4.89500700
C	-0.20677900	5.84517300	-0.01933500	H	-3.67100000	-1.43254300	3.53686300
H	0.65512900	6.47273800	0.20421300	C	-1.06849100	-2.28973400	-1.38326100
C	-1.45399100	6.42462300	-0.23639300	H	-0.03117000	-2.06249300	-1.65457300
H	-1.57381000	7.50529400	-0.18125200	H	-1.06635200	-3.13408500	-0.68310700
C	-2.54681100	5.61177500	-0.53257700	C	-1.75904200	-1.08336900	-0.85223400
H	-3.52557200	6.05594400	-0.70786500	H	-1.66632700	-0.23984300	-1.54396600
C	-2.39062100	4.23193900	-0.60963100	C	-2.95317500	-1.15357700	-0.06970900
H	-3.24609200	3.59047100	-0.83455000	H	-3.23643700	-2.14620300	0.28639200
C	0.82831200	2.03604900	-2.06654100	O	-1.74619000	-2.73476100	-2.59337800
H	0.41773900	3.04827100	-2.19632900	C	-0.99810900	-3.50897900	-3.37376200
C	0.17738800	1.17670100	-3.13479500	O	0.12781600	-3.90748500	-3.15101900
C	-1.04879700	1.59135000	-3.67161200	O	-1.70997800	-3.77895100	-4.48276800
H	-1.46984000	2.54708200	-3.35200900	C	-1.02383600	-4.61043200	-5.41461700
C	-1.73280100	0.81214300	-4.60114300	H	-0.12381000	-4.11303500	-5.79346300
H	-2.69362200	1.14868200	-4.98750200	H	-1.73136800	-4.78312000	-6.22671400
C	-1.18432000	-0.39062800	-5.03435300	H	-0.73027000	-5.55819500	-4.95245500
H	-1.71861500	-1.01659000	-5.74712400	C	-4.09784500	-0.24845500	-0.20058000
C	0.05566700	-0.79407500	-4.54273400	C	-5.21219600	-0.41353900	0.65726100
H	0.50385000	-1.72623900	-4.88516900	C	-4.18903500	0.77238500	-1.15340800
C	0.72786900	-0.02393500	-3.59790200	C	-6.31639100	0.47014300	0.56289700
H	1.68690300	-0.36537900	-3.21435000	C	-5.53365600	-1.36309800	1.67421700
C	2.33354000	2.18158200	-2.19324500	C	-5.29537000	1.63310500	-1.22874200
H	2.72720600	2.83235100	-1.40324800	H	-3.39581300	0.88442600	-1.89195000
H	2.87299000	1.23252200	-2.15362500	C	-6.37470100	1.51111400	-0.36491100
H	2.55729200	2.65033700	-3.15881600	C	-6.77344100	-1.03331100	2.15548800
C	-1.95641900	-0.24182500	3.17447700	H	-4.93608200	-2.20828000	1.99340000
H	-2.57987400	0.65666300	3.18724100	H	-5.30942600	2.40558200	-1.99722900
C	-0.53891000	-0.04296100	3.19150300	H	-7.23257700	2.17870900	-0.42693300

H	-7.37864300	-1.50088500	2.92376500	P	0.60916500	0.36970200	0.25833600
N	-7.25186600	0.07955200	1.49656100	N	-0.22232700	1.50174200	-0.67082900
C	-8.52243100	0.71816600	1.71013000	C	-1.76134600	1.13230200	1.23305300
H	-9.14259600	0.68169900	0.80487100	H	-1.42788500	1.89728900	1.95318800
H	-8.39237000	1.76945100	1.99751000	H	-2.83553400	0.97888900	1.41798500
H	-9.05288400	0.20276700	2.51463900	C	-1.60360700	1.70510900	-0.18216800
IM2b				H	-2.29577400	1.16143100	-0.85098700
Atomic				C	-1.99803100	3.16548700	-0.20725900
Coordinates (Angstroms)				C	-1.05841100	4.18881900	-0.05563000
Type	X	Y	Z	H	-0.00191800	3.92666400	0.01594400
Ir	-0.75875900	-0.70742700	1.68587600	C	-1.45929100	5.52078100	-0.01233900
O	1.68628800	-0.11483500	-0.92683800	H	-0.71283500	6.30605400	0.10079700
O	1.71804600	1.17498900	1.25099500	C	-2.80844700	5.85093800	-0.11741300
C	2.83176600	-0.78697600	-0.54844900	H	-3.12218700	6.89299800	-0.08643600
C	2.88461000	-2.17174900	-0.80226200	C	-3.75229900	4.83723900	-0.27049300
H	2.04558000	-2.65057200	-1.30662200	H	-4.81009900	5.08472000	-0.35986500
C	4.00414000	-2.87651800	-0.43871800	C	-3.34928000	3.50655000	-0.31850400
H	4.06481100	-3.94631100	-0.63713600	H	-4.08492000	2.71038800	-0.44311500
C	5.08567400	-2.23707700	0.21351100	C	0.01824000	1.89374600	-2.09191500
C	6.21562000	-2.96767100	0.65309000	H	-0.69548800	2.71823300	-2.23666900
H	6.24091800	-4.04124500	0.46560200	C	-0.39938000	0.79758500	-3.05806400
C	7.25143900	-2.34751800	1.30964600	C	-1.74072700	0.72836100	-3.45343200
H	8.11199200	-2.92333200	1.64515200	H	-2.43018600	1.50350000	-3.11137800
C	7.19005600	-0.96155700	1.55991600	C	-2.20273800	-0.30230200	-4.26899400
H	7.99980800	-0.47339600	2.09935600	H	-3.25301300	-0.34045500	-4.55760500
C	6.11305400	-0.21897600	1.13419200	C	-1.31988500	-1.27825200	-4.72459600
H	6.07551200	0.84802200	1.34244000	H	-1.67767100	-2.09433800	-5.35105400
C	5.03535400	-0.82158500	0.43730600	C	0.02891200	-1.19025800	-4.38614700
C	3.89557000	-0.07794400	-0.01109900	H	0.73593400	-1.93422300	-4.74993300
C	3.80710200	1.39420200	0.10063100	C	0.48514700	-0.16146200	-3.56595900
C	4.78569200	2.26869000	-0.47593700	H	1.53875000	-0.11522000	-3.30353500
C	5.85080200	1.79583800	-1.28338300	C	1.39443700	2.47875000	-2.35679100
H	5.93318600	0.72874900	-1.47662700	H	1.60635000	3.29381700	-1.65523100
C	6.76715200	2.66169900	-1.83456500	H	2.20014100	1.74571900	-2.27126300
H	7.56932200	2.27023000	-2.45797300	H	1.41845100	2.88933700	-3.37335600
C	6.67247400	4.04961400	-1.60741200	C	-1.91575400	-0.86543600	3.49070800
H	7.40675200	4.72437500	-2.04337300	H	-2.85462300	-0.30567900	3.41999200
C	5.64053500	4.54503400	-0.84754300	C	-0.72351200	-0.08515400	3.70651200
H	5.54111500	5.61742900	-0.67842400	H	-0.85170900	1.00063200	3.73477300
C	4.67141800	3.68415600	-0.27939700	C	0.46078800	-0.59200500	4.51447500
C	3.58087800	4.19562400	0.46412300	H	0.90208400	0.24123300	5.07517800
H	3.51349300	5.27104500	0.62764600	H	0.10983000	-1.30486400	5.27400800
C	2.60998500	3.35645700	0.94720800	C	1.53636400	-1.22573900	3.62683800
H	1.75238400	3.72663500	1.50592000	H	2.15402900	-1.93388000	4.20487600
C	2.71506900	1.96565800	0.73684300				

H	2.21807000	-0.44183800	3.27255200
C	0.97362200	-1.91043900	2.40903200
H	1.69703500	-2.05206600	1.60288800
C	-0.15508300	-2.74915400	2.40056900
H	-0.21973800	-3.45072300	1.56572400
C	-0.88671600	-3.17886900	3.66167000
H	-1.24581100	-4.20734200	3.52590900
H	-0.16869500	-3.23406300	4.49181500
C	-2.06593000	-2.26804700	4.03301800
H	-2.20915500	-2.26052900	5.12844400
H	-2.99361100	-2.69857500	3.62782300
C	-0.88248300	-2.70685000	-1.05865900
H	-0.50708400	-1.83204600	-1.60925900
H	-0.04592000	-3.13252600	-0.49067800
C	-2.05283300	-2.36786500	-0.20630500
H	-2.28732900	-3.03709900	0.62301400
C	-2.91712300	-1.39367300	-0.57826900
H	-2.66749500	-0.84821200	-1.49442700
O	-1.32117700	-3.69358500	-2.03942600
C	-0.34601700	-4.16715300	-2.81158100
O	0.84199100	-3.93400600	-2.71740300
O	-0.90835000	-4.96616900	-3.73257800
C	0.02868600	-5.54515200	-4.63809700
H	0.52838300	-4.76952100	-5.22863100
H	-0.55838900	-6.19609300	-5.28688600
H	0.78859500	-6.12080400	-4.10083600
C	-4.14351000	-0.98015900	0.07732100
C	-5.00630700	-0.05941700	-0.56280500
C	-4.49570400	-1.39870600	1.36371000
C	-6.14539700	0.42840500	0.13205600
C	-5.01505800	0.55477300	-1.85012400
C	-5.62710200	-0.91152800	2.02305300
H	-3.83335300	-2.08605100	1.88614000
C	-6.46824000	0.02195300	1.42449700
C	-6.11138300	1.37642500	-1.89348700
H	-4.30856300	0.39413100	-2.65434800
H	-5.83951900	-1.25488700	3.03431100
H	-7.33774400	0.41614300	1.94812200
H	-6.47591800	2.02014000	-2.68590200
N	-6.79863500	1.31227500	-0.70084800
C	-7.98767300	2.04778500	-0.35941000
H	-7.80173800	2.73656800	0.47481400
H	-8.80057600	1.36798600	-0.07541500
H	-8.31067100	2.62988700	-1.22583300

TS1a			
Atomic	Coordinates (Angstroms)		
Type	X	Y	Z
Ir	-1.14031000	-0.91190600	0.62993000
O	1.93492800	0.12304700	-0.84570700
O	1.73850500	0.19788300	1.68550200
C	2.80503400	-0.95988300	-0.75570900
C	2.61800800	-1.99266800	-1.69194800
H	1.85675000	-1.86908500	-2.46978300
C	3.44826800	-3.08317900	-1.63469600
H	3.33579000	-3.89132000	-2.35683000
C	4.45334600	-3.18733200	-0.64286600
C	5.26594000	-4.34160800	-0.54328100
H	5.10589000	-5.14738500	-1.25947300
C	6.22662600	-4.45244000	0.43276700
H	6.84261400	-5.34726800	0.49821400
C	6.40395400	-3.40592600	1.36021500
H	7.14871900	-3.50337400	2.14807700
C	5.64120900	-2.26292400	1.28323700
H	5.78475000	-1.46823800	2.01216900
C	4.65666200	-2.10523600	0.27607500
C	3.83574700	-0.93326000	0.17085400
C	4.04207900	0.26915300	1.00920200
C	5.29401100	0.96985100	1.05417900
C	6.39719600	0.61767700	0.23618900
H	6.29644500	-0.21130600	-0.46012400
C	7.58094800	1.31591000	0.29739000
H	8.40792000	1.02789800	-0.34897000
C	7.73049100	2.40437800	1.18018300
H	8.67433500	2.94461900	1.22290900
C	6.67424400	2.79030500	1.96878600
H	6.76507600	3.64383200	2.64057100
C	5.43674000	2.10469900	1.91930400
C	4.33377900	2.53682200	2.69321400
H	4.45775100	3.39287000	3.35559500
C	3.12106400	1.90606100	2.59044500
H	2.25201000	2.22817900	3.16050800
C	2.98611200	0.79494400	1.73722600
P	0.79287900	0.33600000	0.31643400
N	0.38245400	1.92395300	0.01350600
C	-1.64490600	1.10270700	1.14653500
H	-1.33298800	1.26576000	2.19045200
H	-2.73712300	1.19401000	1.13108900
C	-1.04363300	2.20677300	0.28925000

H	-1.56908200	2.24695300	-0.68019900	H	-2.76619600	-4.50472200	1.37717500
C	-1.24981100	3.54250000	0.96516900	H	-1.33648800	-4.36194800	2.36567200
C	-0.41931100	3.97021000	2.00442200	C	-2.74899000	-2.71632900	2.58705300
H	0.44381800	3.35771300	2.27188800	H	-2.84749800	-3.05710100	3.63240100
C	-0.67507300	5.16503200	2.66842300	H	-3.77366600	-2.58827600	2.21722400
H	-0.01639100	5.49100100	3.47214700	C	-1.02094300	-1.20205800	-1.81687600
C	-1.77141300	5.94602200	2.30555600	H	-0.15095600	-0.71388500	-2.24392900
H	-1.97218800	6.88120900	2.82538300	H	-1.00763000	-2.28443700	-1.82167400
C	-2.60167500	5.52986200	1.26826300	C	-2.13200500	-0.47849900	-1.36168100
H	-3.45380600	6.13951800	0.97243000	H	-2.16833700	0.58643100	-1.59108700
C	-2.33746800	4.33748200	0.59998900	C	-3.17604800	-1.08022700	-0.61438000
H	-2.97419200	4.01711700	-0.22697600	H	-3.26533300	-2.16273300	-0.69364300
C	1.01682000	2.95684000	-0.87216300	O	-1.39121900	-1.54603900	-4.01721200
H	0.79158100	3.89891600	-0.34941700	C	-0.29550700	-1.31843100	-4.58988100
C	0.29643200	3.00598300	-2.20516200	O	0.84448400	-1.14621400	-4.10676000
C	-0.50542500	4.10911700	-2.51004200	O	-0.43432400	-1.22697600	-5.97520300
H	-0.56934100	4.93340200	-1.79696000	C	0.77751800	-1.04168000	-6.67799600
C	-1.23333100	4.15545400	-3.69692300	H	1.28003200	-0.10721900	-6.39326000
H	-1.85672500	5.02090400	-3.91765300	H	0.51010500	-1.00920100	-7.73889000
C	-1.16897800	3.09069700	-4.59073700	H	1.48237800	-1.86369300	-6.49834600
H	-1.74673400	3.11383400	-5.51312800	C	-4.40395600	-0.40436000	-0.21416900
C	-0.36554700	1.98888500	-4.30096000	C	-5.47459100	-1.16373400	0.31900600
H	-0.31482100	1.15204500	-4.99479000	C	-4.61087400	0.97468400	-0.34932600
C	0.36685900	1.94674100	-3.11737200	C	-6.66832800	-0.50772400	0.71794300
H	0.98608900	1.07153800	-2.91768000	C	-5.67794400	-2.55832400	0.54797500
C	2.52825400	2.89614400	-1.00478300	C	-5.79882900	1.59708800	0.05367900
H	3.01609000	2.80387700	-0.02766000	H	-3.83230400	1.58918900	-0.80036800
H	2.87068300	2.08361000	-1.64870700	C	-6.84650300	0.87051600	0.60402000
H	2.85779500	3.83903600	-1.45558000	C	-6.93896300	-2.69960200	1.06563900
C	-2.07161700	-1.37195300	2.55174900	H	-4.99284100	-3.37059600	0.33441700
H	-2.71903500	-0.53433800	2.82381200	H	-5.90105000	2.67328000	-0.07251200
C	-0.67097800	-1.18965600	2.73515400	H	-7.76963100	1.35626500	0.91590500
H	-0.35973600	-0.22267700	3.13175100	H	-7.47878000	-3.58967700	1.36729600
C	0.28856700	-2.32643900	3.04941300	N	-7.54433100	-1.46738300	1.17683100
H	1.07313400	-1.94772600	3.71485900	C	-8.87193800	-1.20969500	1.66909900
H	-0.24359600	-3.09652500	3.62501800	H	-9.34919600	-2.15822400	1.92685400
C	0.94572400	-2.93558800	1.80665800	H	-9.48252700	-0.70942400	0.90713400
H	1.23999500	-3.98178500	1.99482400	H	-8.84720900	-0.57740100	2.56574000
H	1.87759300	-2.39994000	1.58986300				
C	0.07609400	-2.87926600	0.57969000	TS1b			
H	0.60927300	-2.89386000	-0.37205000	Atomic	Coordinates (Angstroms)		
C	-1.27931400	-3.20942800	0.56018800	Type	X	Y	Z
H	-1.70039100	-3.45605900	-0.41491300	Ir	-1.36619700	-0.66938400	0.35500900
C	-2.03149800	-3.77782300	1.74761500	O	1.92144900	0.14103600	-0.82743200
				O	1.60310700	-0.31171500	1.65271000

C	2.56069900	-1.08313000	-0.99354100	C	-0.98856200	5.66199900	3.47317700
C	2.23212200	-1.81544100	-2.14994700	H	-1.06043900	6.47400500	4.19469000
H	1.54758500	-1.36933800	-2.87513100	C	-1.65107000	5.75014100	2.25231600
C	2.82967200	-3.03504500	-2.34735100	H	-2.24116000	6.63309800	2.01287700
H	2.60121200	-3.61513200	-3.24090900	C	-1.55004400	4.71373900	1.32694900
C	3.73478700	-3.56921700	-1.39827800	H	-2.04725800	4.79042200	0.35900300
C	4.29913400	-4.85685500	-1.56406800	C	1.57442200	3.03802800	0.00301100
H	4.02938200	-5.42791100	-2.45227200	H	1.50587500	3.75621500	0.83416500
C	5.15658600	-5.38300800	-0.62780400	C	1.07081600	3.74434200	-1.23946100
H	5.58000200	-6.37583500	-0.76748200	C	0.77931500	5.10885900	-1.17703900
C	5.47554700	-4.63737400	0.52463000	H	0.90154400	5.63669100	-0.22920800
H	6.13591900	-5.06285600	1.27820200	C	0.33233700	5.79130300	-2.30537000
C	4.95557400	-3.37694600	0.71019400	H	0.10936600	6.85569600	-2.24273000
H	5.20498100	-2.81827000	1.60952000	C	0.16071400	5.10741100	-3.50530500
C	4.08739600	-2.79359100	-0.24649500	H	-0.20163300	5.63346300	-4.38710300
C	3.52064100	-1.48584900	-0.07845000	C	0.44514800	3.74463800	-3.57864100
C	3.90990300	-0.59359000	1.03574500	H	0.28931200	3.20390100	-4.51032600
C	5.27453200	-0.21627300	1.27059100	C	0.90450500	3.06685600	-2.45180300
C	6.32681600	-0.57374300	0.39025700	H	1.13178000	2.00128800	-2.52499900
H	6.09536000	-1.14755800	-0.50370800	C	3.04405500	2.67600700	-0.12725100
C	7.62488200	-0.19362800	0.64041600	H	3.43224100	2.18555300	0.77034200
H	8.41060200	-0.47519300	-0.05831800	H	3.25552000	2.05002600	-0.99641600
C	7.94598700	0.56291800	1.78550500	H	3.59356800	3.61589500	-0.25386100
H	8.97816900	0.85032500	1.97601800	C	-2.43783300	-1.31213200	2.15246000
C	6.94831000	0.94940400	2.64667200	H	-3.00329900	-0.46205800	2.54467200
H	7.17620200	1.55296700	3.52507400	C	-1.03106100	-1.30778700	2.39550500
C	5.59964400	0.59049100	2.41022900	H	-0.65051900	-0.45050800	2.95464000
C	4.56550600	1.03162900	3.26917600	C	-0.18913000	-2.56553100	2.56211800
H	4.82425100	1.63251600	4.14019800	H	0.63436300	-2.33773700	3.24866500
C	3.25617300	0.73594000	2.99176300	H	-0.79152100	-3.33239200	3.06914300
H	2.44028200	1.08827700	3.61913300	C	0.40564600	-3.11847200	1.25629900
C	2.94203600	-0.05121100	1.86688200	H	0.50325500	-4.21524300	1.31616000
P	0.76596600	0.28896500	0.33706300	H	1.42423900	-2.73718100	1.13136200
N	0.63170600	1.94360600	0.40615500	C	-0.39404400	-2.77088300	0.02730000
C	-1.65563300	1.30588100	1.12721700	H	0.16094500	-2.70647400	-0.91033100
H	-1.53122500	1.22549200	2.21823800	C	-1.77001000	-2.94897700	-0.03792700
H	-2.69529500	1.61689100	0.96653600	H	-2.22397900	-2.98413200	-1.02515200
C	-0.75009500	2.42943500	0.62955700	C	-2.58790200	-3.58864200	1.06069800
H	-1.12193000	2.81472300	-0.33492700	H	-3.36141700	-4.21179900	0.59510000
C	-0.79591800	3.57636100	1.61456600	H	-1.94743900	-4.27519100	1.62976500
C	-0.13612600	3.49457200	2.84502600	C	-3.25212500	-2.56814300	1.98438800
H	0.46517500	2.60900100	3.06216700	H	-3.45268800	-3.01317100	2.97411300
C	-0.22738100	4.53078400	3.76699300	H	-4.23152700	-2.29568800	1.57555800
H	0.29802200	4.45943000	4.71827500	C	-1.13640700	0.36349900	-1.93189600

H	-1.25764500	1.40925100	-1.66730200	H	3.23933600	-4.14031600	-2.82920700
H	-0.20765200	0.05447700	-2.40372800	C	4.33841900	-3.53868000	-1.06449700
C	-2.18425700	-0.54465200	-1.75151000	C	5.13082400	-4.71011000	-1.00972800
H	-2.10262500	-1.50311200	-2.26352100	H	4.97984000	-5.47414600	-1.77129800
C	-3.28819300	-0.26364100	-0.90547100	C	6.06318100	-4.88736200	-0.01644800
H	-3.43099800	0.78926500	-0.65861600	H	6.66565400	-5.79236100	0.01537500
O	-1.32821000	1.04922200	-4.09653000	C	6.22773300	-3.89740800	0.97295200
C	-0.25406600	0.68865800	-4.64182600	H	6.94881800	-4.04963700	1.77339800
O	0.67389600	-0.02304200	-4.20008000	C	5.48406800	-2.74011600	0.94075500
O	-0.11105000	1.21646300	-5.92626300	H	5.62076300	-1.99147500	1.71708800
C	1.10199600	0.87646300	-6.56664400	C	4.53140100	-2.51150100	-0.08319500
H	1.97235600	1.25182300	-6.01144900	C	3.74233300	-1.31301400	-0.14689200
H	1.06408800	1.34385200	-7.55575100	C	3.96651300	-0.17299400	0.77137700
H	1.21649300	-0.20952600	-6.67205400	C	5.24274300	0.47177700	0.90022300
C	-4.49690200	-1.07021500	-0.77356200	C	6.34528500	0.15456400	0.06898400
C	-5.49139900	-0.64963000	0.14195700	H	6.23066900	-0.60535400	-0.70006600
C	-4.74662200	-2.24386100	-1.49097100	C	7.54972000	0.80487800	0.20857100
C	-6.66442000	-1.42813900	0.31087200	H	8.37790400	0.54806200	-0.44872800
C	-5.58725300	0.44438900	1.05272800	C	7.72049700	1.80294600	1.18858400
C	-5.91427000	-2.99740000	-1.30327900	H	8.68147500	2.30152500	1.29407400
H	-4.02971800	-2.57355500	-2.24193200	C	6.66571100	2.15338500	1.99571600
C	-6.89123900	-2.60946900	-0.39564700	H	6.77648600	2.93740400	2.74382300
C	-6.77930700	0.30731300	1.71574300	C	5.40692900	1.51893000	1.86629500
H	-4.87110800	1.24429900	1.20182800	C	4.30546800	1.91715300	2.66127900
H	-6.06070900	-3.90057300	-1.89255700	H	4.44877800	2.69529900	3.40952600
H	-7.79507500	-3.19919000	-0.25157800	C	3.06883200	1.35288700	2.47455000
H	-7.23475100	0.92894200	2.47800400	H	2.20187600	1.65298600	3.05932700
N	-7.43834600	-0.81966000	1.27454000	C	2.91766000	0.33862000	1.51354000
C	-8.71259200	-1.30095800	1.74006900	C	1.50383900	2.71185700	-1.18996800
H	-8.61775600	-2.29449700	2.19664800	H	1.21483800	3.72140500	-0.86382700
H	-9.43412300	-1.36437000	0.91610200	C	1.02455800	2.55714100	-2.62002500
H	-9.10420100	-0.61029500	2.49057000	C	-0.07190800	3.31727300	-3.04840900

IM3a

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Ir	-1.29373400	-0.68083200	0.06885500
P	0.80644300	0.20193700	-0.02530800
N	0.69605400	1.84489100	-0.25589700
O	1.63344600	-0.18369500	1.34741200
O	1.89197400	-0.16250300	-1.18816400
C	2.73572100	-1.26674500	-1.09802300
C	2.55469400	-2.25656900	-2.08040000
H	1.78893200	-2.10045100	-2.83899000
C	3.35685500	-3.36888700	-2.06976000

H	-0.49875200	4.06060000	-2.37243800
C	-0.60235400	3.16089800	-4.32640600
H	-1.45315000	3.76372900	-4.63811400
C	-0.02864500	2.24942400	-5.20839500
H	-0.43524900	2.12625800	-6.21020000
C	1.08847700	1.51705200	-4.81070200
H	1.56232100	0.82708500	-5.50683400
C	1.61240700	1.67079800	-3.52996600
H	2.48971200	1.09754300	-3.23874200
C	3.00308200	2.61284400	-0.98960300
H	3.26317800	2.75996400	0.06527500
H	3.43005700	1.66037700	-1.31445200

H	3.48600100	3.40644000	-1.57024000	C	-4.86492200	-0.05684500	-0.40982300
C	-0.65588200	2.35909300	0.04294100	C	-5.94363700	-0.94899600	-0.17784300
H	-1.17437100	2.51001900	-0.91976600	C	-5.03760300	1.27934800	-0.01421700
C	-1.42156100	1.31857600	0.85074400	C	-7.12692400	-0.46211700	0.44259800
H	-1.05367000	1.32297600	1.88929900	C	-6.16096800	-2.33017800	-0.44647600
H	-2.48363600	1.59125600	0.89802400	C	-6.21210700	1.72753100	0.59417000
C	-0.61787000	3.68678100	0.76376100	H	-4.24301100	2.00174500	-0.19519500
C	0.40264400	3.99829900	1.66602600	C	-7.27656000	0.86395700	0.83632200
H	1.22482200	3.29441600	1.80168400	C	-7.42292500	-2.62868900	0.00465800
C	0.38749800	5.20355700	2.35954500	H	-5.49106100	-3.02929900	-0.93366200
H	1.19350700	5.43921300	3.05229000	H	-6.29650400	2.77314500	0.88039900
C	-0.65019600	6.11192300	2.16300500	H	-8.19085400	1.21968000	1.30767400
H	-0.66003800	7.05621400	2.70329500	H	-7.96919600	-3.56436400	-0.01774700
C	-1.66931700	5.81170500	1.26247000	N	-8.01210000	-1.51161300	0.54370000
H	-2.47623500	6.52229500	1.09459500	C	-9.34014100	-1.43204800	1.10461600
C	-1.64928900	4.60758200	0.56441900	H	-9.81056900	-2.41570600	1.04789300
H	-2.44237600	4.37743100	-0.15099600	H	-9.95714400	-0.71802400	0.54708500
C	-1.40122800	-0.30221500	-2.07095800	H	-9.30290400	-1.12291000	2.15546500

IM3b

	Coordinates (Angstroms)		
	X	Y	Z
Ir	-1.36518400	-0.60937000	-0.03628800
O	1.88141300	-0.13194200	-1.19456100
O	1.54429600	-0.11770400	1.32753500
C	2.68377500	-1.26441100	-1.07415800
C	2.49370300	-2.25951500	-2.04963200
H	1.75524200	-2.08879600	-2.83116300
C	3.25297500	-3.40064200	-2.00403900
H	3.12723200	-4.17652400	-2.75764000
C	4.19956900	-3.59453700	-0.97030200
C	4.94326700	-4.79551800	-0.87952700
H	4.78445000	-5.56182800	-1.63720400
C	5.83764700	-4.99735600	0.14304900
H	6.40246100	-5.92505700	0.20318300
C	6.01116500	-4.00282400	1.12629600
H	6.70078300	-4.17412300	1.95033700
C	5.31538500	-2.81771500	1.05958500
H	5.45828700	-2.06757500	1.83314100
C	4.40339000	-2.56338400	0.00474800
C	3.66095000	-1.33715500	-0.09451300
C	3.89479100	-0.20060600	0.82490400
C	5.18961800	0.39509400	0.99591900
C	6.30405900	0.03906200	0.19718600
H	6.18394300	-0.71379300	-0.57794900

C	7.52742300	0.64320000	0.37580000	H	3.24862900	2.73788200	0.12740900
H	8.36469400	0.35822600	-0.25785000	H	3.44710000	1.67125600	-1.27572600
C	7.70592100	1.63044100	1.36537400	H	3.54853900	3.42122100	-1.47933000
H	8.68105300	2.09254500	1.50143700	C	-2.43416900	-1.16214300	1.83989000
C	6.64135100	2.01649200	2.14308000	H	-2.98384700	-0.27306700	2.16038800
H	6.75889900	2.79248400	2.89844100	C	-1.04000700	-1.16477400	2.07255900
C	5.36426000	1.43075400	1.97226900	H	-0.64194000	-0.27603800	2.56281700
C	4.25514300	1.86479600	2.73714500	C	-0.20888000	-2.41824500	2.29238100
H	4.40498300	2.63078900	3.49649600	H	0.61442900	-2.16572100	2.96915300
C	3.00431500	1.35078100	2.50732800	H	-0.81764800	-3.15513400	2.83245800
H	2.13211700	1.67934500	3.06836400	C	0.38677900	-3.03583000	1.01762700
C	2.84170900	0.35120600	1.53239500	H	0.51002900	-4.12339400	1.14461600
P	0.75913100	0.25609000	-0.07409000	H	1.39784900	-2.64325200	0.86378800
N	0.66372800	1.89421600	-0.33131400	C	-0.42387200	-2.79010700	-0.22688800
C	-1.53831900	1.42464400	0.64208600	H	0.13153700	-2.76784900	-1.16640100
H	-1.25851000	1.42917400	1.70759100	C	-1.79265300	-2.97073800	-0.28850500
H	-2.58605000	1.74676000	0.60616100	H	-2.23587200	-3.06215000	-1.27792300
C	-0.68021800	2.45175400	-0.08631000	C	-2.63181900	-3.49650400	0.85304700
H	-1.14056400	2.67169100	-1.06495500	H	-3.42350100	-4.12913200	0.43429700
C	-0.63134400	3.74547400	0.69595300	H	-2.01163700	-4.16067000	1.46795200
C	0.34762000	3.97434800	1.66616900	C	-3.27363600	-2.40325800	1.71102500
H	1.13653400	3.23508600	1.80843900	H	-3.49532300	-2.79136300	2.71857800
C	0.33453100	5.14237200	2.42113000	H	-4.24414600	-2.12999100	1.28313800
H	1.10825600	5.31242000	3.16770500	C	-1.31956700	0.03602100	-2.14705800
C	-0.66140700	6.09519300	2.21924800	H	-1.27256500	1.12462700	-2.17957100
H	-0.67095700	7.00951300	2.80866700	H	-0.59539300	-0.44071800	-2.80817800
C	-1.63787200	5.87809300	1.24999400	C	-2.57288600	-0.61495500	-1.98839200
H	-2.41144100	6.62384500	1.07806100	H	-2.68492100	-1.60215400	-2.43302500
C	-1.61892600	4.71171500	0.49013900	C	-3.58179100	-0.14689100	-1.13965000
H	-2.37921600	4.54650100	-0.27608200	H	-3.54738100	0.90511000	-0.86274400
C	1.54043400	2.76376700	-1.19947000	C	-4.81376800	-0.84234400	-0.82817200
H	1.26314100	3.77139800	-0.85756300	C	-5.72919200	-0.24596200	0.07255700
C	1.12575000	2.66392600	-2.65323400	C	-5.13671100	-2.10742200	-1.33679300
C	0.11764200	3.51433000	-3.12503300	C	-6.91949200	-0.94368800	0.41831400
H	-0.29379700	4.27202800	-2.45518700	C	-5.74658400	0.98213300	0.79216600
C	-0.34507900	3.42526900	-4.43535100	C	-6.31204000	-2.77287800	-0.97591400
H	-1.12642600	4.09880700	-4.78237000	H	-4.46755800	-2.58971700	-2.04834300
C	0.20830900	2.48870300	-5.30332100	C	-7.22166200	-2.20537100	-0.08806800
H	-0.14398200	2.41877600	-6.33054800	C	-6.91203200	0.99880300	1.51678600
C	1.23794200	1.66141500	-4.85805200	H	-5.01020500	1.77758200	0.77252600
H	1.69777300	0.95019100	-5.54223400	H	-6.52230100	-3.75042600	-1.40372700
C	1.69470600	1.74902300	-3.54627600	H	-8.13439800	-2.72923000	0.18992100
H	2.50838100	1.10614700	-3.21748200	H	-7.30934500	1.75497800	2.18358500
C	3.02718200	2.62301300	-0.93988900	N	-7.62466700	-0.15664400	1.30045300

C	-8.90008400	-0.49582900	1.88511700	H	2.23227400	-5.82590300	-2.08316300
H	-8.82381500	-1.40421400	2.49398800	C	-2.43057800	-1.43199800	-1.60608400
H	-9.65520500	-0.65475500	1.10682100	C	-3.09458600	-0.30775600	-2.11196700
H	-9.22907600	0.32530700	2.52515000	C	-3.00599100	-2.69937100	-1.76634800
IM4				C	-4.32977200	-0.45123400	-2.74069200
Atomic				H	-2.62948900	0.67507400	-2.01934100
Coordinates (Angstroms)				C	-4.23849400	-2.83743800	-2.39683300
Type	X	Y	Z	H	-2.47822000	-3.58196700	-1.40203900
C	-0.60290200	-0.92265000	2.15262000	C	-4.90517400	-1.71212300	-2.87953500
C	-1.25243800	-1.39534600	3.34032100	H	-4.84022500	0.42791100	-3.13223200
H	-0.97409500	-1.12337800	4.35255800	H	-4.67783600	-3.82637100	-2.51747300
C	-2.34861800	-2.21282000	2.94883800	H	-5.86855600	-1.82183800	-3.37489700
H	-3.06578400	-2.67462800	3.61934100	Cu	0.17225600	0.75266500	-0.79474700
C	-1.30921400	-1.46497200	1.00647800	O	-1.14702400	2.24510500	-1.56291400
C	-2.38127600	-2.26593700	1.52584800	C	-0.46510700	3.07211200	-2.22808100
H	-3.12026300	-2.78184000	0.92057100	O	-1.08914800	4.13883600	-2.80448500
C	1.87148800	1.72925500	1.73448800	C	0.92984600	3.01133600	-2.42050800
C	2.36179300	0.93558400	2.94672000	N	1.54512300	1.94764700	-1.83230100
H	2.54889800	1.53866300	3.84064800	C	2.85917700	1.86593000	-1.75908900
N	0.78249100	0.88274200	1.21311700	H	3.47867600	2.69984400	-2.10793900
C	0.49398900	0.03197100	2.14105500	C	3.55168100	0.74482000	-1.17070700
O	1.26191500	0.04314900	3.25279100	C	4.85803100	0.90986200	-0.66756100
H	3.24063400	0.31376400	2.73547600	C	2.97114800	-0.53332800	-1.04794800
H	2.64984700	1.81907800	0.96470700	C	5.52560200	-0.12097000	-0.02049100
C	1.37059000	3.13583600	2.10189000	H	5.34435000	1.88134300	-0.76650900
C	0.58157900	3.78264800	0.97476800	C	3.62295300	-1.57360200	-0.40260200
C	2.55453300	4.01227600	2.49173800	H	1.99591100	-0.71459900	-1.49667400
H	0.70846500	3.02151000	2.98035400	C	4.89542500	-1.35618800	0.12298000
H	-0.27915500	3.17776800	0.66621400	H	6.52691700	0.02717800	0.37757100
H	0.21625000	4.77235100	1.27658700	H	3.15749900	-2.55485300	-0.32786700
H	1.21374300	3.91791100	0.08681900	C	-2.48421700	4.21600600	-2.56406000
H	3.14697400	3.58933000	3.31311900	H	-3.01333400	3.35805800	-2.99794700
H	3.22740700	4.14350700	1.63237200	H	-2.70282100	4.24937100	-1.48976900
H	2.22275800	5.00860500	2.80550700	H	-2.81608800	5.13872700	-3.04465500
P	-0.84229200	-1.19263400	-0.72729300	C	-2.96892400	1.30990500	1.05533000
C	0.07974800	-2.72798300	-1.12286700	C	-2.53779800	1.67028500	2.36646300
C	0.58804800	-2.87091600	-2.42279300	H	-1.65316700	2.25592900	2.60019800
C	0.36536800	-3.71648400	-0.17412600	C	-3.41349000	1.05748100	3.31125200
C	1.35012200	-3.98080900	-2.76770400	H	-3.32417700	1.10872100	4.39132000
H	0.39113400	-2.09547100	-3.16521100	C	-4.11583700	0.46685200	1.19084300
C	1.13382100	-4.82668100	-0.52164300	H	-4.64596300	-0.01931200	0.37745500
H	-0.01253100	-3.62143700	0.84322600	C	-4.39127100	0.31328200	2.58387100
C	1.62682000	-4.96190900	-1.81605200	H	-5.17486100	-0.30065300	3.01601400
H	1.73958500	-4.07542300	-3.77982200	H	-2.47427500	1.59276500	0.12866700
H	1.34884900	-5.58730400	0.22711000				

C	1.70429300	4.07962000	-3.11043000	H	0.28480700	-2.34174800	6.04717800
H	1.04027300	4.79144900	-3.60504900	H	-3.60368300	-2.11883700	4.22312400
H	2.34201400	4.65034300	-2.41245500	H	-2.16997000	-2.68998400	6.17162500
H	2.38444300	3.65890100	-3.86712400	C	1.63860900	0.22248900	1.87052600
Fe	-2.52534100	-0.34839200	2.14526500	C	1.46857600	1.55211000	2.28433500
Cl	5.72178100	-2.65702600	0.95302100	C	2.93113200	-0.31109500	1.84406200

IM4'

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-0.09168000	-2.70290400	-0.66875100
C	0.40204500	-4.02628000	-0.92834900
H	0.11301600	-4.64071000	-1.77279100
C	1.36845600	-4.34243500	0.06155100
H	1.95470200	-5.25407800	0.10905400
C	0.58848700	-2.19135200	0.51304800
C	1.47555400	-3.23397900	0.94661400
H	2.12531600	-3.18183000	1.81450800
C	-2.40498900	-0.68748800	-2.67494900
C	-2.40875100	-2.07766700	-3.32171400
H	-1.91819400	-2.07995100	-4.30680000
N	-1.35811800	-0.79643100	-1.64032200
C	-1.02995300	-2.04331900	-1.56462000
O	-1.61811100	-2.89575300	-2.44139600
H	-3.39463400	-2.54107400	-3.41633800
H	-3.35011600	-0.48557400	-2.14319200
C	-2.17670400	0.42808200	-3.69630500
C	-2.11480800	1.80187600	-3.05254000
C	-3.28037500	0.37959700	-4.74905000
H	-1.21103100	0.22163000	-4.19207900
H	-1.27237200	1.89500500	-2.36172900
H	-2.01177800	2.58385000	-3.81477700
H	-3.02771700	2.01053400	-2.47632600
H	-3.32244100	-0.58131100	-5.27862000
H	-4.26326500	0.54687900	-4.28700000
H	-3.13654300	1.16128300	-5.50331100
P	0.11432300	-0.64142100	1.34940400
C	-0.56894400	-1.28230200	2.92573300
C	0.23205300	-1.59863800	4.02863000
C	-1.95484000	-1.46808900	3.00480100
C	-0.34367500	-2.10307000	5.19060200
H	1.30942900	-1.43393600	3.98108100
C	-2.52485000	-1.98027700	4.16707200
H	-2.58086500	-1.18812800	2.15451800
C	-1.72181200	-2.29827600	5.25981900

H	0.28480700	-2.34174800	6.04717800
H	-3.60368300	-2.11883700	4.22312400
H	-2.16997000	-2.68998400	6.17162500
C	1.63860900	0.22248900	1.87052600
C	1.46857600	1.55211000	2.28433500
C	2.93113200	-0.31109500	1.84406200
C	2.56267400	2.32855300	2.64744000
H	0.46785300	1.98865600	2.28232200
C	4.02924200	0.47443500	2.18958100
H	3.09270800	-1.33309200	1.50727700
C	3.84858300	1.79496600	2.58941500
H	2.41103900	3.36489900	2.94397500
H	5.03125400	0.04994700	2.13875500
H	4.70889400	2.41153900	2.84346700
Cu	-1.31555100	0.41923400	0.10377900
O	-3.41830000	0.09837900	0.35859200
C	-3.94001800	1.23535400	0.51018100
O	-5.27834100	1.32923800	0.76953100
C	-3.26210300	2.47148200	0.43285500
N	-1.92871100	2.38907500	0.16035700
C	-1.17538000	3.47054800	0.12140600
H	-1.61459700	4.43827500	0.38587400
C	0.22413600	3.50257900	-0.21685000
C	0.95588600	4.66785000	0.09936000
C	0.92787500	2.46202200	-0.86247700
C	2.31322500	4.78010000	-0.15543400
H	0.43561300	5.49609100	0.58158900
C	2.28271700	2.57133700	-1.14191600
H	0.39994000	1.54992700	-1.15054400
C	2.97596400	3.72008100	-0.77002100
H	2.86038800	5.67929500	0.11789000
H	2.80810800	1.77761300	-1.66738100
C	-5.95141300	0.08895700	0.89601500
H	-5.91945400	-0.48435900	-0.03830500
H	-5.50986600	-0.52521000	1.69027900
H	-6.98517000	0.33808900	1.14493300
C	3.03315000	-1.01096700	-1.33761300
C	2.16683500	-1.28608200	-2.43478300
H	1.37471400	-0.63336700	-2.79392300
C	2.45345700	-2.60480700	-2.90373500
H	1.93109400	-3.12545900	-3.69993700
C	3.85251000	-2.15757600	-1.11997300
H	4.59317600	-2.27114700	-0.33456800
C	3.49688300	-3.14361800	-2.08940100

H	3.91565100	-4.14141000	-2.16801700	H	-6.60361300	1.43303000	-1.75357800
H	3.02466200	-0.11335200	-0.73001000	C	-5.75928600	0.52734900	-4.92161100
C	-3.94089900	3.78317200	0.62643300	H	-3.74974100	0.49653500	-5.70448800
H	-5.01564800	3.65117500	0.76454800	H	-7.63413000	0.66531300	-3.86414800
H	-3.55535800	4.32851100	1.50333600	H	-6.21577400	0.20185500	-5.85427000
H	-3.78475400	4.44857000	-0.23842100	C	-2.40153900	2.88377400	-1.34384100
Cl	4.69173500	3.83229700	-1.08340700	C	-1.27412000	2.84552100	-0.51443900
Fe	1.88409300	-2.65301400	-0.96631000	C	-2.38980600	3.72712100	-2.46450700

TS2

Atomic Type	Coordinates (Angstroms)						
	X	Y	Z				
C	-6.07715700	2.75587200	0.72824400	H	-1.26069100	2.17665000	0.34533800
C	-6.84849800	3.95194900	0.91443000	C	-1.27196700	4.50523300	-2.75040500
H	-7.66034800	4.06454200	1.62437500	H	-3.25331700	3.75935000	-3.12868200
C	-6.31902800	4.95666600	0.06111900	C	-0.15525200	4.46238900	-1.91577400
H	-6.65396200	5.98707100	0.01157000	H	0.70920200	3.58929100	-0.14328600
C	-5.05564900	3.03249500	-0.26800900	H	-1.27191800	5.14620500	-3.62984300
C	-5.23230800	4.39867800	-0.66864100	H	0.72220100	5.06567800	-2.14497800
H	-4.60097800	4.92660500	-1.37645500	Cu	-3.63925700	0.29899400	0.64978100
C	-6.02675000	-0.31035500	2.71729600	O	-1.81361800	0.61856200	1.77719500
C	-7.50845100	0.05682000	2.60677600	C	-1.41617700	-0.46470600	2.23401800
H	-8.03079100	0.12651500	3.56512800	O	-0.51394400	-0.50976200	3.22013000
N	-5.38677900	0.63070800	1.77722000	C	-1.86321800	-1.76647000	1.74735900
C	-6.26334800	1.54375000	1.50671600	N	-3.12833600	-1.67951500	1.15043300
O	-7.49784300	1.38365100	2.02469800	C	-3.82080000	-2.77439900	0.99109000
H	-8.07515400	-0.59311200	1.92896600	H	-3.43395800	-3.72051000	1.38786300
H	-5.83522800	-1.33789000	2.37485800	C	-5.08712700	-2.89855800	0.30247200
C	-5.48735700	-0.15689300	4.14930300	C	-5.72720300	-4.15169700	0.35131200
C	-3.96933700	-0.17971100	4.19662400	C	-5.70846200	-1.87054700	-0.43098100
C	-6.06919900	-1.24898300	5.03795600	C	-6.93869200	-4.37641900	-0.28318500
H	-5.83573900	0.82475400	4.51871000	H	-5.25045200	-4.96607700	0.89742900
H	-3.53239500	0.61387000	3.58034600	C	-6.92210800	-2.08021900	-1.07022900
H	-3.60560500	-0.06063000	5.22455600	H	-5.21780500	-0.89967400	-0.52278600
H	-3.58762300	-1.14025600	3.82117100	C	-7.53093100	-3.33228000	-0.99395900
H	-7.16616200	-1.25891000	5.04093500	H	-7.42398600	-5.34785700	-0.23678600
H	-5.73183000	-2.23870800	4.69937100	H	-7.38755300	-1.28393700	-1.64757000
H	-5.74228700	-1.12793000	6.07649400	C	-0.05999500	0.76597200	3.68562400
P	-3.84245600	1.84334500	-0.90919300	H	0.51864500	1.27414200	2.90458200
C	-4.58397800	1.39458700	-2.52421400	H	-0.90995900	1.39338900	3.97203900
C	-3.79436100	1.11978500	-3.64858000	H	0.57994400	0.54982400	4.53977500
C	-5.97134600	1.21571400	-2.61630000	C	-3.15101400	3.72094400	2.25638000
C	-4.37871300	0.69679600	-4.83905200	C	-4.22745900	3.77564700	3.19084000
H	-2.71341600	1.25111700	-3.59829900	H	-4.60117900	2.93874500	3.77418300
C	-6.55355200	0.78557100	-3.80543300	C	-4.77466900	5.09153900	3.16537000
				H	-5.63047500	5.43708600	3.73522600
				C	-3.03257400	5.01012600	1.64870100

H	-2.33751700	5.27871600	0.85836700	C	7.72482100	-0.91960900	-1.25490400
C	-4.03613300	5.85543800	2.21281200	H	7.42304800	-1.87668200	-1.67545600
H	-4.23318800	6.88505300	1.93405500	C	6.73496600	0.05142200	-1.01445800
H	-2.56970600	2.83398100	2.01926000	C	3.92710300	-2.96451600	0.77347900
C	-1.47314900	-2.97130900	2.54972700	H	3.14454100	-2.90484600	1.55277500
H	-1.45923300	-3.88160400	1.93938700	C	4.68007900	-4.25733700	0.97199000
H	-0.47563000	-2.83681300	2.97657300	C	5.96385000	-4.44794400	0.45201400
H	-2.17174200	-3.14506500	3.38251800	H	6.46201300	-3.61452800	-0.04619000
Fe	-4.87463500	4.23899200	1.31910600	C	6.60274700	-5.67618600	0.58552100
Cl	-9.02992200	-3.60820700	-1.82886500	H	7.60434400	-5.81205800	0.18110300
Ir	2.27438000	-1.07649100	-1.02709200	C	5.96595600	-6.73180400	1.23643000
P	4.31311500	-0.54392700	-0.11835100	H	6.46816100	-7.69142600	1.34138800
O	4.63568000	0.74972100	0.86250000	C	4.68800900	-6.55099700	1.75827700
O	5.42747200	-0.28770800	-1.32590700	H	4.18740600	-7.36827700	2.27406900
N	4.79882500	-1.77457800	0.91102200	C	4.05341000	-5.31866200	1.62860200
C	4.79280100	2.01088000	0.30710900	H	3.05121100	-5.17104400	2.03901400
C	3.78030900	2.95340200	0.56942300	C	3.25132200	-2.93832800	-0.58810300
H	2.94262000	2.64827100	1.19665500	H	3.99873800	-3.16077600	-1.36765700
C	3.87690300	4.21596100	0.04150600	H	2.50435300	-3.74115900	-0.63286800
H	3.10749500	4.96129400	0.24384600	C	5.48561300	-1.66309400	2.23946300
C	4.97198800	4.57044200	-0.78295000	H	5.77246900	-2.70488100	2.44210500
C	5.05304800	5.84813600	-1.38735600	C	4.52394000	-1.26654900	3.34457300
H	4.25760000	6.56665500	-1.18975100	C	3.76577500	-2.26455500	3.97074100
C	6.10371700	6.17742500	-2.20929900	H	3.90965600	-3.30428800	3.66959400
H	6.15350500	7.16254100	-2.66848500	C	2.86695600	-1.95716000	4.98842700
C	7.11437300	5.22956300	-2.46644700	H	2.29614800	-2.75101500	5.46719700
H	7.93491500	5.48387700	-3.13439400	C	2.73363400	-0.64009300	5.41820600
C	7.07272600	3.98367500	-1.88539600	H	2.05827000	-0.39818300	6.23827200
H	7.85539600	3.26071800	-2.10161600	C	3.49122000	0.36245900	4.81450200
C	6.01579900	3.61601300	-1.01544000	H	3.40611800	1.39227600	5.15980500
C	5.94187700	2.32031700	-0.40344000	C	4.37537600	0.05300500	3.78563200
C	7.02408500	1.31941400	-0.53908900	H	4.96889100	0.84371600	3.33258600
C	8.37777100	1.59694800	-0.15598700	C	6.77750800	-0.87034100	2.20952600
C	8.75653200	2.79874200	0.49303700	H	7.44013900	-1.24880700	1.42367000
H	7.99607000	3.54241800	0.71958300	H	6.63179100	0.20013400	2.04411600
C	10.06388600	3.03135400	0.85236000	H	7.28736700	-0.99254000	3.17171400
H	10.32527400	3.95911900	1.35780800	C	1.45819500	-0.69401500	0.93593500
C	11.06542500	2.07745300	0.58148100	H	0.92663900	0.26575700	0.95102700
H	12.09682800	2.27757600	0.86375400	H	2.14286900	-0.81302800	1.78051800
C	10.72984800	0.89063600	-0.02334800	C	0.75727200	-1.85311500	0.46634000
H	11.48912600	0.13423900	-0.21942700	H	1.13281400	-2.81440000	0.82264900
C	9.39153900	0.61119600	-0.39076300	C	-0.60214400	-1.87683400	-0.01033500
C	9.03496300	-0.63132900	-0.96803500	H	-1.00250800	-0.92898200	-0.37861700
H	9.81551400	-1.36701300	-1.15755800	C	3.02460000	-1.21657700	-3.06041500

H	3.94823600	-1.79789700	-3.04750100	H	6.15384500	-5.36656700	-0.58449700
C	1.81016000	-1.96052000	-2.96693900	C	5.14627300	-2.27179000	0.31520400
H	1.90100500	-3.04866600	-2.91109200	C	5.90418700	-3.46505000	0.57102000
C	0.49858700	-1.47697700	-3.53595600	H	6.56042400	-3.61759800	1.42226900
H	0.49479400	-1.59146800	-4.63375200	C	2.95380900	0.30268400	-2.74820200
H	-0.29625900	-2.13651800	-3.16596000	C	2.40647700	-0.93616200	-3.45375700
C	0.16338900	-0.03261200	-3.14796500	H	2.54608900	-0.94528900	-4.53857000
H	0.47268200	0.67313900	-3.93230500	N	3.53912600	-0.26497800	-1.52396900
H	-0.92907100	0.07143400	-3.07772400	C	3.72669600	-1.52673000	-1.75251500
C	0.77164500	0.39774600	-1.82581200	O	3.20519300	-2.01427500	-2.90427200
H	0.06044000	0.60084700	-1.02380200	H	1.35284000	-1.14628100	-3.21820600
C	2.00685100	1.05109400	-1.71520300	H	2.15058300	0.99937500	-2.46488700
H	2.13655800	1.70873400	-0.85452000	C	4.00911600	1.04453400	-3.59077800
C	2.93046600	1.32858100	-2.87256100	C	4.90635800	1.95039600	-2.75818300
H	3.90427300	1.63538700	-2.46849800	C	3.33129300	1.80842200	-4.72138100
H	2.55417400	2.19780100	-3.44032200	H	4.64268000	0.26087300	-4.04428200
C	3.12837500	0.11534500	-3.79110000	H	5.45723700	1.38553500	-1.99646700
H	2.40623400	0.13455200	-4.61936100	H	5.63785000	2.45580100	-3.40082400
H	4.11530100	0.18518800	-4.26322500	H	4.33412400	2.72139400	-2.22677300
C	-1.16930100	-3.05274000	-0.65408300	H	2.68370900	1.16651700	-5.33319800
C	-2.24959500	-2.90032300	-1.55803900	H	2.70400600	2.62138500	-4.32986400
C	-0.75068600	-4.36477800	-0.38080300	H	4.07214700	2.25746100	-5.39250600
C	-2.90036100	-4.04966600	-2.08406600	P	4.93436800	-0.82078400	1.38932400
C	-2.90346800	-1.76750000	-2.11383700	C	4.30218700	-1.49047600	2.97040500
C	-1.39573200	-5.47968600	-0.92825600	C	3.91899600	-0.53613100	3.92675000
H	0.09180900	-4.52981100	0.29006000	C	4.15954700	-2.84643300	3.27688100
C	-2.49255400	-5.34360200	-1.77543000	C	3.42749300	-0.92979900	5.16532800
C	-3.90952800	-2.24110700	-2.91882200	H	4.00794900	0.52628400	3.68860600
H	-2.68323100	-0.72496500	-1.91838300	C	3.66732500	-3.23905000	4.52076700
H	-1.03557600	-6.47537200	-0.67868600	H	4.41741900	-3.60589700	2.54073700
H	-2.99756500	-6.21655300	-2.18579600	C	3.30336100	-2.28612900	5.46695600
H	-4.64672800	-1.70153700	-3.50471200	H	3.14042700	-0.17673000	5.89789700
N	-3.92078000	-3.61497300	-2.90400800	H	3.56425000	-4.29974100	4.74513900
C	-4.86875400	-4.46559700	-3.58038100	H	2.92170800	-2.59771000	6.43762500
H	-5.41776000	-5.08454700	-2.85936100	C	6.62614300	-0.29716700	1.85213300
H	-5.58932500	-3.84037700	-4.11329600	C	7.10208300	0.92928200	1.37387900
H	-4.36779600	-5.12096800	-4.30276700	C	7.44663200	-1.07268700	2.68071800

TS2'

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	4.46132000	-2.48646400	-0.95194300
C	4.80163100	-3.79948000	-1.42577000
H	4.47522300	-4.22428800	-2.36833600
C	5.68374200	-4.39422800	-0.48560600

C	8.38939400	1.35668000	1.69059300
H	6.45169100	1.54818400	0.75061600
C	8.73152000	-0.64433500	2.99728300
H	7.06690400	-2.00445000	3.10178700
C	9.20626400	0.56793900	2.49725900
H	8.75230000	2.31120300	1.31414800
H	9.36162800	-1.25184600	3.64416400

H	10.20994700	0.90420800	2.75004300	C	-3.58772500	-2.41781900	-0.14678600
Cu	3.58279800	0.57007600	0.36363100	C	-2.28379100	-2.94080300	-0.05724100
O	3.63226800	2.67992700	0.29721600	H	-1.56896700	-2.44820500	0.60352800
C	2.78132000	3.17587800	1.05765800	C	-1.95727800	-4.05415500	-0.78867900
O	2.80928800	4.47088500	1.38979600	H	-0.95947400	-4.48740500	-0.72003900
C	1.65545100	2.43945300	1.62422200	C	-2.90396800	-4.64784200	-1.65857100
N	1.81569500	1.06363100	1.45495800	C	-2.55548100	-5.75360200	-2.47027900
C	1.16523400	0.21753500	2.20300800	H	-1.54515600	-6.15475400	-2.39046600
H	0.59408800	0.55003600	3.07985400	C	-3.46170400	-6.30405000	-3.34438700
C	1.13765400	-1.20338800	1.91007000	H	-3.18042700	-7.15218600	-3.96508500
C	0.83050000	-2.13498900	2.91143100	C	-4.75705800	-5.75745300	-3.44500800
C	1.38159800	-1.68156200	0.61029800	H	-5.46575600	-6.17678100	-4.15624000
C	0.82672300	-3.49779800	2.64668100	C	-5.13493700	-4.69596300	-2.65507400
H	0.63125600	-1.78387800	3.92266300	H	-6.13647900	-4.28309400	-2.75005700
C	1.38796300	-3.03986700	0.32907300	C	-4.23489300	-4.11802800	-1.72585300
H	1.54175600	-0.95976000	-0.18921900	C	-4.59787800	-3.01067500	-0.88780000
C	1.12597600	-3.94230400	1.36026000	C	-5.98448800	-2.49624400	-0.79510400
H	0.61876800	-4.21774600	3.43452500	C	-7.09200900	-3.34912500	-0.46165400
H	1.58152700	-3.40209800	-0.67967900	C	-6.93007700	-4.70726100	-0.08832300
C	3.82851000	5.25405700	0.75964400	H	-5.92930000	-5.12925100	-0.03862000
H	4.81301400	4.97969000	1.15198500	C	-8.01401300	-5.49414600	0.22715000
H	3.81331800	5.10030300	-0.32421500	H	-7.85675700	-6.53124900	0.51733300
H	3.58984000	6.28866000	1.00941500	C	-9.32161800	-4.97079600	0.18553400
C	7.57461500	-0.96882400	-1.48726900	H	-10.17032100	-5.60602100	0.42964700
C	6.99392700	-1.40563800	-2.71222200	C	-9.51430100	-3.65153000	-0.14392800
H	6.29649300	-0.83763600	-3.32118100	H	-10.51634900	-3.22365300	-0.15879400
C	7.43032600	-2.73982200	-2.96018400	C	-8.42094000	-2.80914900	-0.45653800
H	7.13231400	-3.36397900	-3.79560200	C	-8.61939500	-1.43753400	-0.74200500
C	8.37248100	-2.03464100	-0.97097100	H	-9.63463400	-1.04280000	-0.75057100
H	8.91312400	-2.02475700	-0.03013000	C	-7.55065100	-0.61218800	-0.97397800
C	8.28646800	-3.12738900	-1.88548600	H	-7.67322500	0.45044400	-1.17153400
H	8.75075700	-4.09988300	-1.76194700	C	-6.24976000	-1.14766300	-0.97653400
H	7.41090200	-0.00997000	-1.00822400	C	-4.26784200	2.34961100	1.31054200
C	0.97088800	2.98442100	2.83984800	H	-3.39574200	2.34408000	1.98996500
H	0.90916200	4.07443900	2.79178400	C	-5.29249300	3.29198800	1.89331200
H	-0.04762100	2.58472800	2.93944900	C	-6.63945500	3.23506500	1.52333600
H	1.51338800	2.71820000	3.76050200	H	-6.96736000	2.44856100	0.84181700
Fe	6.44762800	-2.63981500	-1.18552600	C	-7.54939200	4.15598300	2.03253700
Cl	1.16914700	-5.65085800	1.02968100	H	-8.59688700	4.09920100	1.74181700
Ir	-2.46351000	1.47273000	-1.04114400	C	-7.12495500	5.14863000	2.91447700
P	-4.09547700	0.15893100	-0.10262700	H	-7.83915500	5.86570200	3.31387500
O	-3.86145500	-1.30118100	0.62645900	C	-5.78535600	5.21383500	3.28751700
O	-5.21943300	-0.25856300	-1.24584400	H	-5.44719100	5.98188300	3.98078400
N	-4.77189100	0.96185600	1.20738200	C	-4.87813600	4.28707700	2.78072600

H	-3.82673500	4.33077200	3.07527900	H	-2.23847800	-1.03337400	-4.24478600
C	-3.79921200	2.82785900	-0.05265200	C	-3.37566800	0.80674600	-3.94309300
H	-4.67452400	3.02424900	-0.69240500	H	-2.81673400	1.20528300	-4.80111700
H	-3.27057800	3.78281200	0.06506600	H	-4.37154300	0.56429500	-4.33259400
C	-5.19512600	0.36207600	2.51910300	C	0.23264100	4.24159500	-0.17438100
H	-5.70793300	1.20392200	3.00628600	C	1.09206000	4.76542900	-1.16796400
C	-3.99767500	0.02605400	3.39198800	C	-0.51236600	5.16332900	0.57007900
C	-3.39506500	1.05068300	4.13451200	C	1.16388200	6.16731100	-1.37402100
H	-3.85000700	2.04292500	4.13300100	C	1.97960100	4.16696500	-2.10688500
C	-2.25140800	0.81706200	4.89453700	C	-0.41737200	6.54444000	0.35494200
H	-1.80274200	1.63002400	5.46385100	H	-1.17745600	4.80698200	1.35566900
C	-1.70316400	-0.46147800	4.94526500	C	0.42137500	7.07331300	-0.61883900
H	-0.81756400	-0.65364500	5.55161800	C	2.54757900	5.18585300	-2.83028500
C	-2.31879300	-1.50133200	4.24988000	H	2.19633700	3.11168200	-2.21631200
H	-1.91582600	-2.51184200	4.30810700	H	-1.01603100	7.21654800	0.96559600
C	-3.45480200	-1.26044000	3.48361100	H	0.48768300	8.14741300	-0.78272800
H	-3.92287800	-2.08371800	2.94921500	H	3.27435000	5.15470000	-3.63502300
C	-6.22632000	-0.74038100	2.37898900	N	2.06454200	6.39822300	-2.39158800
H	-7.06509700	-0.40046200	1.76170700	C	2.40027100	7.69588800	-2.92370000
H	-5.83127700	-1.65628600	1.93157700	H	2.79898700	8.34807600	-2.13736500
H	-6.61536600	-0.99400500	3.37150600	H	3.16194600	7.58026200	-3.69778000
C	-1.31692900	0.79900600	0.67389700	H	1.52184900	8.17972300	-3.36758000
H	-0.60038500	0.05166100	0.33120300				
H	-1.89703900	0.46635500	1.54076500	TS3			
C	-1.00609500	2.19315100	0.57002100	Atomic	Coordinates (Angstroms)		
H	-1.59556200	2.84655400	1.21377800	Type	X	Y	Z
C	0.18767800	2.79765000	0.05371800	Ir	2.37725300	1.56802300	-0.99647400
H	0.77710600	2.20442400	-0.64780200	P	4.09021800	0.33659200	-0.09785700
C	-3.51368500	1.88770400	-2.88118100	O	3.90920200	-1.12258300	0.66758300
H	-4.54545500	2.15347400	-2.64165300	O	5.19694400	-0.06703500	-1.26371800
C	-2.53792900	2.91261700	-2.66876700	C	3.48955600	-2.20143600	-0.09451300
H	-2.91058900	3.87516000	-2.30700700	C	2.19051600	-2.69328300	0.14178200
C	-1.24781100	3.00375800	-3.44391100	H	1.59484300	-2.23641500	0.93221000
H	-1.43254900	3.39871200	-4.45793900	C	1.71831800	-3.73184900	-0.61999700
H	-0.60582400	3.74274400	-2.94750800	H	0.72138200	-4.13596900	-0.44198400
C	-0.49923800	1.67068400	-3.51878600	C	2.50074900	-4.26922500	-1.67231400
H	-0.74778100	1.12669800	-4.44147100	C	1.99162900	-5.26480400	-2.54162500
H	0.57920900	1.87603000	-3.58768900	H	0.98596800	-5.64663200	-2.36134400
C	-0.75423200	0.76331900	-2.32479800	C	2.74170100	-5.74471300	-3.58847500
H	0.10186900	0.59882800	-1.66130600	H	2.33378100	-6.50397400	-4.25256600
C	-1.73064800	-0.24654600	-2.31167400	C	4.04311600	-5.24771400	-3.80410600
H	-1.54183600	-1.10589600	-1.66389600	H	4.62824200	-5.61398300	-4.64525300
C	-2.72462600	-0.48214000	-3.42170900	C	4.58115100	-4.30459000	-2.95952000
H	-3.50554300	-1.14976300	-3.03544000	H	5.58675200	-3.92804800	-3.13464800
				C	3.83842700	-3.79246600	-1.86747600

C	4.36582700	-2.78564600	-0.99321800	C	-4.90113100	-2.75049500	0.67125100
C	5.79083000	-2.38441600	-1.00642000	C	-5.55146600	-4.02581700	0.54377800
C	6.83806300	-3.35254100	-0.82831000	H	-5.82274300	-4.66870300	1.37330500
C	6.58245500	-4.71986600	-0.55365900	C	-5.83493200	-4.24342800	-0.83053300
H	5.55533700	-5.06273800	-0.46011600	H	-6.36518900	-5.09618400	-1.24086400
C	7.61082600	-5.61843600	-0.38650900	C	-4.78363100	-2.17437600	-0.65884900
H	7.38232400	-6.65985700	-0.16862300	C	-5.36749400	-3.11987600	-1.56667600
C	8.95369300	-5.20385200	-0.48392100	H	-5.45063500	-2.98332300	-2.64024200
H	9.75679200	-5.92639500	-0.35575900	C	-4.19665700	-0.76805800	3.66460800
C	9.23973000	-3.88163300	-0.72168600	C	-4.32832500	-2.21145200	4.16922400
H	10.27245600	-3.53878000	-0.77802300	H	-5.10085900	-2.34553500	4.93357300
C	8.20636600	-2.92798600	-0.88402300	N	-4.27532300	-0.91122400	2.19996900
C	8.50419500	-1.55829900	-1.07867800	C	-4.60980700	-2.13720000	1.95279400
H	9.54716800	-1.24871000	-1.12999100	O	-4.73962600	-2.96571800	3.00832400
C	7.49959100	-0.63116100	-1.17459300	H	-3.38787300	-2.64583600	4.52919400
H	7.70237500	0.43001800	-1.30261600	H	-3.21202000	-0.34602700	3.92000800
C	6.15841200	-1.05265200	-1.11758900	C	-5.27695400	0.17196400	4.21882000
C	1.32347900	0.88022100	0.77300500	C	-5.25242500	1.52567200	3.52973500
H	0.63435600	0.07201200	0.50684500	C	-5.10200200	0.33339800	5.72399900
H	1.94520500	0.63907200	1.64178300	H	-6.25370500	-0.30540600	4.02247700
C	0.88379500	2.23397800	0.58559200	H	-5.41470200	1.44274100	2.45019700
H	1.41804900	3.01075300	1.13473100	H	-6.01948100	2.19019700	3.94511800
C	-0.41336900	2.59191700	0.10032500	H	-4.27832100	2.01748700	3.67720200
H	-0.98329400	1.78242100	-0.36044400	H	-5.13178400	-0.62164900	6.26303400
C	3.39582200	2.05736900	-2.84848900	H	-4.13816500	0.81051100	5.95096400
H	4.41776800	2.35460200	-2.60472500	H	-5.88840800	0.96893400	6.14539500
C	2.37996100	3.03237000	-2.61122600	P	-3.92474500	-0.63654200	-1.11335500
H	2.70978800	4.00337400	-2.23123100	C	-2.69457300	-1.27045300	-2.31287600
C	1.08544300	3.07427100	-3.38184800	C	-2.30686400	-0.53156100	-3.43750700
H	1.26192800	3.46228200	-4.40014700	C	-2.05464900	-2.49176700	-2.05781100
H	0.42292900	3.80284000	-2.89788800	C	-1.31931100	-1.01482200	-4.29324600
C	0.37760700	1.71694500	-3.44706900	H	-2.78759700	0.42351400	-3.65546300
H	0.61192800	1.20138300	-4.38969900	C	-1.05567400	-2.96120400	-2.90282800
H	-0.70859300	1.88193600	-3.46427900	H	-2.36884500	-3.09265000	-1.20364600
C	0.69961700	0.78303400	-2.28959400	C	-0.68488400	-2.22493300	-4.02575400
H	-0.14293900	0.52958400	-1.64133800	H	-1.04202900	-0.43483400	-5.17187000
C	1.72793400	-0.16921500	-2.31304500	H	-0.57259400	-3.91424200	-2.69386800
H	1.58341100	-1.05267000	-1.68937500	H	0.09386800	-2.60009900	-4.68815200
C	2.72043900	-0.32808100	-3.43505700	C	-5.12941900	0.27990300	-2.13996600
H	3.54586500	-0.95625700	-3.07795500	C	-5.72583000	1.41800400	-1.58378700
H	2.24936000	-0.89302400	-4.25895600	C	-5.52636700	-0.14425100	-3.41578000
C	3.28604500	1.00380700	-3.93919800	C	-6.72643400	2.09839600	-2.27472400
H	2.67590800	1.39795200	-4.76389000	H	-5.39349400	1.77471500	-0.60840400
H	4.28016900	0.82932100	-4.36796100	C	-6.51872900	0.54316100	-4.10828900

H	-5.04931400	-1.00991800	-3.87565100	C	3.63628400	3.00023000	-0.02888000
C	-7.12749400	1.65991900	-3.53422800	N	4.78767500	1.19518300	1.16374700
H	-7.18736600	2.97828000	-1.82851400	Cl	-0.84515900	-5.70618000	2.70539500
H	-6.82159600	0.20446200	-5.09744100	C	-0.71974400	3.91383500	-0.42504300
H	-7.91043100	2.18940900	-4.07394100	C	-1.75721100	4.05146600	-1.37843600
Cu	-3.34569800	0.31481000	0.77671800	C	-0.01833800	5.06812600	-0.06034000
O	-3.75034200	2.41679900	0.84458500	C	-2.02225500	5.32766100	-1.94234800
C	-2.84250300	3.02253900	1.43470300	C	-2.65532000	3.13296000	-1.99813100
O	-2.89792700	4.34542400	1.63171700	C	-0.31081400	6.31750500	-0.61989100
C	-1.62571900	2.39406600	1.92880900	H	0.78616900	4.99564300	0.67156300
N	-1.72826900	1.00426000	1.93241600	C	-1.31283400	6.46969100	-1.57326500
C	-0.96217400	0.28019200	2.69914700	C	-3.41415300	3.85280100	-2.88492500
H	-0.31156400	0.75194800	3.44612400	H	-2.76412300	2.07399100	-1.78291700
C	-0.92417400	-1.17053100	2.65417700	H	0.26519100	7.18646600	-0.30987300
C	-0.48060200	-1.87425600	3.78651300	H	-1.52423900	7.44203100	-2.01499100
C	-1.30734800	-1.91507600	1.52364900	H	-4.21430200	3.52776200	-3.54180200
C	-0.45414600	-3.26189700	3.81690500	N	-3.04179400	5.17982700	-2.85790700
H	-0.15621200	-1.31323700	4.66205500	C	-3.58729500	6.23852600	-3.67013200
C	-1.29505200	-3.30157400	1.54294100	H	-4.38926100	5.83568100	-4.29276300
H	-1.60196400	-1.39148100	0.61115400	H	-4.00055300	7.03876900	-3.04421100
C	-0.87215100	-3.97093700	2.69199300	H	-2.82013600	6.66873900	-4.32530100
H	-0.11442000	-3.79608900	4.70088900	H	5.91667900	1.50029300	2.83975500
H	-1.59970600	-3.87642400	0.67055900	H	3.36578800	2.48389100	2.03380800
C	-4.04046200	4.99794100	1.06863400	H	4.47082000	3.26541500	-0.69741800
H	-4.14575900	4.73728000	0.01009100	H	3.05505800	3.91905800	0.12399600
H	-4.94776700	4.70225000	1.60656000	C	4.30928900	0.27357000	3.43559300
H	-3.85391500	6.06530900	1.19132400	C	3.79231800	1.28338400	4.25719500
C	-7.58645400	-0.75763900	0.32827900	C	3.81888300	-1.02667900	3.59650500
C	-7.93533700	-1.77383800	1.26840300	C	2.79241500	1.01643900	5.18860300
H	-7.69372800	-1.77480800	2.32711700	H	4.20534200	2.29085200	4.17883600
C	-8.57981500	-2.82854300	0.55971300	C	2.82780600	-1.30048300	4.53353500
H	-8.92223600	-3.76572400	0.98508100	H	4.21918300	-1.83479300	2.98887900
C	-8.01827600	-1.18681600	-0.96427600	C	2.30696800	-0.28038600	5.32834600
H	-7.86465100	-0.65313300	-1.89739400	H	2.41407700	1.81655000	5.82323500
C	-8.63035100	-2.46640300	-0.81896600	H	2.46871800	-2.32228100	4.65066800
H	-9.02393200	-3.08001800	-1.62229400	H	1.54727200	-0.50073100	6.07814000
H	-7.04060000	0.15485200	0.55041400	C	5.18863500	3.55978400	1.82583200
C	-0.81305800	3.11047600	2.96081500	C	4.75572700	4.54119800	2.71945500
H	0.21100700	2.71853000	3.01180300	C	6.51149100	3.59186300	1.37504700
H	-0.75811200	4.17797100	2.72991500	C	5.62191500	5.54066200	3.15478300
H	-1.25094800	3.00916100	3.96602900	H	3.72188200	4.51671300	3.07327500
Fe	-6.70193100	-2.51445100	-0.16379800	C	7.38122400	4.58494500	1.81392300
C	4.19801600	2.54621500	1.30675000	H	6.85255400	2.81923600	0.68355500
C	5.38030300	0.63664400	2.42192400	C	6.93860500	5.56263300	2.70356900

H	5.27002100	6.29816200	3.85273900	H	-8.31905000	-0.55988900	-1.51541800
H	8.41117300	4.59668300	1.46164400	C	-6.92443800	0.94814800	-0.89163700
H	7.62141900	6.33698300	3.04746800	C	-3.72571800	-1.39210500	-3.06371900
C	6.42709100	-0.43267500	2.17707000	H	-4.66748900	-1.93615300	-2.96151500
H	6.02363900	-1.35346300	1.74624600	C	-2.53377500	-2.17466800	-2.98846000
H	7.20377600	-0.05688900	1.50224200	H	-2.65541500	-3.25217700	-2.84816900
H	6.90343600	-0.69008000	3.12956700	C	-1.24547700	-1.77577100	-3.66938900
TS3'				H	-1.32015000	-1.94945000	-4.75673100
Atomic	Coordinates (Angstroms)			H	-0.45236600	-2.44621100	-3.31550100
Type	X	Y	Z	C	-0.83604500	-0.32602700	-3.38736400
Ir	-2.84648800	-1.15074800	-1.08645600	H	-1.16945400	0.34372000	-4.19361600
P	-4.77073800	-0.46350400	-0.03615600	H	0.26184700	-0.26417800	-3.39333400
O	-4.85527500	0.77325800	1.06567700	C	-1.35666000	0.20478300	-2.06291600
O	-5.89507500	0.05615700	-1.13535300	H	-0.60049900	0.44635000	-1.30990600
C	-4.47397400	2.02649800	0.62488400	C	-2.55763800	0.92329300	-1.94639000
C	-3.25609200	2.52932500	1.11903900	H	-2.61345600	1.65374900	-1.13960000
H	-2.72052900	1.93434700	1.85699500	C	-3.51986000	1.15049800	-3.08331000
C	-2.79100000	3.73483200	0.65985900	H	-4.45494900	1.54266500	-2.66549500
H	-1.85516100	4.14761300	1.03539100	H	-3.12831700	1.95195600	-3.73502500
C	-3.50152400	4.44046700	-0.34238700	C	-3.81877700	-0.11804700	-3.89032100
C	-2.98228900	5.62920500	-0.90862600	H	-3.14502400	-0.19786400	-4.75499600
H	-2.02861800	6.00528600	-0.53675300	H	-4.82744000	-0.04106900	-4.31339700
C	-3.65370800	6.28993100	-1.90934000	C	5.69810900	1.61146100	-1.22124200
H	-3.24021900	7.19964000	-2.34001500	C	6.83056600	2.03884400	-2.00000200
C	-4.88040800	5.78193200	-2.38380200	H	6.79387000	2.32710600	-3.04444400
H	-5.40039600	6.29459500	-3.19040800	C	7.96528200	2.07965500	-1.14749000
C	-5.42655300	4.64373600	-1.83658400	H	8.95951800	2.40663600	-1.43251100
H	-6.37424800	4.26014700	-2.20946700	C	6.15582500	1.38608200	0.14542100
C	-4.76700300	3.94329800	-0.79691100	C	7.55644900	1.69491800	0.16038100
C	-5.29963300	2.73718900	-0.22993100	H	8.18970400	1.66257200	1.04161000
C	-6.67592800	2.25417300	-0.49087100	C	2.13129000	1.83813400	-1.99194600
C	-7.81495200	3.09976400	-0.24654600	C	2.82746500	1.97430400	-3.34517400
C	-7.70409600	4.39601900	0.31803600	H	2.54676900	2.86191500	-3.91847200
H	-6.72441400	4.77493500	0.59665700	N	3.23021000	1.37123800	-1.12049700
C	-8.81500700	5.17709700	0.53928100	C	4.33918700	1.65875900	-1.73072300
H	-8.69543600	6.16438900	0.98118500	O	4.22637500	2.11279600	-3.00063500
C	-10.10264600	4.71055100	0.21028600	H	2.72577900	1.08480200	-3.98133700
H	-10.97193600	5.34097400	0.38462100	H	1.33998400	1.07497300	-2.01384200
C	-10.25243700	3.44773300	-0.30912200	C	1.51165200	3.15582700	-1.49517400
H	-11.24210100	3.05821800	-0.54619300	C	1.07357800	3.06973900	-0.04237000
C	-9.13242700	2.61261200	-0.53446500	C	0.33328000	3.55100700	-2.37976900
C	-9.29844900	1.29195100	-1.01436000	H	2.29789400	3.92744400	-1.58130500
H	-10.30293600	0.93435700	-1.23701600	H	1.89111500	2.76397000	0.62142400
C	-8.21757100	0.46711400	-1.17128700	H	0.69030300	4.03900600	0.30099100

H	0.26893100	2.32955300	0.08331800	H	6.68714500	-1.12060900	-2.16790100
H	0.59473200	3.61422900	-3.44356100	C	-0.47804800	0.50559400	3.54652800
H	-0.48666900	2.82524700	-2.28174800	H	0.27734400	1.01023300	4.15761900
H	-0.06258700	4.52982300	-2.08596900	H	-0.76156400	1.16545200	2.71956300
P	5.13565200	0.74643800	1.50793500	H	-1.35010100	0.23841600	4.14587400
C	6.00884600	-0.72800200	2.14552500	C	5.06292500	4.55082500	0.28161500
C	5.34370000	-1.43457400	3.15903700	C	5.37786000	4.88712000	-1.07081600
C	7.21414500	-1.23375100	1.64809800	H	4.69871100	4.85332700	-1.91737400
C	5.88138100	-2.60727600	3.67596700	C	6.76782700	5.19359500	-1.13536800
H	4.38862200	-1.06232000	3.53689500	H	7.32469500	5.43822800	-2.03348600
C	7.74583200	-2.41529600	2.15996400	C	6.26137200	4.65557800	1.05106100
H	7.72831200	-0.72283700	0.83587600	H	6.36333900	4.42622100	2.10760600
C	7.08480500	-3.10188300	3.17473400	C	7.31194000	5.04963300	0.17447300
H	5.35648600	-3.14076000	4.46665000	H	8.35537400	5.17034400	0.44545800
H	8.68012100	-2.80199100	1.75562500	H	4.09385100	4.22751500	0.65133700
H	7.50280600	-4.02519400	3.57129400	C	1.13125300	-3.13614400	2.33134300
C	5.34212600	1.95512400	2.86141500	H	0.15803200	-3.04911800	2.81974600
C	4.28123000	2.82219100	3.14595500	H	1.10881500	-4.02262400	1.68666800
C	6.52748700	2.05589800	3.59984000	H	1.88577700	-3.32062200	3.11184300
C	4.41688300	3.80204900	4.12680200	Fe	6.47698900	3.29487900	-0.45400800
H	3.34639500	2.71982800	2.58954300	C	-4.49660800	-2.91365900	0.84941200
C	6.66044100	3.03190600	4.58248300	C	-6.10849400	-1.53105600	2.21548400
H	7.34425200	1.35799200	3.41158300	C	-3.83951400	-2.96322300	-0.51950800
C	5.60813400	3.91082200	4.84091800	N	-5.34088400	-1.69801300	0.94035500
H	3.58978500	4.47701300	4.33929100	C	0.07677000	-1.96132400	-0.16867300
H	7.58454500	3.10494600	5.15293100	C	-1.26137000	-1.92259000	0.35934200
H	5.71437400	4.67333700	5.60991500	H	0.47431000	-1.00711500	-0.52236800
Cu	3.16931000	0.28988500	0.63064800	H	-1.64182700	-2.86911900	0.74796600
O	1.35266600	0.49173800	1.69105400	C	-1.91207600	-0.73420300	0.82190400
C	0.97350100	-0.62083400	2.09316400	H	-1.34881100	0.20586900	0.77906500
O	0.04165100	-0.73098800	3.04865000	H	-2.55894800	-0.80501500	1.70216100
C	1.44628500	-1.89198600	1.55939400	Cl	8.48790100	-3.32350400	-2.40801800
N	2.66291700	-1.75466700	0.88474800	H	-3.70359700	-2.84407800	1.61839300
C	3.37982700	-2.82330900	0.66246000	H	-4.60625200	-3.20591700	-1.27227500
H	3.06107300	-3.78646200	1.07853800	H	-3.11107900	-3.78430300	-0.53951500
C	4.59817100	-2.88838800	-0.11033400	H	-6.45923100	-2.55148300	2.42533100
C	5.31477000	-4.09978000	-0.10663100	C	-5.28085600	-4.17828400	1.09892200
C	5.10730300	-1.82820800	-0.88087000	C	-4.69571200	-5.21786400	1.82436200
C	6.50182700	-4.24349000	-0.80751100	C	-6.55286600	-4.36857400	0.54965100
H	4.93157100	-4.93919500	0.47459400	C	-5.36134600	-6.42864100	1.99629600
C	6.29544900	-1.95312700	-1.58547600	H	-3.70225300	-5.07105200	2.25507200
H	4.55309200	-0.89286400	-0.92827100	C	-7.22297100	-5.57411300	0.72605700
C	6.98954800	-3.16030900	-1.53906200	H	-7.01410200	-3.55305400	-0.01030800
H	7.05646100	-5.17818000	-0.78588100	C	-6.62822000	-6.60832800	1.44783300

H	-4.89280400	-7.23011200	2.56448900	C	3.35945200	0.79748100	0.43089800
H	-8.21489200	-5.70976100	0.29869100	F	3.92326400	1.67597600	-0.38537900
H	-7.15417500	-7.55103800	1.58541800	F	4.27745700	0.23945600	1.20670000
C	-5.21643100	-1.13752100	3.38063100	F	2.44618500	1.41046700	1.18769900
C	-4.46032000	-2.13084300	4.01651900	O	-1.35835500	0.33804100	1.20659300
C	-5.12557200	0.17162100	3.86465800	S	-2.49700000	-0.47180800	0.60022000
C	-3.60889700	-1.82375100	5.07467700	O	-1.79776700	-1.37574100	-0.40765900
H	-4.56713700	-3.16764000	3.69174500	O	-3.46530600	-1.06269300	1.48964400
C	-4.28516500	0.48223800	4.92926300	C	-3.38597500	0.75409600	-0.46703000
H	-5.71988100	0.95906000	3.40644000	F	-2.50158700	1.33797500	-1.27861500
C	-3.51865600	-0.51251100	5.53464600	F	-3.95901800	1.67129800	0.29838500
H	-3.03690100	-2.61461600	5.55695900	F	-4.30161700	0.12111700	-1.18640800
H	-4.23966600	1.50617200	5.29766100				
H	-2.87168900	-0.26979200	6.37664300				
C	-7.34864900	-0.67782600	2.02971700				
H	-7.12588500	0.36149600	1.76828900				
H	-7.97922300	-1.09565000	1.23698300				
H	-7.93078900	-0.67126600	2.95770400				
C	0.61656200	-3.12348900	-0.85052200				
C	1.64956000	-2.95749100	-1.80655300				
C	0.20085000	-4.43797400	-0.58541700				
C	2.24692500	-4.09767800	-2.40808200				
C	2.28157900	-1.81734900	-2.37310400				
C	0.80136200	-5.54377400	-1.19743400				
H	-0.60443300	-4.60959700	0.12823300				
C	1.84413000	-5.39553800	-2.10840200				
C	3.22424900	-2.28013400	-3.25667500				
H	2.11083600	-0.78179200	-2.11083500				
H	0.44815600	-6.54258500	-0.95053300				
H	2.31310000	-6.26191900	-2.57163700				
H	3.93889500	-1.73699800	-3.86616300				
N	3.21321000	-3.65309700	-3.28667200				
C	4.13913600	-4.49890200	-3.99945000				
H	3.60318100	-5.22713000	-4.61874400				
H	4.76283800	-3.88109400	-4.64998200				
H	4.79333500	-5.03683800	-3.30031600				

Zn(OTf)₂

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
Zn	0.00664400	-0.55464000	0.00123200
O	1.80398800	-1.35319700	0.48649300
S	2.51786500	-0.51565300	-0.56615200
O	1.38622100	0.23640800	-1.25545800
O	3.51419600	-1.15500600	-1.38795100

OTf

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
O	1.23246400	-0.56068800	1.32612300
S	0.92166000	0.00087400	-0.00037400
O	1.23232900	1.43058100	-0.17821400
O	1.22718300	-0.86901700	-1.15001000
C	-0.92780400	0.00100700	0.00091500
F	-1.43672800	0.74576000	1.00555100
F	-1.42858200	-1.24544200	0.14477100
F	-1.43641700	0.49667800	-1.14839900

IM5

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
O	-3.16839900	-1.84594600	-1.43920300
C	-3.28859100	-1.55531000	-0.27038000
O	-4.28184900	-2.02103300	0.51346700
C	-2.34686500	-0.59569200	0.47190000
N	-1.01741800	-1.15726800	0.29029600
C	-0.07971800	-0.80866500	1.08572400
H	-0.23120100	-0.15549400	1.96373300
C	1.31120100	-1.17179300	0.82316900
C	2.33178900	-0.60055100	1.59047700
C	1.65332800	-2.01433800	-0.24378500
C	3.66910100	-0.84508700	1.29937100
H	2.07098700	0.06892200	2.41153500
C	2.98038300	-2.28103700	-0.53815300
H	0.85080200	-2.43916400	-0.84383700
C	3.97859100	-1.68328700	0.23265700
H	4.46526800	-0.39422600	1.88684900
H	3.25310300	-2.93366300	-1.36388600
C	-5.21054900	-2.86809500	-0.16768400

H	-5.68490300	-2.32376800	-0.99049900	C	-0.91614800	-0.65188300	1.40195000
H	-4.70185800	-3.74657000	-0.57596200	O	-1.88564200	-0.24065500	2.24590200
H	-5.94937800	-3.15963400	0.57986200	C	-0.16124800	0.53896200	0.79402900
C	-2.76127900	-0.35207600	1.91692700	N	1.17553000	0.05258700	0.51650600
H	-2.15956700	0.44196500	2.37182800	C	2.19325500	0.79655000	0.70492600
H	-3.81197000	-0.05436600	1.97756500	H	2.13961400	1.81556700	1.12849900
H	-2.63816000	-1.26308200	2.51178700	C	3.54203300	0.34263100	0.36257600
Cl	5.65239500	-1.97593100	-0.16564000	C	4.63852000	1.17622200	0.60648600
C	-4.71206100	1.13979600	-1.27863600	C	3.76233500	-0.91733700	-0.21233300
H	-4.50191600	0.54401100	-2.16701700	C	5.93069600	0.77309100	0.29241300
H	-5.70899600	1.56761200	-1.19714800	H	4.47503800	2.15849200	1.05104400
C	-3.78574800	1.33370000	-0.34006000	C	5.04406300	-1.33437000	-0.53227000
H	-4.03806100	1.92974100	0.53987100	H	2.90251100	-1.55928300	-0.39421200
C	-2.40559300	0.74870800	-0.39485400	C	6.11976500	-0.48289500	-0.27521300
H	-2.22296600	0.40165500	-1.41947900	H	6.78461300	1.41762200	0.48357600
C	-1.30780700	1.70391300	-0.00947800	H	5.22202800	-2.31119000	-0.97503600
C	-0.07270300	1.63590100	-0.68754400	C	-2.76305300	-1.28235300	2.67944500
C	-1.40843000	2.60412500	1.04998700	H	-3.15438100	-1.82819400	1.81428300
C	1.01461500	2.43709500	-0.24741500	H	-2.23467000	-1.98383000	3.33307300
C	0.41114800	0.83682600	-1.76758400	H	-3.56668000	-0.78117000	3.22093600
C	-0.32690300	3.40434800	1.45442900	C	-0.26196800	1.79712800	1.64478000
H	-2.34821100	2.69213800	1.59406000	H	0.19809500	2.65248700	1.13519100
C	0.90574300	3.32708200	0.82030700	H	-1.30649300	2.04130800	1.84750300
C	1.73063600	1.15832800	-1.93580800	H	0.24374600	1.66191800	2.60808800
H	-0.13376800	0.07588300	-2.31370000	Cl	7.73493600	-1.00727300	-0.67076900
H	-0.45843900	4.09259500	2.28737700	C	-2.33679400	0.90645400	-0.55675200
H	1.74814700	3.93666400	1.14502400	C	-3.17245400	-0.21019300	-0.76767000
H	2.46722400	0.76397900	-2.62697500	C	-2.95195100	2.11490000	-0.23855000
N	2.10638300	2.12712800	-1.02798000	C	-4.58044500	-0.06134800	-0.63875500
C	3.43030900	2.66266100	-0.85512500	C	-2.93342700	-1.57838200	-1.10920900
H	3.79363300	2.48322000	0.16542200	C	-4.34501100	2.23835900	-0.11616000
H	4.11050100	2.16708700	-1.55256300	H	-2.34129700	3.00097900	-0.07009400
H	3.45464300	3.74283000	-1.04894900	C	-5.18419800	1.15198100	-0.31186800

IM6

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	0.88722900	1.72365700	-2.17882800
H	1.33254700	0.74328800	-2.35097300
H	1.34548800	2.56612900	-2.69298800
C	-0.16719800	1.87652000	-1.37830100
H	-0.57740800	2.87758800	-1.23026700
C	-0.83485600	0.75268800	-0.64357000
H	-0.60796500	-0.18548300	-1.16772000
O	-0.72529000	-1.81005900	1.11282000

C	-4.15516600	-2.19129800	-1.17363800
H	-1.97512600	-2.06312200	-1.24627800
H	-4.77141400	3.20758400	0.13602200
H	-6.26547200	1.24621600	-0.22072100
H	-4.41510600	-3.21936900	-1.39840200
N	-5.15799000	-1.28571600	-0.88701900
C	-6.57252800	-1.54875300	-0.88947900
H	-6.73915100	-2.61260700	-1.07597400
H	-7.02135800	-1.29235400	0.07873300
H	-7.08510000	-0.97331500	-1.67143900

TS4

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	4.04506900	1.23775400	-1.35871300
C	2.98574900	0.33594200	-1.16501500
C	3.26658700	-1.00090400	-0.85512500
C	4.60789300	-1.38573600	-0.85306500
C	5.64588200	-0.47569300	-1.09031900
C	5.38494000	0.86908500	-1.32146700
C	2.15815300	2.43551400	-1.51001500
C	1.74105500	1.11330100	-1.19653400
H	4.85380500	-2.42197800	-0.62490000
H	6.67535400	-0.82464200	-1.06995500
H	6.18866600	1.58750900	-1.46518400
H	1.54840000	3.31906600	-1.66669700
N	3.49094100	2.51429700	-1.54691400
C	4.28162400	3.71645500	-1.72857300
H	4.89723500	3.89740700	-0.84169700
H	4.93371900	3.60007900	-2.59943100
H	3.61684200	4.56661300	-1.88698800
C	2.18763400	-1.93285000	-0.34847100
C	0.97952900	0.99511700	0.56688600
H	1.83776800	1.35729800	1.13244600
C	1.64202500	-1.37863600	1.03348300
N	0.65283900	-0.31174500	0.80279400
H	2.64758400	-2.90361100	-0.12103900
C	-0.18842200	1.91852700	0.54339900
C	-0.32537800	2.87747400	1.55207700
C	-1.20314700	1.80295600	-0.41476300
C	-1.45650900	3.68259800	1.61772600
H	0.45039500	2.97866500	2.30974800
C	-2.34384200	2.59588600	-0.35908400
H	-1.10637800	1.11680600	-1.25860000
C	-2.46507600	3.53248800	0.66535500
H	-1.56587200	4.42008900	2.40837900
H	-3.12589000	2.49493500	-1.10721200
C	0.92291200	-2.48324000	1.81102600
H	1.58690500	-3.32975100	2.00453900
H	0.55758300	-2.09520900	2.76769200
H	0.05204700	-2.86952300	1.26171600
C	2.85128300	-0.93947300	1.87398900
O	3.07572500	0.16783700	2.31077600
O	3.65914000	-1.99392100	2.05881000
C	4.87146700	-1.70850200	2.77848200

H	4.63900700	-1.34641700	3.78269100
H	5.41142300	-2.65372000	2.82161900
H	5.45082300	-0.94982700	2.24403400
C	1.06023800	-2.14200300	-1.32885500
C	0.24557100	-3.20660200	-1.36758800
H	0.91688000	-1.36548900	-2.08538900
H	-0.53979900	-3.29106300	-2.11692000
H	0.35859000	-4.05104600	-0.68806000
Cl	-3.87446900	4.53058500	0.74488300
Zn	-0.95834200	-1.04055200	0.08834500
O	-2.36167900	-1.00285700	-1.42087300
S	-3.23649700	-2.01816300	-0.69706300
O	-2.48665700	-2.26968500	0.60598600
O	-3.69253700	-3.16556000	-1.44221200
C	-4.71470300	-1.03026200	-0.17869300
F	-5.36590700	-0.63797600	-1.26361500
F	-4.29299700	0.03693900	0.50453300
F	-5.49424800	-1.77370100	0.58721900
H	0.85188200	0.74409800	-1.70230100

TS4'

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-3.93162200	1.39795100	-1.43081600
C	-2.93859400	0.46393300	-1.10171900
C	-3.29666700	-0.81766000	-0.67460100
C	-4.65708700	-1.13113900	-0.69284000
C	-5.63120500	-0.19263900	-1.05864000
C	-5.29080200	1.10659000	-1.41439800
C	-1.96782400	2.46391400	-1.60541800
C	-1.64724500	1.15873600	-1.13335700
H	-4.98153600	-2.12971300	-0.40922300
H	-6.67801800	-0.48533800	-1.04861300
H	-6.04827100	1.84495900	-1.66625500
H	-1.29780200	3.29165300	-1.81290200
N	-3.28879000	2.61527000	-1.72014700
C	-3.99226300	3.83075700	-2.08251400
H	-4.58666000	3.65631000	-2.98453400
H	-4.65874800	4.13490900	-1.26924100
H	-3.26943200	4.62477100	-2.27444200
C	-2.23339900	-1.74929100	-0.13487500
C	-1.10576600	1.17660500	0.67912600
H	-2.05490900	1.49946700	1.12647600
C	-1.66739500	-1.16917800	1.24558100
N	-0.70277600	-0.08566300	1.00347200

H	-1.36915800	-1.73558600	-0.82173500	C	-4.75320700	-1.87509500	-0.45192800
C	-0.04035400	2.21575300	0.78306300	C	-5.91885100	-1.10789000	-0.56720400
C	-0.14560700	3.19421700	1.77469300	C	-5.85982800	0.26655400	-0.76441900
C	1.09370900	2.20640500	-0.03750700	C	-2.89348000	2.26175900	-1.11337600
C	0.86826400	4.12575700	1.96552300	C	-2.27610300	0.99006300	-0.90456100
H	-1.02178100	3.21773800	2.42206300	H	-4.84216800	-2.94364100	-0.25971000
C	2.12180400	3.12440400	0.14703500	H	-6.88696800	-1.59410400	-0.47774300
H	1.17355700	1.49968400	-0.86535200	H	-6.76086300	0.87326200	-0.81563400
C	2.00243200	4.07934400	1.15583000	H	-2.41711400	3.22562000	-1.26118800
H	0.78883900	4.88004800	2.74363100	N	-4.22014200	2.16110300	-1.05225800
H	3.00347600	3.09772300	-0.48818800	C	-5.17577500	3.24969100	-1.13138900
C	-2.78624500	-0.78002900	2.20222500	H	-5.85369900	3.08107200	-1.97346800
H	-3.45647300	-1.62445000	2.38801900	H	-5.75985400	3.30280800	-0.20719000
H	-2.37846100	-0.45130200	3.16319400	H	-4.64295600	4.19002900	-1.27841000
H	-3.39510600	0.02834400	1.78593500	C	-2.24316300	-2.13111300	-0.25724300
C	-0.81740500	-2.30366000	1.81974100	C	-1.37814500	0.86987400	0.71134100
O	0.36125000	-2.48968400	1.47966100	H	-2.22867900	1.01167600	1.39246800
O	-1.43677800	-3.08668000	2.66266800	C	-1.50885700	-1.58141200	1.03948400
C	-0.69612400	-4.23755300	3.13968600	N	-0.76178800	-0.35109000	0.77807100
H	0.22216400	-3.90840900	3.62927700	C	-0.43384300	2.02738500	0.70899600
H	-1.36427700	-4.72973200	3.84327100	C	-0.47515100	2.97647200	1.73345000
H	-0.45706900	-4.88947800	2.29618100	C	0.53318200	2.16389200	-0.29594000
C	-2.68397000	-3.17328700	0.00101700	C	0.44130100	4.02182400	1.77119500
C	-2.11084800	-4.19216800	-0.63838100	H	-1.21951600	2.88936400	2.52467600
H	-3.50468700	-3.36880800	0.69515500	C	1.46206700	3.19710100	-0.26818100
H	-2.45530900	-5.21532000	-0.50976700	H	0.56549800	1.46398700	-1.13514300
H	-1.28273700	-4.04027200	-1.33086200	C	1.40927100	4.12297400	0.77235900
Cl	3.27261700	5.22834400	1.39819000	H	0.41481400	4.75343000	2.57440600
Zn	1.04805200	-0.76629200	0.56963500	H	2.22097200	3.28227600	-1.04121400
O	1.60031700	-0.85981100	-1.50535500	C	-2.48555200	-1.46432400	2.20945600
S	3.04310500	-0.65274700	-1.10472600	H	-2.96663400	-2.42570700	2.41116400
O	3.01988400	-0.66416500	0.42519200	H	-1.96716800	-1.13656000	3.11683500
O	3.77432900	0.42562600	-1.73097300	H	-3.27829900	-0.74356100	1.98502100
C	3.87263100	-2.25107700	-1.53495700	C	-0.45341700	-2.64374100	1.36627800
F	5.09094500	-2.26771700	-1.01992000	O	0.76493000	-2.48635900	1.22352400
F	3.92656000	-2.35759700	-2.85405400	O	-0.96421800	-3.78096600	1.77583100
F	3.15301100	-3.25443500	-1.03060400	C	-0.02231900	-4.85161600	2.03218700
H	-0.74953900	0.68175600	-1.52735100	H	0.67169700	-4.55158700	2.81954600
TS5				H	-0.63297000	-5.69598000	2.34580200
Atomic	Coordinates (Angstroms)			H	0.53137000	-5.07819300	1.11825600
Type	X	Y	Z	Cl	2.55273000	5.41915700	0.81717000
C	-4.58767300	0.81148200	-0.88899900	Zn	1.10237800	-0.63222700	0.38067700
C	-3.40802900	0.05490600	-0.82514000	O	2.10066300	-0.66192900	-1.45109500
C	-3.47851000	-1.31375600	-0.55033000	S	3.34441800	-0.07727500	-0.80825600

O	2.98412700	0.04493600	0.66599100	H	-1.16380100	1.48291800	-1.22876900
O	3.95424400	1.06900800	-1.44229300	C	-2.03179200	4.18202900	0.60946800
C	4.56566600	-1.46660100	-0.83529800	H	-0.85773800	5.06859100	2.18011100
F	5.62874500	-1.12717300	-0.12268300	H	-2.98867100	3.11747800	-1.00438900
F	4.91277400	-1.71784400	-2.08940700	C	0.23264700	-2.23525500	1.70164600
F	3.99271700	-2.54761300	-0.30136500	H	0.71044300	-3.16982800	2.00284300
H	-1.41446000	0.77279000	-1.53322100	H	-0.19895400	-1.76423800	2.59378400
H	-2.57427200	-3.14707700	0.00172000	H	-0.57477700	-2.51687500	1.00601100
C	-1.28360900	-2.22723500	-1.41191600	C	2.41857600	-1.04747300	1.93204400
C	-0.71233100	-3.36208900	-1.81459200	O	2.79557000	0.01971100	2.36305100
H	-1.02675600	-1.29911900	-1.92702900	O	3.03116500	-2.21441200	2.17682900
H	0.00099200	-3.38234700	-2.63463400	C	4.22798300	-2.11327100	2.97022700
H	-0.94585200	-4.31945300	-1.34602100	H	3.99535800	-1.68999200	3.94994200

TSS'

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	3.98141800	0.94028900	-1.45753100
C	2.83087000	0.16745800	-1.24193700
C	2.94013300	-1.15936900	-0.81891600
C	4.22921600	-1.68420000	-0.71968500
C	5.36735600	-0.90500000	-0.97262500
C	5.27045100	0.43551500	-1.32578400
C	2.22412000	2.29068500	-1.79630500
C	1.67403200	1.05002500	-1.38173100
H	4.36365600	-2.72318900	-0.42633300
H	6.35085000	-1.35891600	-0.87668700
H	6.15568900	1.04550100	-1.49025300
H	1.71222800	3.21167800	-2.05495400
N	3.56116600	2.24041600	-1.78147100
C	4.47000400	3.33793300	-2.05052300
H	5.08526400	3.54113400	-1.16825600
H	5.12313300	3.07688600	-2.88870300
H	3.89681500	4.23044700	-2.30554300
C	1.69168400	-1.89068300	-0.36937200
C	1.00330700	1.16745600	0.45876400
H	1.95656900	1.40202300	0.93461500
C	1.21089700	-1.28274400	1.01636200
N	0.45892700	-0.03879900	0.78297400
C	-0.00226500	2.26374900	0.44159300
C	0.08326100	3.30679600	1.36763800
C	-1.11565000	2.21396100	-0.41631300
C	-0.92243900	4.26335500	1.45299600
H	0.93171900	3.35557800	2.04829200
C	-2.13524700	3.16011300	-0.33255500

H	-1.16380100	1.48291800	-1.22876900
C	-2.03179200	4.18202900	0.60946800
H	-0.85773800	5.06859100	2.18011100
H	-2.98867100	3.11747800	-1.00438900
C	0.23264700	-2.23525500	1.70164600
H	0.71044300	-3.16982800	2.00284300
H	-0.19895400	-1.76423800	2.59378400
H	-0.57477700	-2.51687500	1.00601100
C	2.41857600	-1.04747300	1.93204400
O	2.79557000	0.01971100	2.36305100
O	3.03116500	-2.21441200	2.17682900
C	4.22798300	-2.11327100	2.97022700
H	3.99535800	-1.68999200	3.94994200
H	4.60014200	-3.13269800	3.06558700
H	4.95730000	-1.47440300	2.46347500
Cl	-3.27691500	5.37289800	0.71443900
Zn	-1.39829600	-0.21510900	0.50339500
H	0.73719100	0.71045800	-1.81924500
O	-2.20125100	-0.93308600	-1.37188300
S	-3.56196700	-0.98595300	-0.72559100
O	-4.68513700	-0.37378700	-1.38944500
O	-3.29818400	-0.53197300	0.72658300
C	-3.91424900	-2.79406500	-0.52398800
F	-4.08412700	-3.33513700	-1.71897100
F	-2.86501500	-3.36357900	0.08056600
F	-4.99610800	-2.94983300	0.21685800
H	0.87139900	-1.64061400	-1.06490900
C	1.81117800	-3.38395100	-0.36128600
C	1.00659300	-4.17418500	-1.07053900
H	2.57911600	-3.82167400	0.27732500
H	1.10258000	-5.25675000	-1.05331200
H	0.21917700	-3.76527300	-1.70606300

(6*S*,7*S*,9*R*)-3a

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.58806500	2.54366200	0.06546100
C	-1.37759600	1.13921200	0.17782400
C	-2.37832300	0.35633200	0.78572100
C	-3.53090400	1.00045700	1.22438000
C	-3.72100100	2.38251300	1.08730100
C	-2.74512400	3.18055200	0.50976800
C	0.41834400	2.08089300	-0.79254900
C	-0.08555700	0.86859000	-0.38938400
H	-4.30529400	0.40261800	1.70624600

				Atomic	Coordinates (Angstroms)		
				Type	X	Y	Z
H	-4.64410700	2.83355300	1.44663200				
H	-2.87555800	4.25686700	0.40832400				
H	1.37126200	2.30906800	-1.25877300	C	1.82255700	2.31430100	-0.45226100
N	-0.47538700	3.09241300	-0.52728300	C	1.54946300	0.92961400	-0.58448300
C	-0.27716300	4.49467500	-0.77896100	C	2.60725700	0.01424400	-0.68254800
H	-1.03858800	4.88440200	-1.46672800	C	3.90063300	0.52148400	-0.69699100
H	-0.32291500	5.07315500	0.15265700	C	4.15518200	1.89877400	-0.59036500
H	0.70658400	4.64227300	-1.23079000	C	3.12338400	2.81809700	-0.44944600
C	-2.22170300	-1.12118000	1.06688700	C	-0.39525600	2.01979000	-0.37692000
C	0.60391200	-0.44145100	-0.64888200	C	0.12849300	0.76131600	-0.53308000
H	0.49339700	-0.67375000	-1.72378600	H	4.73851200	-0.17333500	-0.76091500
C	-1.35413100	-1.90386300	0.04697100	H	5.18552500	2.24986400	-0.59489000
N	0.06463400	-1.53690500	0.17057500	H	3.32500100	3.88251700	-0.33820600
H	-3.22614300	-1.56677800	1.02941800	H	-1.43004600	2.33838700	-0.31418100
H	0.61986800	-2.35779600	-0.05685300	N	0.61468300	2.96180100	-0.32831900
C	2.08879200	-0.35263100	-0.36773400	C	0.44844700	4.37797900	-0.13776900
C	3.02100300	-0.50705200	-1.39182800	H	0.87065100	4.70673300	0.82113100
C	2.55053900	-0.11261900	0.93038000	H	0.93931100	4.93865200	-0.94298900
C	4.38948400	-0.42096800	-1.14123500	H	-0.61713800	4.61926600	-0.14853000
H	2.67272500	-0.70239300	-2.40655200	C	2.33869500	-1.47452300	-0.65832200
C	3.90886300	-0.02823800	1.20346800	C	-0.61484400	-0.51375500	-0.82471600
H	1.82372000	0.00847600	1.73256000	C	1.22413300	-1.86388400	0.36424100
C	4.81876300	-0.18280300	0.15837300	N	-0.13140300	-1.75264600	-0.16952000
H	5.11532000	-0.54332100	-1.94090800	H	3.25670100	-1.95437100	-0.29021600
H	4.26858700	0.15681500	2.21257500	H	-0.75889400	-1.95377200	0.60534100
C	-1.44568300	-3.39834900	0.37724000	C	1.40609200	-3.34024500	0.74010300
H	-2.48866800	-3.73325500	0.40291400	H	2.36855300	-3.50566300	1.23704100
H	-0.91114400	-3.98983100	-0.37557700	H	0.60907000	-3.66980200	1.41788600
H	-1.00290800	-3.58271700	1.36207200	H	1.35758300	-3.95112200	-0.16729400
C	-1.87795900	-1.78115900	-1.38729400	C	1.37933000	-1.05594000	1.66166400
O	-1.21589500	-2.02432200	-2.37549900	O	0.46089600	-0.58266900	2.29894700
O	-3.18092200	-1.43910500	-1.43296400	O	2.66690300	-0.99329800	2.05322000
C	-3.72227300	-1.34005200	-2.75209000	C	2.90666600	-0.17358900	3.19811700
H	-3.65086700	-2.30088900	-3.27096200	H	2.31975800	-0.51838100	4.05445400
H	-4.76431900	-1.04675000	-2.62136600	H	3.97535800	-0.25331900	3.40090200
H	-3.17827600	-0.58661500	-3.32939800	H	2.63781900	0.86503300	2.97553300
C	-1.69638600	-1.29346100	2.46578400	C	2.05812800	-2.03332000	-2.02366100
C	-2.37525300	-1.86745000	3.45774200	C	2.78087800	-2.99270700	-2.59966200
H	-0.69784000	-0.88962500	2.64048300	H	1.21564300	-1.59690100	-2.56425600
H	-1.96925200	-1.94746500	4.46399000	H	2.55695300	-3.36340700	-3.59747900
H	-3.37343900	-2.27973800	3.30229900	H	3.63265500	-3.44569700	-2.09086700
Cl	6.53012900	-0.07771200	0.49071200	H	-0.51525100	-0.68630200	-1.91288600
				C	-2.09178700	-0.36918800	-0.54184100
				C	-3.03974500	-0.47702400	-1.55751500

(6S,7S,9S)-3a

C	-2.52847400	-0.11952500	0.76486900
C	-4.39938600	-0.33631700	-1.29158900
H	-2.71227700	-0.67877600	-2.57731400
C	-3.88131700	0.02222000	1.05001900
H	-1.78802200	-0.03431600	1.56148700
C	-4.80631400	-0.08729300	0.01420600
H	-5.13742000	-0.42502200	-2.08443400
H	-4.22186000	0.21709900	2.06396600
Cl	-6.50863700	0.08783800	0.36246800

(6R,7S,9S)-3a

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	0.90501600	3.16473800	-0.04756400
C	1.04701300	1.74799200	-0.09565300
C	2.28804200	1.18400700	0.27043300
C	3.30689300	2.05472300	0.64861800
C	3.14258900	3.44615400	0.68157000
C	1.93122000	4.02524900	0.33701800
C	-1.03783500	2.30752100	-0.73245100
C	-0.21344100	1.22582400	-0.54757400
H	4.26551600	1.62775000	0.94557000
H	3.97652500	4.07635200	0.98441400
H	1.78712100	5.10437700	0.36271900
H	-2.07533200	2.33692200	-1.04848500
N	-0.37571900	3.47720400	-0.44028300
C	-0.92797500	4.80476700	-0.48402800
H	-0.33826300	5.45211600	-1.14525000
H	-0.95208200	5.25953100	0.51484400
H	-1.94952400	4.75531900	-0.86839700
C	2.56464300	-0.30240800	0.35118400
C	-0.59326900	-0.19801200	-0.85403900
H	-0.55926600	-0.33230900	-1.95669500
C	1.69617000	-1.17396800	-0.59815000
N	0.29208900	-1.13580800	-0.17332500
C	-2.01961100	-0.48220200	-0.43603400
C	-3.01938600	-0.66648200	-1.38917400
C	-2.36490900	-0.52670900	0.91832700
C	-4.34364100	-0.88282700	-1.01404900
H	-2.76021600	-0.64016000	-2.44820800
C	-3.67719300	-0.74941500	1.31402100
H	-1.58441900	-0.38397900	1.66432900
C	-4.65846300	-0.92130800	0.33868000
H	-5.12212300	-1.02384900	-1.75932100
H	-3.94703700	-0.78560200	2.36662900

C	1.95079600	-0.78741200	-2.06322200
H	3.01511200	-0.88770400	-2.29829300
H	1.38584400	-1.43234700	-2.74757400
H	1.65892300	0.25128900	-2.25100000
C	2.13810900	-2.63105100	-0.43231500
O	1.39531400	-3.56321800	-0.20874800
O	3.46589400	-2.76627900	-0.60396100
C	3.95272400	-4.09772100	-0.41910800
H	3.48014200	-4.78369400	-1.12823600
H	5.02831800	-4.04436000	-0.59134300
H	3.74017300	-4.43886800	0.59885200
H	-0.08447300	-2.07804100	-0.25470900
Cl	-6.31331700	-1.18755400	0.82594200
H	3.61191700	-0.45887200	0.05652700
C	2.42005700	-0.77507600	1.77232200
C	3.40510200	-1.32703900	2.47995400
H	1.42694200	-0.64872400	2.20616000
H	3.26293400	-1.65724600	3.50689400
H	4.39949200	-1.46936900	2.05390100

(6R,7S,9R)-3a

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.69006100	2.98176700	-0.07751500
C	-1.53112900	1.57777700	-0.04380900
C	-2.61937500	0.74947300	0.27672500
C	-3.81707900	1.36598900	0.61729200
C	-3.95021100	2.76629100	0.61810700
C	-2.89924800	3.59660300	0.25247500
C	0.42316500	2.49100200	-0.63928400
C	-0.17645400	1.28324500	-0.38951200
H	-4.68232600	0.74854200	0.85939800
H	-4.90775800	3.20702600	0.88970400
H	-3.01817900	4.67880400	0.22773000
H	1.44972800	2.71956900	-0.90449400
N	-0.48271200	3.52207700	-0.46369200
C	-0.21021900	4.92671500	-0.61188200
H	-0.35758300	5.46188500	0.33541600
H	-0.86283900	5.37873700	-1.36981500
H	0.82785400	5.05966300	-0.92632600
C	-2.51227700	-0.73919900	0.04746000
C	0.42087800	-0.09219100	-0.28135100
C	-1.37930900	-1.44542500	0.87476800
N	-0.12140400	-0.70055700	0.95880100
H	0.16247300	-0.70695700	-1.16263400

C	1.92619500	-0.08898400	-0.18449400	N	-0.77424700	3.16408300	-0.54914600
C	2.69488400	-0.88477000	-1.03430900	C	-0.70635400	4.58086100	-0.83043000
C	2.57544700	0.65967400	0.80318500	H	-1.48464100	4.86438300	-1.54674700
C	4.08215700	-0.92188700	-0.92803000	H	-0.83656700	5.16723900	0.08605500
H	2.19680200	-1.49646500	-1.78603800	H	0.26817400	4.81466600	-1.26311700
C	3.95964500	0.63260500	0.92883600	C	-2.09377200	-1.09273900	1.19802000
H	1.98027500	1.26845900	1.48255500	C	0.63052400	-0.20609600	-0.62510500
C	4.70161200	-0.15697200	0.05386300	H	0.43900500	-0.51990700	-1.65746400
H	4.67886200	-1.54033400	-1.59334700	C	-1.27770400	-1.94890600	0.20048700
H	4.46449400	1.21333500	1.69691100	N	0.17616800	-1.47387900	0.15929400
Cl	6.44201700	-0.18759900	0.19596600	H	-3.01035600	-1.67312200	1.36597900
H	0.57642800	-1.36325600	1.29118500	H	0.73503500	-2.23338600	-0.24307100
C	-1.87149600	-1.61404800	2.31472300	C	2.11557700	-0.10602900	-0.40323300
H	-2.76074200	-2.25011600	2.36500000	C	2.99023000	-0.73061500	-1.29830900
H	-1.09206800	-2.06133400	2.94347100	C	2.64012800	0.54561700	0.71867100
H	-2.10716100	-0.62693900	2.72698500	C	4.36320800	-0.70622900	-1.08719500
C	-1.14034400	-2.82146200	0.24039700	H	2.59409800	-1.22940100	-2.18409900
O	-0.09616400	-3.18377100	-0.25971600	C	4.00971900	0.57492800	0.94484000
O	-2.24065400	-3.60011300	0.31131000	H	1.96836700	1.05610300	1.40927800
C	-2.11102400	-4.86385100	-0.34433600	C	4.86442100	-0.05405100	0.03847800
H	-1.29989100	-5.44749300	0.10088100	H	5.04490800	-1.17866700	-1.78900300
H	-3.06895600	-5.36773800	-0.20875400	H	4.42166000	1.08361000	1.81231900
H	-1.89860600	-4.71647000	-1.40831200	C	-1.22031100	-3.40611000	0.65781700
H	-3.44024200	-1.21596400	0.39382500	H	-2.23268700	-3.81996200	0.68699200
C	-2.43808900	-0.97727200	-1.44411200	H	-0.62989500	-4.02145500	-0.03145300
C	-3.20745300	-1.83692700	-2.11110100	H	-0.79561900	-3.48235200	1.66529700
H	-1.73448600	-0.35335900	-1.99869100	C	-1.79857800	-1.94338200	-1.23236500
H	-3.13577900	-1.94794800	-3.19098100	O	-1.07008700	-2.03317700	-2.19949600
H	-3.94252200	-2.46094200	-1.60218000	O	-3.12390900	-1.93477500	-1.24746800

(6*S*,7*S*,9*R*)-**3a**-H⁺

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.88043000	2.50754400	-0.05643300
C	-1.53281600	1.14295000	0.12916200
C	-2.48016600	0.27926800	0.71131500
C	-3.74065100	0.78479300	1.00023100
C	-4.07648600	2.12577100	0.75837600
C	-3.14246400	3.01456200	0.24983300
C	0.24583800	2.26532500	-0.68091100
C	-0.16503700	1.00710800	-0.28752200
H	-4.47905100	0.12531600	1.45513600
H	-5.07611500	2.47716000	1.00194300
H	-3.38440400	4.06460400	0.09910200
H	1.20169100	2.58155800	-1.08406400

N	-0.77424700	3.16408300	-0.54914600
C	-0.70635400	4.58086100	-0.83043000
H	-1.48464100	4.86438300	-1.54674700
H	-0.83656700	5.16723900	0.08605500
H	0.26817400	4.81466600	-1.26311700
C	-2.09377200	-1.09273900	1.19802000
C	0.63052400	-0.20609600	-0.62510500
H	0.43900500	-0.51990700	-1.65746400
C	-1.27770400	-1.94890600	0.20048700
N	0.17616800	-1.47387900	0.15929400
H	-3.01035600	-1.67312200	1.36597900
H	0.73503500	-2.23338600	-0.24307100
C	2.11557700	-0.10602900	-0.40323300
C	2.99023000	-0.73061500	-1.29830900
C	2.64012800	0.54561700	0.71867100
C	4.36320800	-0.70622900	-1.08719500
H	2.59409800	-1.22940100	-2.18409900
C	4.00971900	0.57492800	0.94484000
H	1.96836700	1.05610300	1.40927800
C	4.86442100	-0.05405100	0.03847800
H	5.04490800	-1.17866700	-1.78900300
H	4.42166000	1.08361000	1.81231900
C	-1.22031100	-3.40611000	0.65781700
H	-2.23268700	-3.81996200	0.68699200
H	-0.62989500	-4.02145500	-0.03145300
H	-0.79561900	-3.48235200	1.66529700
C	-1.79857800	-1.94338200	-1.23236500
O	-1.07008700	-2.03317700	-2.19949600
O	-3.12390900	-1.93477500	-1.24746800
C	-3.72441600	-2.00400400	-2.55901000
H	-3.39879300	-2.91163200	-3.07224900
H	-4.79822500	-2.01591200	-2.38146600
H	-3.43397700	-1.12777100	-3.14291400
C	-1.37008600	-0.95285100	2.51925000
C	-1.57296400	-1.71918800	3.59169100
H	-0.67637800	-0.10805900	2.58718300
H	-1.04914100	-1.54406100	4.52811800
H	-2.29565700	-2.53542300	3.58586400
Cl	6.57076100	-0.01694700	0.31365500
H	0.47970700	-1.38439300	1.13897300

(6*S*,7*S*,9*S*)-**3a**-H⁺

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	1.88742600	2.30757400	-0.48885700

C	1.56157400	0.93610200	-0.61767900	H	-1.86131500	0.38673300	1.58311000
C	2.58371200	-0.01318300	-0.76895000	C	-4.86916000	-0.02525300	0.07316900
C	3.89202000	0.44600200	-0.83136100	H	-5.18428200	-0.63112500	-1.96795300
C	4.19655600	1.81361200	-0.72870600	H	-4.29046100	0.56259300	2.06357200
C	3.20375500	2.76537500	-0.54102800	Cl	-6.56006100	0.10929500	0.40764800
C	-0.33369300	2.11392200	-0.31965000	H	-0.61817000	-2.43016700	-0.28095800
C	0.13700000	0.83132700	-0.50207300	H	-0.57784600	-1.44219900	1.05590000
H	4.70272900	-0.27359900	-0.94096300	(6<i>R</i>,7<i>S</i>,9<i>S</i>)-3a-H⁺			
H	5.23551400	2.13010900	-0.77846800	Atomic Coordinates (Angstroms)			
H	3.44730000	3.82094100	-0.43944800	Type	X	Y	Z
H	-1.35230000	2.47239900	-0.22441000	C	1.38977100	3.10814100	-0.06374900
N	0.70763700	3.00140200	-0.31145200	C	1.32876600	1.68817700	-0.10471000
C	0.60443100	4.43375500	-0.14110100	C	2.49021400	0.95780300	0.22817900
H	1.11583100	4.75387200	0.77354600	C	3.64449800	1.66870000	0.53611200
H	1.04826300	4.95404300	-0.99665700	C	3.68288900	3.07059000	0.54246100
H	-0.44857100	4.71239600	-0.07057300	C	2.54920000	3.81271400	0.25610400
C	2.26200900	-1.48943600	-0.76927400	C	-0.69419300	2.55100400	-0.62151500
C	-0.67880100	-0.37902000	-0.75003700	C	-0.02183500	1.35525900	-0.47459500
C	1.29578900	-1.88018800	0.38779900	H	4.54315500	1.11356100	0.80340100
N	-0.18135800	-1.59169500	0.11289200	H	4.61193800	3.57831600	0.78926400
H	3.18542200	-2.02657400	-0.51169100	H	2.56368500	4.90033300	0.27871000
C	1.38154200	-3.37172400	0.69746200	H	-1.72751400	2.72907500	-0.89840800
H	2.38667500	-3.61702200	1.05200800	N	0.14328500	3.60053900	-0.38163500
H	0.67167700	-3.66794100	1.47911000	C	-0.20888500	5.00264000	-0.42557400
H	1.18578500	-3.96179900	-0.20609000	H	0.41767700	5.53251200	-1.15094500
C	1.57711800	-1.09413700	1.67451200	H	-0.08186700	5.46599500	0.55903100
O	0.69150900	-0.60730900	2.35294300	H	-1.25320100	5.10030500	-0.72777100
O	2.86797000	-1.09011600	1.95289000	C	2.49224800	-0.53909700	0.41909300
C	3.25358600	-0.30483300	3.10113500	C	-0.63266400	0.04879900	-0.85635700
H	2.70443600	-0.63299700	3.98603300	H	-0.53658200	-0.14366600	-1.93527100
H	4.32354600	-0.46907400	3.21492600	C	1.61227000	-1.32004700	-0.58162200
H	3.04106200	0.74936500	2.90058400	N	0.14023200	-1.11511500	-0.23640200
C	1.80267900	-1.99944900	-2.11268300	H	0.06873600	-1.05719000	0.78872200
C	2.14946200	-3.17776000	-2.63179700	C	-2.07768300	-0.12432800	-0.46599000
H	1.19115800	-1.31646400	-2.70629600	C	-2.98902800	-0.67248800	-1.37101700
H	1.81453500	-3.48990400	-3.61776200	C	-2.51310900	0.21102600	0.82149400
H	2.81037100	-3.86636200	-2.10466100	C	-4.31511800	-0.87924600	-1.00922700
H	-0.53724700	-0.74913800	-1.77434600	H	-2.66542200	-0.93189900	-2.37946000
C	-2.14755000	-0.24696200	-0.46630300	C	-3.83133200	-0.00034600	1.20109200
C	-3.08932800	-0.53434300	-1.45580500	H	-1.81770100	0.66476900	1.52902300
C	-2.58800800	0.15004000	0.80354900	C	-4.72708600	-0.54437900	0.27924900
C	-4.44993400	-0.41824000	-1.19640000	H	-5.02749400	-1.29378700	-1.71655200
H	-2.75965400	-0.84128400	-2.44833700	H	-4.17324800	0.26086100	2.19890900
C	-3.94438600	0.25792500	1.07958800	C	1.89069900	-0.96250300	-2.03369100

H	2.93427000	-1.20496200	-2.25393100	C	-2.71957600	-0.80444800	1.01752000
H	1.26215200	-1.53505600	-2.72573900	C	-2.61909700	0.85890900	-0.72483200
H	1.75263900	0.10676200	-2.21769000	C	-4.10397500	-0.84275400	0.91455600
C	1.78552200	-2.83802500	-0.40522300	H	-2.21894500	-1.45244300	1.73639000
O	0.84096900	-3.59584600	-0.29476400	C	-4.00221600	0.82505200	-0.84508200
O	3.05961600	-3.19114100	-0.44768200	H	-2.04697100	1.53215300	-1.36387500
C	3.30708400	-4.61145700	-0.32750200	C	-4.73827700	-0.02393000	-0.01759200
H	2.79515800	-5.14636200	-1.13000200	H	-4.69207500	-1.50067800	1.54804300
H	4.38697400	-4.72104900	-0.40703500	H	-4.51385200	1.45109600	-1.57110800
H	2.94363300	-4.96655800	0.64000300	Cl	-6.46116500	-0.05945900	-0.15418900
H	-0.32815500	-2.00738100	-0.47043800	H	-0.60252700	-1.47995900	-1.10706000
Cl	-6.37385200	-0.79490100	0.73949700	H	0.10821200	-0.08720500	-1.69217000
H	3.50870300	-0.91220700	0.23920200	C	1.97806900	-1.52074700	-2.26707400
C	2.11788900	-0.87487300	1.84776800	H	2.85325400	-2.17394900	-2.30964000
C	2.68026200	-1.84105100	2.57481400	H	1.24033900	-1.90893000	-2.97924900
H	1.36150200	-0.23029900	2.30848100	H	2.29017100	-0.51748500	-2.58269800
H	2.38572500	-2.02760900	3.60425600	C	1.05116800	-2.88084000	-0.36093400
H	3.47916400	-2.46530600	2.17506500	O	-0.09011000	-3.18942800	-0.07631900

(6R,7S,9R)-3a-H⁺

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	1.85980700	2.92659400	0.05201000
C	1.62526700	1.53307100	0.07504000
C	2.69238800	0.63824200	-0.12813200
C	3.94294900	1.17644800	-0.40224700
C	4.15016600	2.56621900	-0.45627300
C	3.12040200	3.46286800	-0.21443000
C	-0.31130700	2.60730100	0.48581300
C	0.22910600	1.34710600	0.33698100
H	4.79048200	0.50710500	-0.54701200
H	5.14683300	2.94413600	-0.67045900
H	3.29432500	4.53676500	-0.23025900
H	-1.33039600	2.90495200	0.70473700
N	0.66217300	3.55618200	0.32462100
C	0.48202000	4.98814900	0.42519600
H	0.76660900	5.47870600	-0.51197600
H	1.09036500	5.39724600	1.23907300
H	-0.56800400	5.20482300	0.62985400
C	2.48715200	-0.83832800	0.11552500
C	-0.46551400	0.03556600	0.33024400
C	1.43652100	-1.48072600	-0.84282800
N	0.09305900	-0.74635800	-0.90811300
H	-0.18560400	-0.62149700	1.16348300
C	-1.96222700	0.05251200	0.21294600

C	1.85422100	-5.01224700	0.16673900
H	1.10844100	-5.50669800	-0.45920000
H	2.81360900	-5.52388900	0.11243900
H	1.49406200	-4.95854900	1.19724300
H	3.41013100	-1.36979800	-0.15534500
C	2.24981500	-1.08948000	1.58927700
C	2.82669600	-2.06739200	2.28675400
H	1.62473700	-0.36300600	2.11119300
H	2.65859100	-2.17671400	3.35524400
H	3.50645700	-2.78228500	1.82442800

TS6

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.78594600	2.62482500	-0.28361900
C	-1.47748100	1.26277800	-0.04860600
C	-2.52813200	0.37892200	0.28480300
C	-3.82710700	0.88250200	0.16247600
C	-4.10549100	2.20969900	-0.17583700
C	-3.07847400	3.12541300	-0.36032000
C	0.44250100	2.47666600	-0.25590300
C	-0.03299200	1.16700700	-0.09015500
H	-4.65873500	0.21905600	0.39678500
H	-5.13963300	2.53852600	-0.24231000
H	-3.27874400	4.17811500	-0.54632800
H	1.46004100	2.81449600	-0.41715000

N	-0.58933000	3.32927200	-0.40048600	C	0.90110900	1.80341100	-0.15135900
C	-0.49918900	4.74614000	-0.68625800	C	2.15930700	1.16011200	-0.07332700
H	-0.99979300	4.97199500	-1.63336700	C	3.28024600	1.99368200	-0.20239600
H	-0.97128400	5.32510400	0.11435300	C	3.21053400	3.38388600	-0.30123100
H	0.55106900	5.03325500	-0.76002900	C	1.98651300	4.03431000	-0.22370400
C	-2.38660900	-0.93592800	1.03487500	C	-1.25940300	2.56290500	0.03093100
C	0.77567100	0.05362600	-0.42200200	C	-0.49349400	1.37944700	-0.11031800
H	0.37304800	-0.63772200	-1.15564500	H	4.26504400	1.52954200	-0.17280500
C	-1.44818100	-2.05178800	0.49326500	H	4.12738600	3.96192300	-0.38396700
N	-0.04420400	-1.72457600	0.77643600	H	1.91216500	5.11919600	-0.21953100
H	-3.38490900	-1.39184600	1.03609200	H	-2.33761200	2.67595600	0.01232400
H	0.56305700	-2.42930900	0.36006100	N	-0.46386100	3.63213000	-0.02776100
C	2.19899600	-0.00787200	-0.23371800	C	-0.88681300	5.01887300	-0.04313500
C	2.95502100	-0.87054700	-1.05379900	H	-0.58110900	5.49179400	-0.98162100
C	2.86503200	0.73882200	0.75953000	H	-0.43029300	5.55624700	0.79387500
C	4.32991600	-0.95198400	-0.92494100	H	-1.97264500	5.06690300	0.04959200
H	2.44377100	-1.46837400	-1.80859000	C	2.45583900	-0.26080600	0.38663400
C	4.23882900	0.66258800	0.89999600	C	-1.09131900	0.20680000	-0.57292500
H	2.28779000	1.36292100	1.44034600	H	-0.51085700	-0.40067300	-1.25517800
C	4.96612300	-0.17827100	0.05059700	C	1.98532500	-1.48549200	-0.46506900
H	4.91619200	-1.60488700	-1.56554000	N	0.62845500	-1.87128900	-0.08829300
H	4.75689500	1.23177500	1.66685100	H	0.65747000	-2.24224700	0.86152500
C	-1.83272100	-3.39021100	1.14404100	C	-2.42912800	-0.22868800	-0.33081800
H	-2.85944000	-3.67338900	0.88880900	C	-3.00161400	-1.17469800	-1.21004500
H	-1.16493100	-4.19143100	0.80709600	C	-3.19388100	0.20812800	0.77474100
H	-1.75739800	-3.31187400	2.23458000	C	-4.29638700	-1.62214000	-1.03654000
C	-1.57749400	-2.23515400	-1.01463800	H	-2.41371900	-1.53990300	-2.05120400
O	-0.63139600	-2.38709900	-1.76480900	C	-4.48645200	-0.24093000	0.96506400
O	-2.85631400	-2.26854400	-1.38703800	H	-2.74253800	0.86948400	1.51269600
C	-3.08112300	-2.49924000	-2.79115100	C	-5.03818800	-1.14655900	0.05021300
H	-2.66538500	-3.46642200	-3.08420600	H	-4.74000200	-2.33838500	-1.72201400
H	-4.16282600	-2.48617200	-2.91678500	H	-5.07033900	0.07868000	1.82360500
H	-2.60979900	-1.70822900	-3.37973200	C	2.05882800	-1.18031700	-1.95679600
C	-2.03380400	-0.60199400	2.46503200	H	3.07616600	-0.89578000	-2.24192600
C	-2.71256000	-1.02131500	3.53168500	H	1.77456000	-2.05238500	-2.55848800
H	-1.17083600	0.05735800	2.59710700	H	1.39408400	-0.34867700	-2.22051000
H	-2.42570000	-0.73892500	4.54172400	C	2.93413600	-2.66106400	-0.14265900
H	-3.59473900	-1.65460800	3.43602200	O	2.56177300	-3.71039800	0.33245600
Cl	6.67773200	-0.27912400	0.22813500	O	4.20784400	-2.38354700	-0.46389200
H	0.11856200	-1.72014100	1.78255800	C	5.14119200	-3.44307400	-0.18850300
TS7				H	4.85962600	-4.34630200	-0.73564200
Atomic	Coordinates (Angstroms)			H	6.11061100	-3.07309500	-0.52100600
Type	X	Y	Z	H	5.15379600	-3.66444000	0.88248100
C	0.86905200	3.21846200	-0.14262700	H	0.34928100	-2.67038400	-0.65733400

Cl	-6.64765600	-1.70696000	0.28430400
H	3.54972300	-0.32738200	0.36801100
C	2.02839200	-0.42042600	1.82434400
C	2.82281900	-0.88634000	2.78610900
H	0.99404600	-0.14966300	2.05252400
H	2.47632700	-1.01433200	3.80857800
H	3.86019200	-1.15897300	2.58719400

IM7

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	-1.73289500	2.47487000	0.24696900
C	-1.37392000	1.11937900	0.43047000
C	-2.39021900	0.19570200	0.75447200
C	-3.69465400	0.70747500	0.82195000
C	-4.01660700	2.04826300	0.61612900
C	-3.02208900	2.97457600	0.33010900
C	0.48217400	2.39841200	-0.03386600
C	0.07934600	1.06708500	0.24979200
H	-4.50041900	0.01261900	1.05350200
H	-5.05209800	2.37002800	0.69290800
H	-3.24440200	4.02902700	0.18318900
H	1.46078700	2.76529800	-0.32076000
N	-0.57153400	3.20710200	-0.04494100
C	-0.56852800	4.62063400	-0.36738600
H	-1.21039900	4.80440700	-1.23447500
H	-0.94383100	5.19677700	0.48405100
H	0.44973100	4.93755200	-0.59675100
C	-2.23050600	-1.28180600	1.08772200
C	0.91109300	-0.03538800	0.16793700
H	0.43325800	-1.02431000	0.08697900
C	-1.88498600	-2.27209500	-0.11655000
N	-0.50766800	-2.76028300	0.01475400
H	-3.23166100	-1.59484400	1.40790800
H	-0.26947300	-3.29026000	-0.82125200
C	2.33847500	-0.05339300	0.11990100
C	2.95121000	-1.17677900	-0.48289300
C	3.17096200	0.95556800	0.65677100
C	4.32389500	-1.25681800	-0.61792000
H	2.31546700	-1.96640800	-0.87979300
C	4.54544600	0.87191600	0.55195500
H	2.73116600	1.77380200	1.22429200
C	5.11674000	-0.22650700	-0.10333700
H	4.79224400	-2.10653300	-1.10678500
H	5.18817100	1.63185600	0.98730500

C	-2.90142600	-3.41529800	-0.09402400
H	-3.92631600	-3.05760900	-0.23362100
H	-2.68790600	-4.14841400	-0.88103600
H	-2.84549700	-3.93388500	0.87212200
C	-1.95193000	-1.49981300	-1.42909800
O	-0.98711200	-1.14504200	-2.07405400
O	-3.22337800	-1.22456000	-1.75720500
C	-3.37970200	-0.39261000	-2.91521900
H	-2.93781300	-0.87212400	-3.79228100
H	-4.45440800	-0.26489500	-3.04179100
H	-2.89018600	0.57380000	-2.75246500
C	-1.32920000	-1.49887600	2.27108900
C	-1.69708600	-2.17409400	3.35912600
H	-0.32289700	-1.07871600	2.22068800
H	-1.02419800	-2.31541900	4.20139800
H	-2.69401700	-2.60487500	3.45627300
Cl	6.82935000	-0.32342700	-0.24524500
H	-0.46946900	-3.41196900	0.79633600

IM8

Atomic Type	Coordinates (Angstroms)		
	X	Y	Z
C	0.95083000	3.14966200	-0.04459700
C	0.94751800	1.73686200	0.04021400
C	2.15038000	1.08197300	0.38537100
C	3.27527600	1.90068600	0.56498500
C	3.25388800	3.28883500	0.42891100
C	2.06903500	3.94931400	0.12957400
C	-1.17520800	2.53036100	-0.33220000
C	-0.44375200	1.33345200	-0.15019600
H	4.21510400	1.42081100	0.83601800
H	4.16620500	3.85852200	0.58573100
H	2.02069700	5.03348500	0.05728900
H	-2.22083600	2.65198400	-0.59191400
N	-0.35692100	3.58309300	-0.30023600
C	-0.72381600	4.96560800	-0.53404000
H	-0.15732200	5.36486900	-1.38093200
H	-0.50700400	5.56496800	0.35593500
H	-1.79080900	5.02400700	-0.75423900
C	2.34411800	-0.40770100	0.58657600
C	-0.98497400	0.05915300	-0.28761000
H	-0.27863100	-0.71439000	-0.61039100
C	2.69029400	-1.16125500	-0.73880300
N	1.52816400	-1.14834500	-1.63169900
H	1.51930800	-2.02708300	-2.14862800

C	-2.35800700	-0.30287200	-0.15613400
C	-2.80668200	-1.49556600	-0.77027800
C	-3.28789000	0.45509100	0.59387500
C	-4.13345700	-1.87541900	-0.70879200
H	-2.09377900	-2.10511300	-1.32338300
C	-4.61234300	0.07536000	0.67663400
H	-2.94199500	1.31403900	1.16609600
C	-5.03500200	-1.08124600	0.00873900
H	-4.48116300	-2.78061800	-1.19884400
H	-5.32313900	0.64386900	1.26988500
C	3.94805200	-0.59019300	-1.40015200
H	4.80514900	-0.59047300	-0.71752700
H	4.21743900	-1.18410200	-2.28108900
H	3.77727300	0.44136400	-1.73021100
C	2.97583600	-2.63032300	-0.41030500
O	2.46776600	-3.56503400	-0.99246000
O	3.87672100	-2.74575200	0.57276700
C	4.23132100	-4.09821000	0.91221300
H	4.66121100	-4.60384300	0.04401500
H	4.96245600	-4.01443800	1.71534500
H	3.34657400	-4.64705800	1.24581600
H	1.63349700	-0.40153600	-2.31452900
Cl	-6.68587200	-1.55272200	0.11007200
H	3.24830200	-0.50473900	1.20674200
C	1.23881900	-1.10873000	1.33574300
C	0.55059200	-0.60586400	2.36203000
H	1.02121700	-2.13138700	1.01426000
H	-0.19700600	-1.19623800	2.88644300
H	0.71351900	0.40855600	2.72741600