

Supporting Information

Substituent-dependent generation of tricyclic frameworks by the rhodium-catalyzed cycloisomerization of homopropargyl allene-alkynes: a theoretical study

Ping Wang^{a,b}, Jing Zhang^{a,b}, Lingli Han^{a,b,*}, Siwei Bi^{b,*}, Tao Liu^{a,b,*}

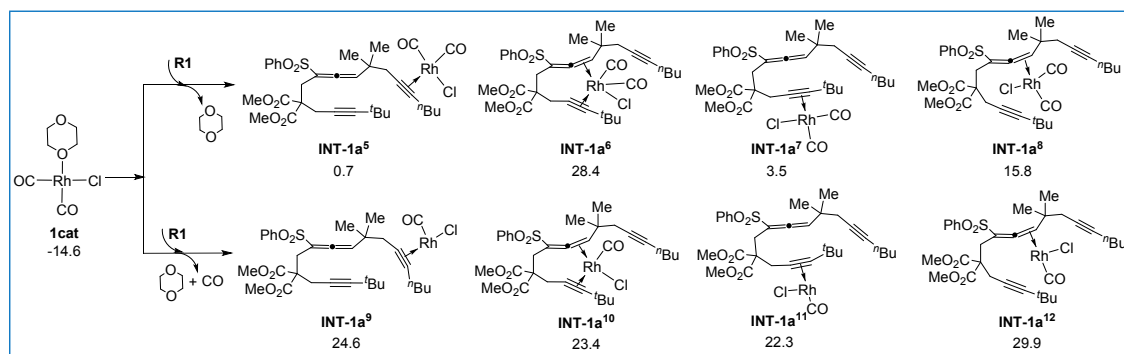
^a Department of Chemistry and Chemical Engineering, Jining University, Qufu 273155, Shandong, China

^b School of Chemistry and Chemical Engineering, Qufu Normal University, Qufu 273165, Shandong, China

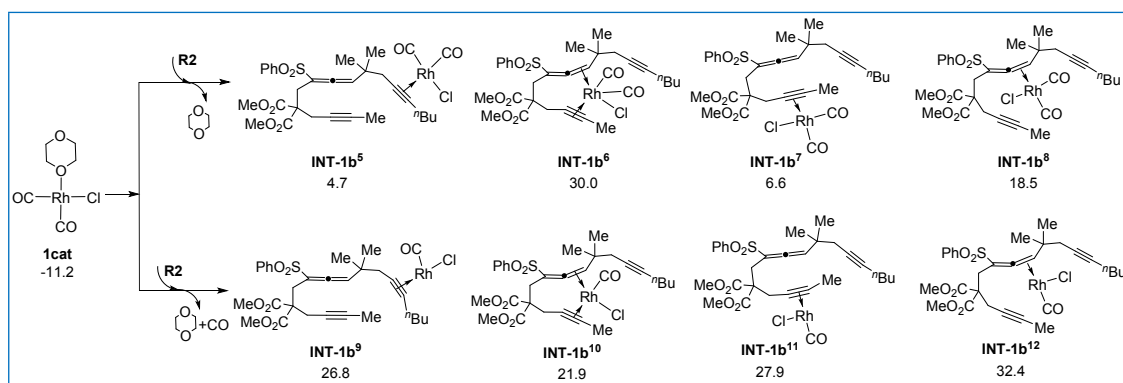
Correspondent author email addresses: hll_2002@sina.com, siwei@126.com and liutao_2005@126.com

Table of Contents

1. Other unfavorable cat-R1 coordination without the participant of 1,4-dioxane.....	S2
2. Other unfavorable cat-R2 coordination without the participant of 1,4-dioxane.....	S3
3. The unfavorable alkyne insertion process in reaction A.....	S4
4. The unfavorable stepwise pathway for the formation of P2^A from INT-4aa	S5
5. The unfavorable stepwise pathway for the formation of INT-3b from INT-3bb	S6
6. The unfavorable stepwise pathway for the formation of P2^B from INT-4bb	S7
7. The unfavorable free energy diagram for the alkyne insertion mechanism in reaction C.....	S8
8. Comparisons for the β -hydride elimination mechanism and alkyne insertion one by replacing the dimethyl of substrate R2 with other groups.....	S9
9. Calculated solution-phase Gibbs free energies ΔG_{sol} of all species (in Hartree).....	S10
10. Cartesian coordinates of all calculated species.....	S12



Scheme S1 Other unfavorable **cat–R1** coordination without the participant of 1,4-dioxane. The relative free energies are given in kcal/mol.



Scheme S2 Other unfavorable **cat–R2** coordination without the participant of 1,4-dioxane. The relative free energies are given in kcal/mol.

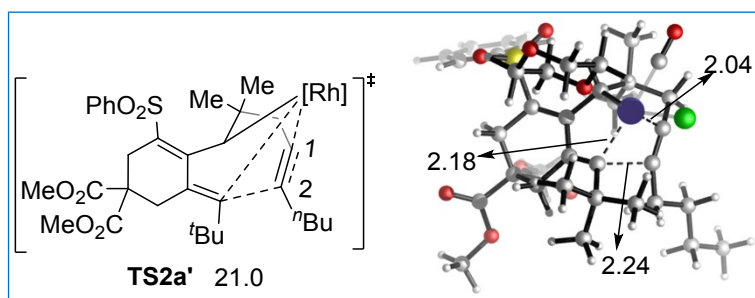


Fig. S1 The unfavorable alkyne insertion process in reaction A. The relative free energies are given in kcal/mol. Bond distances are given in Å.

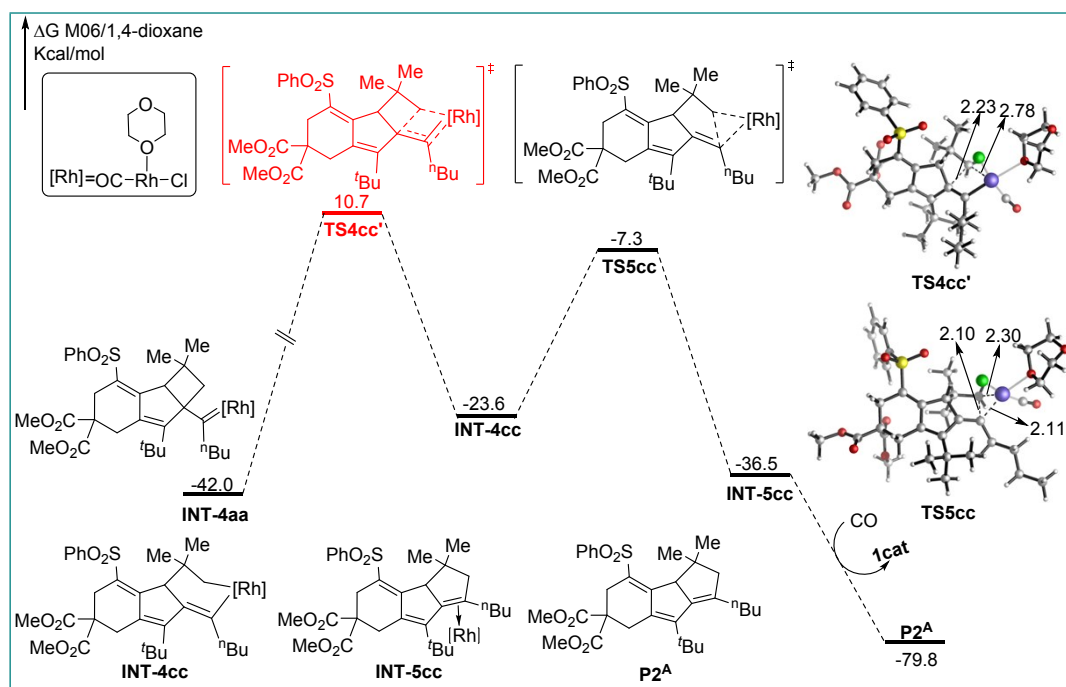


Fig. S2 The unfavorable stepwise pathway for the formation of **P2^A** from **INT-4aa**. Bond distances are given in Å.

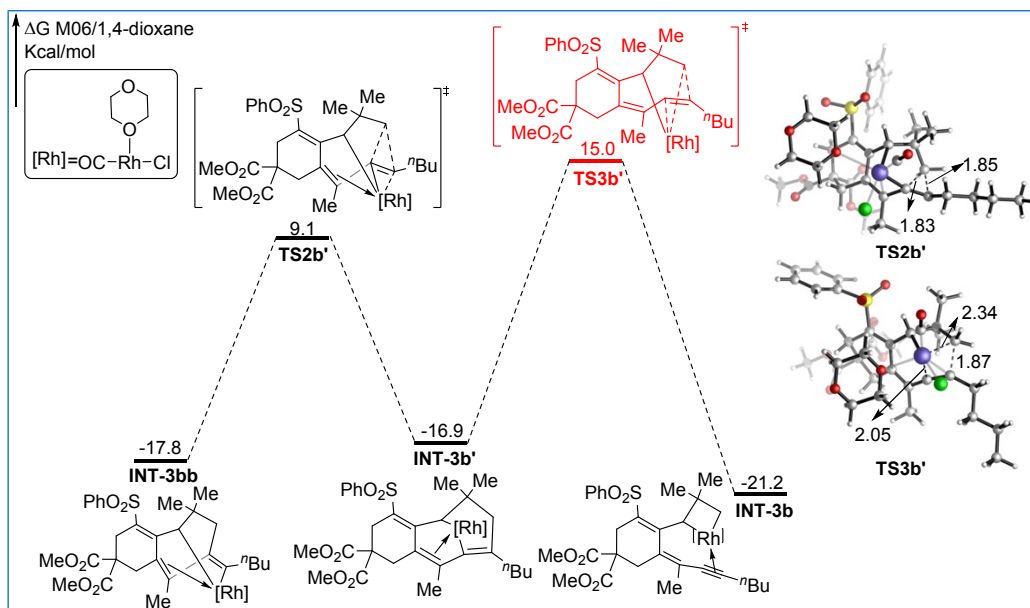


Fig. S3 The unfavorable stepwise pathway for the formation of **INT-3b** from **INT-3bb**. Bond distances are given in \AA .

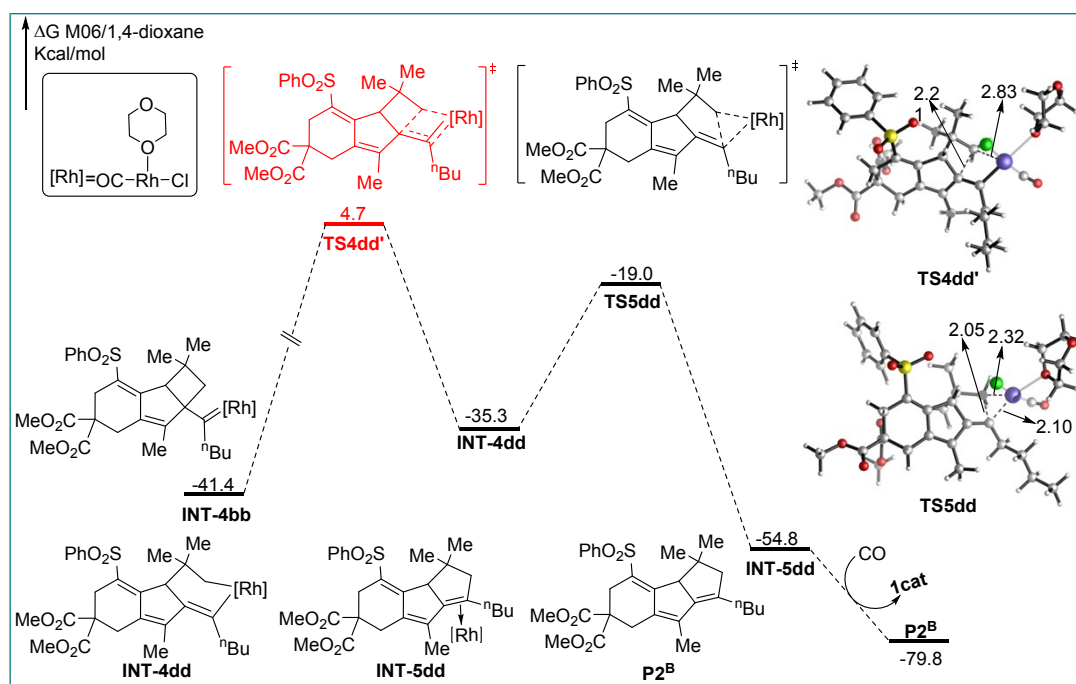


Fig. S4 The unfavorable stepwise pathway for the formation of **P2^B** from **INT-4bb**. Bond distances are given in Å.

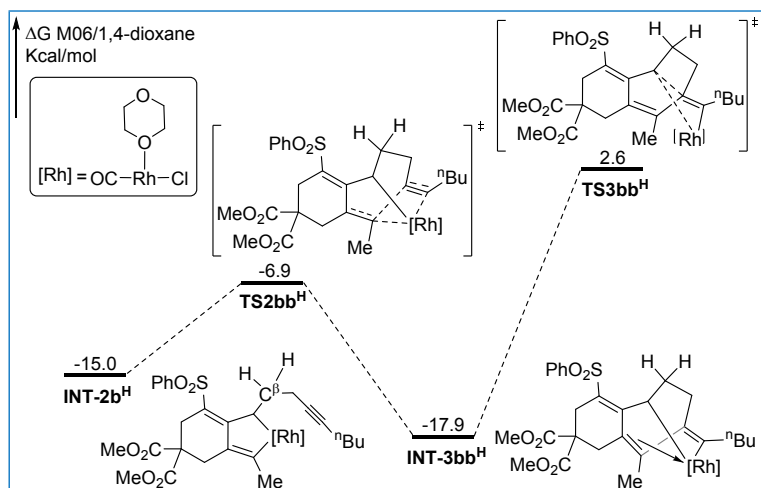


Fig. S5 The unfavorable free energy diagram for the alkyne insertion mechanism in reaction C. The relative free energies are given in kcal/mol.

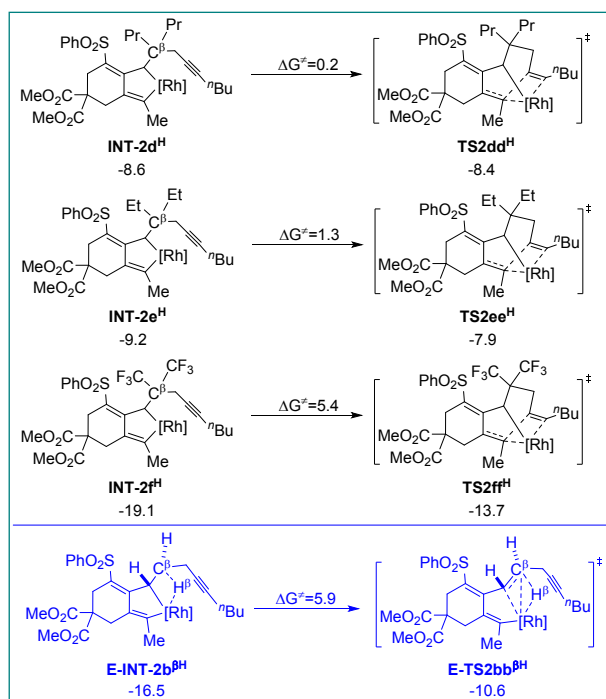


Fig. S6 Comparisons for the β -hydride elimination mechanism and alkyne insertion one by replacing the dimethyl of substrate **R2** with other groups. The relative free energies are given in kcal/mol.

Table S1 Calculated solution-phase Gibbs free energies ΔG_{sol} of all species (in Hartree)

species	ΔG_{sol}	species	ΔG_{sol}
R1	-2093.3393744	TS4aa	-3085.0921967
R2	-1975.4612779	INT-5aa	-3085.1444069
R3	-1896.870631	P1^A	-2093.4428887
cat	-1594.9340247	TS4cc	-3085.0847564
1cat	-1105.0120917	INT-5cc	-3085.1295697
INT-1a¹	-3085.0535606	P2^A	-2093.4617369
INT-1b¹	-2967.1796995	TS1b	-2967.1466189
INT-1a²	-3085.0486479	INT-2b	-2967.212839
INT-1b²	-2967.1692998	TS2bb	-2967.2072953
INT-1a³	-3085.0423748	INT-3bb	-2967.2217311
INT-1b³	-2967.1659642	TS3b	-2967.1205848
INT-1a⁴	-3085.0490936	INT-3b	-2967.2242651
INT-1b⁴	-2967.1702044	TS3bb	-2967.1941075
INT-1a⁵	-2890.8119917	INT-4bb	-2967.2574653
INT-1b⁵	-2772.9343421	TS4bb	-2967.2335504
INT-1a⁶	-2890.7746613	INT-5bb	-2967.2734843
INT-1b⁶	-2772.8978798	P2^B	-1975.5971111
INT-1a⁷	-2890.81184	TS4dd	2967.2236369
INT-1b⁷	-2772.9316904	INT-5dd	-2967.2813073
INT-1a⁸	-2890.7928596	P1^B	-1975.5708947
INT-1b⁸	-2772.9155608	TS1b^H	-2888.5662912
INT-1a⁹	-2777.4755529	INT-2b^H	-2888.6280989
INT-1b⁹	-2659.5974905	Z-TS2bb^{BH}	-2888.579266
INT-1a¹⁰	-2777.4859046	E-TS2bb^{BH}	-2888.5802073
INT-1b¹⁰	-2659.6124096	E-INT-2b^{BH}	-2888.6268495
INT-1a¹¹	-2777.4814708	Z-INT-2b^{BH}	-2888.6281663
INT-1b¹¹	-2659.5984711	Z-TS2bb^{BH}	-2888.6151145
INT-1a¹²	-2777.471632	E-TS2bb^{BH}	-2888.6190998
INT-1b¹²	-2659.5946024	Z-INT-3bb^{BH}	-2888.6188524
INT-1b^{10H}	-2581.0297263	E-INT-3bb^{BH}	-2888.6211714
TS1a	-3085.0274894	Z-TS3bb^{BH}	-2888.6025001
INT-2a	-3085.0880188	E-TS3bb^{BH}	-2888.6045799
TS2a	-3085.035783	Z-INT-4bb^{BH}	-2888.644573
TS2aa	-3085.0679239	E-INT-4bb^{BH}	-2888.6437505
INT-3a	-3085.0507604	Z-P3	-1896.9305039
INT-3aa	-3085.0858027	E-P3	-1896.9295784
TS3aa	-3085.0580163	R-INT-2c^H	-2927.9233139
INT-4aa	-3085.1318858	R-TS2cc^H	-2927.9166715

species	ΔG_{sol}	species	ΔG_{sol}
E-INT-2c^{βH}	-2927.9256123	TS4dd'	-2967.1776302
E-TS2cc^{βH}	-2927.9183804	INT-4dd	-2967.249833
S-INT-2c^H	-2927.9377781	TS5dd	-2967.2244001
S-TS2cc^H	-2927.9113779	TS2bb^H	-2888.6203517
Z-INT-2c^{βH}	-2927.9243005	INT-3bb^H	-2888.6389323
Z-TS2cc^{βH}	-2927.916897	TS3bb^H	-2888.6038909
TS2a'	-3085.0349292	INT-2d^H	-3124.3639097
TS4cc'	-3085.0453402	TS2dd^H	-3124.3682051
INT-4cc	-3085.1063445	INT-2e^H	-3045.7791304
TS5cc	-3085.0798629	TS2ee^H	-3045.7816931
TS2b'	-2967.1759248	INT-2f^H	-3562.6769827
INT-3b'	-2967.2217489	TS2ff^H	-3562.6695862
TS3b'	-2967.1651217		

Cartesian coordinates of all calculated species

R1

C	0.09751200	-4.46076300	-4.92556400
C	-0.77658200	-3.43780500	-5.71441100
H	-0.17326900	-3.04137400	-6.53393400
H	-1.59294300	-4.00687900	-6.16296800
C	-0.66217200	-5.09297900	-3.72414800
H	0.03420100	-5.73982700	-3.18161500
H	-0.92827600	-4.28481100	-3.03802500
C	-1.38370900	-2.28652300	-4.93132200
C	-2.56764300	-2.26382200	-4.37085400
C	-3.77494300	-2.16203700	-3.87697100
H	-4.55571700	-1.85691400	-4.57909300
C	-4.25466500	-2.42122100	-2.45420600
C	-5.25912500	-3.61992000	-2.54583100
H	-6.04080200	-3.37003800	-3.27684600
H	-4.71611500	-4.48204900	-2.95412500
C	-5.88493300	-3.98795700	-1.27528100
C	-6.39475800	-4.29303400	-0.21998300
C	-7.03753400	-4.69692100	1.03221900
C	-8.13066900	-5.76892800	0.83534200
H	-7.47783100	-3.81632800	1.52034300
H	-6.27774600	-5.07889700	1.72821600
C	-8.79072000	-6.19139300	2.15294900
H	-8.89031600	-5.38079300	0.14540900
H	-7.68634000	-6.64359700	0.34417900
C	-9.87651100	-7.25526500	1.96269800
H	-8.02096600	-6.57093700	2.83883900
H	-9.22439500	-5.30818800	2.64172000
H	-10.32932300	-7.53929600	2.91812000
H	-10.67764400	-6.89075800	1.30991500
H	-9.46597300	-8.16284300	1.50588400
C	-1.84116700	-5.85991500	-4.12753200
C	-2.78669100	-6.52032100	-4.49915300
C	0.49985000	-5.57479400	-5.90856300
O	0.14583200	-5.65922900	-7.06204000
O	1.29165100	-6.48028500	-5.29804800
C	1.36476700	-3.78116200	-4.38684900
O	1.50061500	-3.40584900	-3.23964400
O	2.28858300	-3.64825900	-5.34453700
C	1.72447300	-7.57501500	-6.12306300
H	2.29168000	-7.20560200	-6.98073100
H	2.35352200	-8.19395000	-5.48367700
H	0.86463500	-8.14447600	-6.48405500
C	3.46285800	-2.89175100	-4.99063200
H	4.12787500	-2.97008000	-5.85010500
H	3.17981900	-1.85305900	-4.81471500

H	3.93132300	-3.31197900	-4.09798900
S	-0.50048800	-0.68141900	-5.01668900
O	0.91285500	-0.99496100	-5.30101300
O	-1.24389100	0.21060300	-5.92183100
C	-0.60513100	0.02509700	-3.36284300
C	0.20068000	-0.48307100	-2.34011700
C	-1.46689700	1.10290000	-3.15510300
C	0.12201700	0.10267700	-1.07588700
H	0.86853400	-1.31758300	-2.52723100
C	-1.53083800	1.68035300	-1.88552700
H	-2.05790900	1.48045300	-3.98205700
C	-0.74061200	1.17891100	-0.84872200
H	0.74037600	-0.27949400	-0.26923000
H	-2.19208400	2.52362700	-1.70972200
H	-0.79269100	1.63085300	0.13767500
C	-4.98396900	-1.15399900	-1.96066500
H	-5.79078700	-0.86609700	-2.64421200
H	-5.42418200	-1.33407900	-0.97555300
H	-4.28704200	-0.31384800	-1.88486600
C	-3.10322600	-2.77293400	-1.50301400
H	-2.60535900	-3.69625500	-1.81260800
H	-2.35905800	-1.97240300	-1.47073500
H	-3.49012800	-2.92787400	-0.49218900
C	-3.90884200	-7.35660400	-4.96710000
C	-4.69423400	-7.89790400	-3.74929000
C	-4.84703400	-6.51377400	-5.86209000
C	-3.34091900	-8.54023700	-5.78661300
H	-4.04647500	-8.49478600	-3.10027400
H	-5.11272400	-7.08212400	-3.15203500
H	-5.52026200	-8.53278800	-4.08841000
H	-4.31086900	-6.12415500	-6.73242600
H	-5.68000700	-7.12985000	-6.21848800
H	-5.26061900	-5.66537300	-5.30894000
H	-4.15812500	-9.17158400	-6.15300900
H	-2.77033700	-8.17864400	-6.64721400
H	-2.67863300	-9.15779600	-5.17236500
R2			
C	0.16549900	-4.45735100	-4.95123100
C	-0.72847200	-3.44847700	-5.73573100
H	-0.13253700	-3.03682500	-6.55308300
H	-1.53314200	-4.03144700	-6.18736800
C	-0.57313400	-5.09679000	-3.74153400
H	0.12804600	-5.75882700	-3.22419200
H	-0.81232200	-4.29420100	-3.03884700
C	-1.35963100	-2.31293000	-4.94893600
C	-2.54728700	-2.31414200	-4.39579000
C	-3.75918400	-2.23683000	-3.90905900
H	-4.54089500	-1.94072900	-4.61399200

C	-4.24067000	-2.50399500	-2.48851300	H	-2.08638300	1.44150700	-3.96622300
C	-5.25770000	-3.69192000	-2.58451900	C	-0.76379500	1.12757900	-0.83632300
H	-6.02997900	-3.43633800	-3.32338700	H	0.73459300	-0.31842200	-0.27067500
H	-4.72180200	-4.56333400	-2.98268200	H	-2.23116500	2.46298200	-1.68475500
C	-5.89896700	-4.04313600	-1.31685900	H	-0.82064400	1.57003200	0.15410300
C	-6.42293800	-4.33027400	-0.26353700	C	-4.95663200	-1.23230900	-1.98607300
C	-7.08425600	-4.71179900	0.98607900	H	-5.76299600	-0.93354000	-2.66553200
C	-8.16680000	-5.79534900	0.79405800	H	-5.39543400	-1.41320000	-1.00053200
H	-7.53890200	-3.82395400	1.44723700	H	-4.25153000	-0.39922300	-1.90885000
H	-6.33429200	-5.07320600	1.70337800	C	-3.09093200	-2.87454400	-1.54244600
C	-8.85108200	-6.18917300	2.10821000	H	-2.60078100	-3.79746700	-1.86533200
H	-8.91461300	-5.42924100	0.07960300	H	-2.34130100	-2.07940400	-1.50140300
H	-7.70762600	-6.67916700	0.33388100	H	-3.47769900	-3.03834500	-0.53292200
C	-9.92582400	-7.26505600	1.92282000	R3			
H	-8.09325900	-6.54583100	2.81919800	C	0.01359800	-4.49567900	-4.94836200
H	-9.30043700	-5.29689900	2.56529200	C	-0.62891400	-3.37763400	-5.82721100
H	-10.39709800	-7.52739400	2.87551400	H	0.14798300	-2.97016000	-6.47698700
H	-10.71512500	-6.92311900	1.24393600	H	-1.36450600	-3.86504200	-6.46988000
H	-9.49989400	-8.18134600	1.49860300	C	-1.00863000	-5.15857700	-3.98061200
C	-1.77514100	-5.84077300	-4.11839000	H	-0.47245700	-5.88574800	-3.36313600
C	-2.75321800	-6.47270800	-4.44902200	H	-1.37203600	-4.38528200	-3.29797000
C	-3.92566500	-7.24735300	-4.84824600	C	-1.31536000	-2.24810400	-5.08097200
H	-4.08631400	-8.09758500	-4.17590100	C	-2.54426200	-2.24234900	-4.63122800
H	-4.83496900	-6.63602900	-4.83326900	C	-3.76630800	-2.19202100	-4.16684600
H	-3.80860800	-7.64290100	-5.86332100	H	-4.55494000	-1.86184100	-4.84612000
C	0.58020100	-5.56404500	-5.93771700	C	-4.18771900	-2.58635000	-2.77029500
O	0.23367100	-5.64423700	-7.09358500	C	-5.09756700	-3.84178300	-2.77898100
O	1.37758600	-6.46607300	-5.32881900	H	-5.95398200	-3.66012500	-3.44312500
C	1.42827000	-3.75989100	-4.42307000	H	-4.53984000	-4.67838000	-3.21877200
O	1.57172700	-3.38756900	-3.27589200	C	-5.57634700	-4.19685200	-1.44292700
O	2.33917900	-3.60907200	-5.39033700	C	-5.95225600	-4.46778900	-0.32468100
C	1.82813300	-7.54911400	-6.15999900	C	-6.43726900	-4.82401800	1.01008400
H	2.40170300	-7.16630000	-7.00752600	C	-7.72521100	-5.67434800	0.98433600
H	2.45523800	-8.16934100	-5.51997400	H	-6.61993800	-3.90879300	1.59036700
H	0.97708100	-8.12167700	-6.53644400	H	-5.65274500	-5.37141900	1.55099900
C	3.50411000	-2.83334500	-5.04689100	C	-8.22154400	-6.04144300	2.38745900
H	4.15925500	-2.89464500	-5.91526900	H	-8.50553700	-5.12232400	0.44566100
H	3.20449500	-1.80102300	-4.86104300	H	-7.53761300	-6.58681300	0.40471700
H	3.99151200	-3.25013900	-4.16283200	C	-9.49918100	-6.88660700	2.36798900
S	-0.50438100	-0.69218100	-5.02128300	H	-7.43039800	-6.58540200	2.92152500
O	0.91329400	-0.97959600	-5.31209700	H	-8.39879500	-5.12190600	2.96208900
O	-1.26487600	0.19580600	-5.91612500	H	-9.83042800	-7.13341900	3.38188200
C	-0.61634700	-0.00223100	-3.36079200	H	-10.31825100	-6.35507300	1.87044000
C	0.19620800	-0.50974100	-2.34303900	H	-9.34264300	-7.82857900	1.83040900
C	-1.49041000	1.06360200	-3.14300800	C	-2.12025000	-5.81301800	-4.67092900
C	0.11120000	0.06358500	-1.07353100	C	-3.02115900	-6.36520400	-5.26141900
H	0.87483900	-1.33375300	-2.53790600	C	-4.10378700	-7.03988300	-5.97299800
C	-1.56025500	1.62904200	-1.86830400	H	-4.46987400	-7.90519900	-5.40915600

H	-4.95296800	-6.36783100	-6.13974400	C	-4.42149200	-0.72856500	-5.30025900
H	-3.76727200	-7.39859700	-6.95204300	C	-3.21719200	-1.10258100	-6.16684000
C	0.57773500	-5.56335200	-5.90220600	O	-4.55037300	-1.66663600	-4.18661200
O	0.49782600	-5.54195000	-7.10871100	O	-3.14367300	-2.50809800	-6.32185600
O	1.16366400	-6.55895100	-5.20561800	H	-4.32457500	0.28632200	-4.90266200
C	1.15956600	-3.91104400	-4.10836900	H	-5.35498400	-0.82720600	-5.85959100
O	1.05409400	-3.59409000	-2.94059800	H	-3.34257000	-0.67323700	-7.16467100
O	2.27478100	-3.78054200	-4.83417600	H	-2.28649400	-0.69380400	-5.74632500
C	1.72774900	-7.61616200	-5.99994500	H	-3.51958900	-2.98549400	-3.01464600
H	2.50717000	-7.22416800	-6.65778800	H	-2.56448800	-1.60643600	-3.57450500
H	2.14716000	-8.32677500	-5.28812400	H	-1.82261500	-3.43105300	-4.99247400
H	0.95470900	-8.09129200	-6.60854200	H	-3.45948000	-4.11479800	-5.12676100
C	3.37145600	-3.09789600	-4.19474100	Rh	-5.67744600	-0.92169700	-2.45312100
H	4.20788800	-3.18099300	-4.88792500	Cl	-3.93023700	0.64688100	-2.10810300
H	3.10036300	-2.05252600	-4.04039000	C	-6.54051300	-0.23076400	-0.96491600
H	3.60974900	-3.57173700	-3.24008400	O	-7.05000700	0.21476300	-0.03894500
S	-0.38892700	-0.67376200	-4.95315300	C	-7.03938300	-2.18389600	-2.79239700
O	1.04215500	-1.03309400	-4.96292000	O	-7.86261700	-2.95515500	-3.01396300
O	-0.90973900	0.26481600	-5.96062100	INT-1a¹			
C	-0.79996400	-0.01346800	-3.32882900	C	-1.96460600	-5.63531300	-5.20765800
C	-0.26094300	-0.60953100	-2.18506200	C	-1.33073100	-4.35294500	-5.82390500
C	-1.61912700	1.11326400	-3.25683100	H	-0.48955900	-4.65136600	-6.44945700
C	-0.56764100	-0.06009000	-0.94021900	H	-2.06044300	-3.88639500	-6.48615300
H	0.37787100	-1.48302400	-2.26703000	C	-2.82443500	-5.36064900	-3.94759600
C	-1.91188400	1.65414000	-2.00363800	H	-3.24175500	-6.31235400	-3.60481300
H	-2.00282500	1.55300100	-4.17073900	H	-2.15296500	-5.01880200	-3.15736000
C	-1.38930200	1.06736400	-0.84944800	C	-0.89664000	-3.31991300	-4.80534100
H	-0.15917400	-0.51037300	-0.04045600	C	-1.72609400	-2.42048200	-4.29971800
H	-2.54492400	2.53346300	-1.93093000	C	-2.16946600	-1.34286700	-3.56443400
H	-1.61972700	1.49078900	0.12400500	H	-1.95706800	-0.36690100	-4.00299900
H	-3.30942700	-2.77154900	-2.14640900	C	-2.47749500	-1.23224100	-2.06526400
H	-4.73699900	-1.75382100	-2.31440100	C	-3.83021600	-0.46022800	-1.92956200
cat				H	-3.73589200	0.50540200	-2.44557000
Rh	-1.83770600	0.46649000	0.56164800	H	-4.59856500	-1.01612700	-2.47666500
Rh	0.15453700	0.21170400	-2.08930800	C	-4.26838100	-0.23506800	-0.55205100
Cl	-1.52613300	1.86976900	-1.42843400	C	-4.64207100	-0.06030100	0.58680600
Cl	-1.29916800	-1.39711700	-0.94078500	C	-5.11006100	0.18860900	1.95189800
C	-2.21392600	1.96486100	1.62012700	C	-5.53663600	1.65167300	2.19630000
O	-2.43756400	2.89782800	2.24798300	H	-4.31812400	-0.08148700	2.66438300
C	-2.03107500	-0.69884100	2.01424300	H	-5.95500700	-0.47741300	2.17610000
C	1.19758100	1.52981500	-2.91401000	C	-6.02432000	1.89312300	3.62949500
C	1.38386800	-1.13392300	-2.52068600	H	-4.68919000	2.31209400	1.97425400
O	-2.14172800	-1.43335400	2.88757900	H	-6.32792600	1.91575100	1.48378000
O	1.82019700	2.35644800	-3.40777900	C	-6.45040200	3.34303200	3.88022800
O	2.12294300	-1.97435300	-2.76985900	H	-6.86632200	1.22084500	3.84414000
1cat				H	-5.22830400	1.61748400	4.33487700
C	-2.89098400	-3.18019600	-5.08847900	H	-6.79250500	3.48627300	4.91024500
C	-3.31236800	-2.34601900	-3.87448900	H	-5.61926200	4.03567700	3.70606700

H	-7.26923700	3.63631000	3.21364700	O	-1.43245800	-2.11266000	-8.18502000
C	-3.95283900	-4.41967200	-4.06625600	H	1.45372600	-2.75319700	-9.81234600
C	-5.04765700	-3.89738000	-3.85348800	H	0.55795900	-3.88486600	-8.76600900
C	-2.79244200	-6.33481500	-6.30210200	H	0.49112400	-1.66354700	-7.69500800
O	-2.91720800	-5.95443700	-7.44252900	H	-0.08225200	-0.91702600	-9.21687700
O	-3.37046300	-7.45286700	-5.81639300	H	-1.72173800	-4.48103900	-9.47743600
C	-0.83407500	-6.58840000	-4.77523400	H	-2.29236600	-3.75412200	-11.00424900
O	-0.51550300	-6.80208100	-3.62272900	H	-2.34753100	-1.51567000	-9.95292600
O	-0.22350100	-7.12235900	-5.83766700	H	-3.26170300	-2.63904000	-8.90285700
C	-4.15703600	-8.20088000	-6.76318800	C	-6.48596100	-3.77334100	-3.46231400
H	-3.53768400	-8.51652600	-7.60582600	C	-7.02856200	-2.33119400	-3.45792700
H	-4.53089100	-9.06501400	-6.21474900	C	-7.32047600	-4.64036100	-4.43661000
H	-4.98358700	-7.59196100	-7.13631900	C	-6.58627600	-4.35925600	-2.02922100
C	0.97893300	-7.87050300	-5.56340200	H	-6.51540600	-1.71178900	-2.71737400
H	1.29892700	-8.26653300	-6.52632400	H	-6.92931300	-1.86861400	-4.44077600
H	1.73407600	-7.19856500	-5.15113900	H	-8.08944000	-2.35624500	-3.18788800
H	0.77353700	-8.67940900	-4.85920100	H	-6.97694100	-5.67947000	-4.42735100
S	0.90971200	-3.22253800	-4.52451300	H	-8.37145800	-4.62265000	-4.12785800
O	1.45948600	-4.48949300	-5.04833100	H	-7.24142300	-4.25496700	-5.45445300
O	1.37779300	-1.93725800	-5.07682400	H	-7.63330800	-4.34737100	-1.70829100
C	1.24413800	-3.19075500	-2.75446700	H	-6.23066800	-5.39343800	-1.99518600
C	0.98978200	-4.32349000	-1.97476800	H	-6.00419300	-3.76842500	-1.31584500
C	1.87230500	-2.06168900	-2.22691600	INT-1b¹			
C	1.34821800	-4.29979200	-0.62648000	C	-1.88282100	-5.67043300	-5.21825900
H	0.53587500	-5.20815100	-2.41016800	C	-1.25651100	-4.36852800	-5.80335900
C	2.23759500	-2.05990600	-0.87891900	H	-0.40205200	-4.64666500	-6.42058200
H	2.07664200	-1.21490600	-2.87279500	H	-1.98102300	-3.90148000	-6.47075100
C	1.96996400	-3.17315300	-0.08019600	C	-2.72507400	-5.44058200	-3.93754400
H	1.15379900	-5.16954400	-0.00624700	H	-3.13357400	-6.40429200	-3.61879700
H	2.73184200	-1.19015100	-0.45672900	H	-2.04418400	-5.11863400	-3.14629900
H	2.25368900	-3.16736400	0.96818900	C	-0.84817400	-3.34025100	-4.76993500
C	-1.35614800	-0.37258300	-1.43651700	C	-1.69268500	-2.44739700	-4.27763100
H	-1.26260500	0.59414200	-1.94402300	C	-2.15497400	-1.36613900	-3.55619700
H	-1.59293200	-0.17799800	-0.38615100	H	-1.93489600	-0.39359200	-3.99873000
H	-0.39166900	-0.88109700	-1.48653600	C	-2.49125800	-1.24343600	-2.06258300
C	-2.54933600	-2.58865800	-1.35347600	C	-3.87970100	-0.52928300	-1.95249100
H	-3.34012900	-3.21758700	-1.76818600	H	-3.82919400	0.42070300	-2.50217600
H	-1.59792900	-3.12186500	-1.43345500	H	-4.62675600	-1.13550300	-2.47800700
H	-2.76260800	-2.43430800	-0.29241200	C	-4.32328100	-0.27384400	-0.58177700
Rh	-3.69238700	-2.21828500	-5.03950800	C	-4.69788200	-0.07072500	0.55195900
Cl	-5.46081800	-2.46479200	-6.66465900	C	-5.16592100	0.21376000	1.91006300
C	-3.27343700	-0.72201700	-6.09762800	C	-5.55135800	1.69241100	2.12751000
O	-3.07133900	0.21503100	-6.72531000	H	-4.38575300	-0.06711400	2.63131100
C	-2.27253000	-2.40431000	-9.30574300	H	-6.03064100	-0.42422500	2.14025400
C	-1.70289100	-3.57312100	-10.09969900	C	-6.03498500	1.97365500	3.55473900
C	0.46366000	-2.99723900	-9.41351200	H	-4.68490600	2.32432200	1.89591000
C	-0.09566400	-1.83221200	-8.60292300	H	-6.33312400	1.96610400	1.40813600
O	-0.37178600	-3.28761900	-10.52802300	C	-6.42124000	3.43922000	3.77743500

H	-6.89573900	1.32907300	3.77979000	C	-1.78172800	-3.59490500	-10.11275100
H	-5.24830300	1.68926200	4.26708800	C	0.35718000	-2.86684500	-9.48711100
H	-6.76160900	3.61091700	4.80366000	C	-0.26144900	-1.76996400	-8.62572600
H	-5.57085300	4.10532900	3.59286100	O	-0.49390300	-3.19338000	-10.57911500
H	-7.23009300	3.74255400	3.10323000	O	-1.55607800	-2.16524400	-8.17067400
C	-3.85426700	-4.49797100	-4.00541400	H	1.30992400	-2.53562900	-9.91298400
C	-4.91746500	-3.94135300	-3.74766700	H	0.54320800	-3.76004300	-8.86793100
C	-2.72831400	-6.33588500	-6.32148200	H	0.34303600	-1.57866200	-7.73373500
O	-2.87667500	-5.91647200	-7.44541500	H	-0.34093900	-0.84097700	-9.21311000
O	-3.29303700	-7.47149600	-5.86345400	H	-1.70553100	-4.51447900	-9.51271500
C	-0.74625900	-6.63666200	-4.83372200	H	-2.38754900	-3.80172500	-11.00071700
O	-0.42045200	-6.90006700	-3.69373000	H	-2.57956000	-1.59878000	-9.88842800
O	-0.13795000	-7.11888900	-5.92217800	H	-3.36445100	-2.81515400	-8.83812700
C	-4.10393200	-8.18538400	-6.81648300	C	-6.27792700	-3.55681500	-3.36032200
H	-3.50594600	-8.47112800	-7.68478200	H	-6.27193500	-2.77533600	-2.59450500
H	-4.46507400	-9.06805200	-6.28959500	H	-6.82786900	-3.19356800	-4.23119000
H	-4.93871900	-7.56290000	-7.14638200	H	-6.79105400	-4.43463000	-2.95112300
C	1.06917700	-7.87284900	-5.68694800	INT-1a²			
H	1.38670200	-8.22373300	-6.66799400	C	-2.76883400	-0.97844100	-5.21317700
H	1.82352200	-7.21687900	-5.24808400	C	-3.55584000	0.36794300	-5.19318200
H	0.87088700	-8.71331700	-5.01864900	H	-3.17652200	0.98195200	-6.01383900
S	0.95056300	-3.22367300	-4.45098600	H	-4.59477300	0.13598500	-5.42827800
O	1.53274600	-4.45874900	-5.01434500	C	-3.21981300	-1.97527900	-4.10282900
O	1.40476200	-1.90742100	-4.93655900	H	-2.49944800	-2.79572700	-4.07247500
C	1.24245000	-3.26257100	-2.67319200	H	-3.15994800	-1.46967400	-3.13455600
C	1.01333900	-4.44021100	-1.95481500	C	-3.54600800	1.19507800	-3.91833600
C	1.80229100	-2.13372100	-2.07336300	C	-4.44868500	1.19566200	-2.96813300
C	1.32694300	-4.46484800	-0.59532000	C	-5.35624400	1.34992700	-2.03678900
H	0.61239200	-5.32172700	-2.44482800	H	-6.17521200	2.03212400	-2.28176100
C	2.12243400	-2.17916400	-0.71474000	C	-5.41284800	0.75252600	-0.63693400
H	1.99267200	-1.25078300	-2.67352000	C	-6.81766900	0.07842700	-0.48692500
C	1.87915900	-3.33918900	0.02287600	H	-7.58921400	0.81860200	-0.74125100
H	1.15157200	-5.37043500	-0.02251000	H	-6.90215100	-0.72553800	-1.22809500
H	2.56402800	-1.30996400	-0.23671200	C	-7.08814900	-0.46230400	0.84524000
H	2.12810300	-3.37024600	1.07961900	C	-7.30912900	-0.90592900	1.94997000
C	-1.41514600	-0.32526400	-1.43716400	C	-7.61836800	-1.46817700	3.26605200
H	-1.36211200	0.63844400	-1.95602900	C	-8.85002400	-2.39855200	3.25428800
H	-1.66602900	-0.12921600	-0.39055600	H	-7.78610300	-0.65364000	3.98460200
H	-0.42844000	-0.79108400	-1.47618500	H	-6.74819400	-2.02543900	3.64011000
C	-2.51142200	-2.58906400	-1.32611600	C	-9.16219300	-2.98595800	4.63541900
H	-3.27000700	-3.26036600	-1.73435700	H	-9.71664700	-1.83700300	2.88367600
H	-1.53818700	-3.08359800	-1.38888600	H	-8.67672300	-3.20812800	2.53462400
H	-2.74087200	-2.42417000	-0.26997800	C	-10.38406700	-3.91006600	4.62919800
Rh	-3.66064100	-2.26189800	-4.99846100	H	-8.28613800	-3.53903500	5.00110900
Cl	-5.55691600	-2.48056700	-6.47567400	H	-9.32471000	-2.16751200	5.35011700
C	-3.29820000	-0.77210500	-6.08048800	H	-10.58388300	-4.31547100	5.62635200
O	-3.12918500	0.16544200	-6.71714300	H	-11.28281500	-3.37594300	4.30068200
C	-2.41212300	-2.49435000	-9.26909400	H	-10.23643200	-4.75638300	3.94888000

C	-4.56955400	-2.54104400	-4.31598700	H	-2.85853500	-8.55909100	-1.10782000
C	-5.71812000	-2.75479800	-4.76147800	H	-4.04636700	-7.63246200	-0.16107700
C	-3.00797100	-1.64745400	-6.58272800	H	-3.24109700	-6.02088400	-1.73374800
O	-3.85267100	-1.30564900	-7.38400300	H	-3.15494700	-7.17149800	-3.07488000
O	-2.18505500	-2.68942700	-6.74195800	H	-5.99279000	-9.68554800	-2.98989400
C	-1.26616200	-0.71519500	-5.02694600	H	-4.37131000	-9.17110500	-3.47488300
O	-0.67425700	-0.87065300	-3.97684000	H	-5.77809100	-7.39309300	-4.29436700
O	-0.70779500	-0.28154600	-6.15920800	H	-6.82639100	-7.43905400	-2.83674300
C	-2.37071400	-3.47737200	-7.93545700	C	-6.99268200	-2.58939600	-5.52091100
H	-2.42657700	-2.82891600	-8.81182900	C	-8.20404100	-2.97266600	-4.64377700
H	-1.50176000	-4.13222200	-7.98732100	C	-7.10847100	-1.10515700	-5.94472400
H	-3.28075300	-4.07165100	-7.83814300	C	-6.95375400	-3.48110000	-6.78325800
C	0.67415100	0.11758600	-6.07672400	H	-8.15328000	-4.02237700	-4.34135400
H	0.98017900	0.31423600	-7.10372500	H	-8.25433800	-2.35690100	-3.74008900
H	0.75070300	1.02215000	-5.47206500	H	-9.12815500	-2.82078000	-5.21110700
H	1.27470700	-0.68290800	-5.63958500	H	-6.27923600	-0.82383900	-6.59846700
S	-2.34218300	2.58392800	-3.84717600	H	-8.04423000	-0.95685200	-6.49449100
O	-1.25126300	2.24121500	-4.77865100	H	-7.11782100	-0.44327400	-5.07262800
O	-3.08185200	3.84435400	-4.02509400	H	-7.88636200	-3.35654400	-7.34464000
C	-1.67670200	2.58681600	-2.17209000	H	-6.11787300	-3.19715500	-7.42738900
C	-0.79114200	1.58117200	-1.77395400	H	-6.83656100	-4.53484000	-6.51962900
C	-2.02011400	3.64284200	-1.32718100	INT-1b²			
C	-0.25581800	1.63602100	-0.48639400	C	-2.51940700	-1.13159400	-5.06765900
H	-0.52771400	0.77570400	-2.45187800	C	-3.38461600	0.15248200	-5.25076500
C	-1.46944000	3.68712600	-0.04466400	H	-2.98206000	0.69762800	-6.10732300
H	-2.69482100	4.41296800	-1.68404900	H	-4.38613200	-0.17515400	-5.53644800
C	-0.59316000	2.68402000	0.37506000	C	-2.96187200	-2.00997000	-3.86355100
H	0.43230800	0.86219700	-0.15959900	H	-2.25989900	-2.84035400	-3.77227600
H	-1.72212000	4.50616600	0.62206300	H	-2.86699900	-1.41761600	-2.94841700
H	-0.16743000	2.72117000	1.37368600	C	-3.51391500	1.10236800	-4.07331200
C	-5.28880700	1.91809500	0.37014200	C	-4.46020000	1.11423200	-3.16740300
H	-6.05455700	2.68136000	0.19130300	C	-5.42351200	1.25639100	-2.29230400
H	-5.41839200	1.54367500	1.38972900	H	-6.29068500	1.83344400	-2.62550300
H	-4.30825200	2.39531600	0.29116700	C	-5.49841800	0.75130700	-0.85736300
C	-4.29678800	-0.27358600	-0.40025400	C	-6.78552600	-0.13572400	-0.75972900
H	-4.37632700	-1.11083400	-1.10048100	H	-7.64280700	0.44810100	-1.12305000
H	-3.31015400	0.18344300	-0.51963300	H	-6.67286500	-0.98144300	-1.45006600
H	-4.37063300	-0.67802400	0.61282000	C	-7.07358800	-0.63414000	0.58511500
Rh	-5.12641400	-4.48604000	-3.55576600	C	-7.30123800	-1.04022800	1.70285000
Cl	-4.06887700	-5.55748700	-5.43099900	C	-7.60723300	-1.55758400	3.03787300
C	-5.94708700	-3.77470800	-2.05567700	C	-8.82595900	-2.50447400	3.06080100
O	-6.47063000	-3.36092900	-1.11216500	H	-7.78792500	-0.71886200	3.72468500
C	-5.80567100	-7.54968000	-3.21189300	H	-6.73007100	-2.08823500	3.43336700
C	-5.23041300	-8.91658300	-2.83659500	C	-9.13035100	-3.04115900	4.46419300
C	-3.82543800	-8.03254300	-1.15581100	H	-9.70017900	-1.97018000	2.66825000
C	-3.71854500	-6.89628200	-2.17825900	H	-8.64042200	-3.33975000	2.37425900
O	-4.88052000	-8.94310600	-1.46404000	C	-10.33892300	-3.98201700	4.49561900
O	-5.04825000	-6.48494000	-2.56203600	H	-8.24645600	-3.56672600	4.85078000

H	-9.30412300	-2.19713800	5.14569800	C	-5.17024200	-3.97262600	-1.66810300
H	-10.53198300	-4.35088500	5.50814900	O	-5.29317200	-3.66645800	-0.56144200
H	-11.24560100	-3.47411000	4.14784200	C	-6.18897000	-7.40798800	-3.14375200
H	-10.17957100	-4.85221100	3.84891000	C	-5.88883000	-8.90988400	-3.09797000
C	-4.33812600	-2.53119300	-3.99676000	C	-3.75531900	-8.61879500	-2.13298800
C	-5.55419300	-2.60189800	-4.26991000	C	-3.77879500	-7.37176900	-3.02489400
C	-6.88772400	-2.30519300	-4.81128700	O	-5.04772200	-9.20846300	-1.99817800
H	-7.66381900	-2.41496100	-4.04764400	O	-5.00209900	-6.64831900	-2.77178500
H	-6.91581500	-1.27724500	-5.19063200	H	-3.03731400	-9.34308300	-2.55086700
H	-7.11376300	-2.99051500	-5.63355800	H	-3.43137800	-8.36092300	-1.11996200
C	-2.64063000	-1.95152300	-6.37007300	H	-2.96012600	-6.69599300	-2.77107400
O	-3.33658900	-1.65182900	-7.31314200	H	-3.71047200	-7.60003200	-4.09273000
O	-1.87706600	-3.05334600	-6.30353600	H	-6.82013800	-9.46430300	-2.95280400
C	-1.04542600	-0.75255000	-4.84845600	H	-5.44484000	-9.25120200	-4.04514300
O	-0.50131400	-0.73607900	-3.76192000	H	-6.51120300	-7.09861000	-4.14300100
O	-0.45179900	-0.43628900	-6.00185900	H	-6.94230800	-7.13247600	-2.40150100
C	-1.94788400	-3.93056800	-7.44763300	INT-1a³			
H	-1.74764600	-3.37120400	-8.36383100	C	0.07343900	-3.07350000	-5.52559000
H	-1.18119000	-4.68654700	-7.27941500	C	-1.21065300	-2.28374500	-5.92701800
H	-2.93589900	-4.39175600	-7.49277100	H	-0.88845600	-1.43585700	-6.53398200
C	0.89408000	0.07001600	-5.90682100	H	-1.77389200	-2.94869600	-6.58596100
H	1.23707500	0.17383400	-6.93562400	C	-0.26852000	-4.49884900	-4.98828400
H	0.87786400	1.03879800	-5.40572800	H	0.64031600	-4.94485700	-4.57236100
H	1.52550800	-0.63052900	-5.35613300	H	-0.98498800	-4.41570600	-4.16663000
S	-2.41336200	2.57435400	-4.09262100	C	-2.17842800	-1.76049700	-4.87465600
O	-1.24172500	2.20754300	-4.91036600	C	-3.31342200	-2.32959500	-4.48519800
O	-3.21966600	3.75028400	-4.45894300	C	-4.63777500	-2.21324700	-4.03922900
C	-1.86526000	2.80899300	-2.39285800	H	-5.26964300	-1.73451500	-4.79001800
C	-0.91192900	1.94513500	-1.84655700	C	-5.29944200	-2.11916600	-2.65172500
C	-2.37338800	3.89354400	-1.67679900	C	-6.39144300	-3.23795000	-2.54607300
C	-0.47496400	2.17449900	-0.54117500	H	-7.00510000	-3.21904300	-3.45791400
H	-0.52311400	1.11402100	-2.42610700	H	-5.88230900	-4.20760200	-2.52478300
C	-1.92090100	4.11296800	-0.37413800	C	-7.26235600	-3.11668300	-1.37606800
H	-3.09569800	4.55143700	-2.14703200	C	-7.97956700	-3.02122500	-0.40492300
C	-0.97702000	3.25335100	0.19236500	C	-8.86369400	-2.93299000	0.75887000
H	0.26455700	1.51292000	-0.10015700	C	-10.08533500	-3.87252300	0.67263000
H	-2.30151100	4.95693000	0.19338700	H	-9.21285900	-1.89756900	0.87701700
H	-0.62746700	3.42704200	1.20601400	H	-8.29379100	-3.16431700	1.66960000
C	-5.64169800	1.98311100	0.06335800	C	-11.00000100	-3.76656400	1.89816500
H	-6.50236100	2.59772900	-0.22410600	H	-10.65249600	-3.63767600	-0.23684600
H	-5.78845900	1.66078500	1.09827900	H	-9.73294300	-4.90528300	0.55851300
H	-4.74528400	2.60777100	0.01295700	C	-12.21735200	-4.69327800	1.81888900
C	-4.25939400	-0.06294700	-0.46273200	H	-10.42177400	-3.99707100	2.80334600
H	-4.15395600	-0.95049900	-1.09336400	H	-11.33752000	-2.72705200	2.00996500
H	-3.34886000	0.53607100	-0.55404400	H	-12.85207600	-4.59613000	2.70561100
H	-4.34962200	-0.40166300	0.57267600	H	-12.83321700	-4.46357700	0.94195800
Rh	-4.99356000	-4.51854000	-3.43410700	H	-11.91196500	-5.74293800	1.74169300
Cl	-4.89755300	-5.38024700	-5.67785400	C	-0.78023100	-5.34987700	-6.06866900

C	-1.09905600	-5.97301700	-7.06048800	H	-6.60735700	-6.94746700	-4.66046000
C	0.93738600	-3.21978200	-6.79449800	H	-7.39705800	-8.07226100	-6.62660400
O	0.65900200	-2.79920200	-7.89446500	H	-6.51667100	-6.98621300	-7.72928000
O	2.06065800	-3.91289200	-6.51890200	H	-4.01675600	-7.49754500	-3.99970200
C	0.87056100	-2.30427900	-4.47008100	H	-3.08362700	-7.32056800	-5.50029900
O	0.73738300	-2.45842800	-3.27200900	H	-4.01821000	-9.50259800	-5.83208200
O	1.70731500	-1.42332400	-5.03080900	H	-5.51089900	-9.12578800	-4.96108800
C	2.95725100	-4.09890500	-7.62570100	C	-1.37696600	-6.68681700	-8.32465200
H	3.27209000	-3.13304600	-8.02814600	C	-1.21529100	-8.21087000	-8.11927900
H	3.81082700	-4.64470100	-7.22392700	C	-2.81041200	-6.37762800	-8.81576300
H	2.47300800	-4.67358800	-8.41890000	C	-0.35487500	-6.19971800	-9.38207300
C	2.39341400	-0.52809300	-4.13655600	H	-0.21235200	-8.45447300	-7.75632500
H	3.15149000	-0.03422400	-4.74357700	H	-1.94258200	-8.59246200	-7.39647600
H	1.68416800	0.20504000	-3.74792800	H	-1.37608100	-8.73518100	-9.06751000
H	2.85161000	-1.08358900	-3.31588000	H	-2.95317800	-5.30085400	-8.94773300
S	-2.01268700	0.04725900	-4.54639800	H	-2.98418700	-6.86479300	-9.78178700
O	-0.67187000	0.42474200	-5.03595100	H	-3.56049200	-6.74880500	-8.11224300
O	-3.20842600	0.70921300	-5.10416300	H	-0.55636200	-6.67772900	-10.34724300
C	-2.03460400	0.36174800	-2.76722600	H	-0.40886400	-5.11497300	-9.50872700
C	-1.16535300	-0.30182900	-1.89793600	H	0.66566100	-6.45557400	-9.07986200
C	-2.86580400	1.39287000	-2.32303400	INT-1b³			
C	-1.15406100	0.06723000	-0.55199200	C	0.15559100	-2.87208200	-5.60556300
H	-0.52012600	-1.09848100	-2.25022200	C	-1.13133900	-2.07808800	-5.97869300
C	-2.83601000	1.75579600	-0.97568000	H	-0.81237900	-1.18764600	-6.52308700
H	-3.51663000	1.89593700	-3.02944500	H	-1.67459000	-2.70514900	-6.68828500
C	-1.98424700	1.09211300	-0.09094500	C	-0.16573700	-4.25711200	-4.97275900
H	-0.49303500	-0.45109600	0.13597500	H	0.77418100	-4.73185800	-4.67450600
H	-3.47904500	2.55541300	-0.62035200	H	-0.75183900	-4.11548700	-4.06152800
H	-1.96684500	1.37288400	0.95818200	C	-2.11965300	-1.64023800	-4.90702300
C	-6.00062900	-0.73664400	-2.64060600	C	-3.20806000	-2.29846800	-4.52113900
H	-6.76274600	-0.66581700	-3.42518000	C	-4.54428100	-2.28078700	-4.08180400
H	-6.49556700	-0.59041300	-1.67701100	H	-5.19801600	-1.84847200	-4.84210900
H	-5.28024800	0.07035000	-2.79143400	C	-5.22713700	-2.20212800	-2.70405400
C	-4.32785300	-2.20709500	-1.46733000	C	-6.26372700	-3.37204200	-2.59920000
H	-3.75770400	-3.13578500	-1.48136300	H	-6.86047400	-3.39849900	-3.52192600
H	-3.63175500	-1.36793100	-1.47256600	H	-5.70664200	-4.31428300	-2.55351300
H	-4.90101500	-2.16578300	-0.53619400	C	-7.16237700	-3.27443500	-1.44799900
Rh	-4.12588300	-4.16868800	-4.90722200	C	-7.90341600	-3.19332400	-0.49357900
Cl	-3.25605100	-5.14804600	-2.91488000	C	-8.81442600	-3.11691900	0.65011300
C	-4.71581900	-3.57020500	-6.57742300	C	-10.03073300	-4.05979400	0.53179100
O	-5.06482100	-3.23700600	-7.62345300	H	-9.17005300	-2.08340100	0.76615000
C	-4.76388700	-8.72146800	-5.66165000	H	-8.26451100	-3.35097000	1.57241600
C	-4.08392100	-7.46742900	-5.09130200	C	-10.97475700	-3.95823700	1.73511400
C	-6.23177900	-6.55000300	-5.61197300	H	-10.57641700	-3.82464700	-0.39066600
C	-6.45188400	-7.52639300	-6.78036400	H	-9.67298100	-5.09143900	0.42422400
O	-4.82679200	-6.28352200	-5.49462300	C	-12.18609300	-4.88994500	1.62765400
O	-5.35886800	-8.42999500	-6.91658200	H	-10.41704600	-4.18614400	2.65374800
H	-6.73040700	-5.59727100	-5.79728200	H	-11.31910300	-2.92012600	1.83878700

H	-12.84218400	-4.79484000	2.49894900	O	-4.82038500	-3.35053200	-7.68009600
H	-12.78208900	-4.66349200	0.73622400	C	-4.44598000	-8.80036300	-5.52293100
H	-11.87484500	-5.93847400	1.55858900	C	-3.91978100	-7.51956100	-4.85511400
C	-0.87252600	-5.12066300	-5.92483500	C	-5.90079500	-6.64652300	-5.86213600
C	-1.37090800	-5.78064000	-6.81314200	C	-5.85589400	-7.65833900	-7.02072600
C	-1.92097100	-6.57506100	-7.91083000	O	-4.55926600	-6.35991500	-5.45008500
H	-1.16645200	-7.26424100	-8.30696600	O	-4.75151700	-8.55035500	-6.88750200
H	-2.78613600	-7.16946800	-7.59896700	H	-6.35445000	-5.70626900	-6.17906100
H	-2.23695300	-5.92667100	-8.73618000	H	-6.47355000	-7.02368500	-5.00476500
C	0.94424200	-3.09371400	-6.91128200	H	-6.80619400	-8.21466000	-7.06162300
O	0.59871400	-2.74314000	-8.01586700	H	-5.71557700	-7.14592400	-7.97685100
O	2.08555200	-3.76911200	-6.66173400	H	-4.09691400	-7.51819000	-3.77497800
C	1.01655800	-2.04970800	-4.64340400	H	-2.85373000	-7.37499500	-5.03129400
O	1.01659000	-2.18342200	-3.43596300	H	-3.67513300	-9.57499000	-5.50232900
O	1.73888700	-1.13645300	-5.30355800	H	-5.32747000	-9.19650100	-4.99583400
C	2.90563800	-4.03568300	-7.81120000	INT-1a⁴			
H	3.20702800	-3.10098400	-8.29021100	C	1.93043600	-0.96094100	-9.43719600
H	3.77588300	-4.57216000	-7.43355500	C	0.77404000	0.02321000	-9.79309900
H	2.36166500	-4.64659100	-8.53570700	H	1.16642800	0.76487600	-10.49186400
C	2.44920500	-0.17532500	-4.49990600	H	0.02204900	-0.55813700	-10.32997100
H	3.10236900	0.35600100	-5.19132900	C	1.46926600	-2.09124300	-8.47235500
H	1.73273500	0.51438000	-4.04973700	H	2.34054500	-2.70116400	-8.21456100
H	3.02936600	-0.67845900	-3.72388000	H	1.13875200	-1.61796400	-7.54447600
S	-2.05515500	0.15933700	-4.51841600	C	0.08692500	0.73204100	-8.63842300
O	-0.76102300	0.64149200	-5.04286500	C	-0.95267100	0.30492600	-7.96598600
O	-3.31128000	0.77084800	-4.99580300	C	-2.04154200	-0.04673900	-7.33102900
C	-2.01730400	0.38653800	-2.72747500	H	-2.98727600	0.20757100	-7.81655000
C	-1.09636200	-0.29413900	-1.92773200	C	-2.17814300	-0.78666500	-6.00406300
C	-2.86650500	1.36118100	-2.19825100	C	-2.75421500	-2.19806400	-6.36249500
C	-1.04985000	-0.00141400	-0.56403200	H	-3.68793900	-2.08354700	-6.92752500
H	-0.43627800	-1.04537100	-2.34609700	H	-2.04523400	-2.70584100	-7.02696500
C	-2.80094700	1.64874200	-0.83421600	C	-3.04209500	-3.05201600	-5.19484700
H	-3.56071500	1.87706100	-2.85211200	C	-3.22929200	-3.42343100	-4.01434500
C	-1.89704700	0.96612900	-0.01801900	C	-3.28499400	-3.41594300	-2.53967900
H	-0.34788300	-0.53365500	0.07059900	C	-4.69411300	-3.63910400	-1.95676400
H	-3.45767800	2.40334900	-0.41181600	H	-2.89305500	-2.44545400	-2.20162500
H	-1.85257800	1.18741500	1.04446700	H	-2.59957600	-4.17856600	-2.14646500
C	-5.99231400	-0.85337700	-2.72232800	C	-4.70556500	-3.58173100	-0.42493100
H	-6.75319300	-0.83390400	-3.51104500	H	-5.37638200	-2.88817300	-2.37083400
H	-6.49794200	-0.71081000	-1.76373000	H	-5.07075000	-4.60900400	-2.30134200
H	-5.30947700	-0.01722600	-2.88973900	C	-6.09863500	-3.81779200	0.16712800
C	-4.27310200	-2.22633800	-1.50234700	H	-4.00644900	-4.33023800	-0.02634900
H	-3.65938900	-3.12643300	-1.49321400	H	-4.32664000	-2.60527100	-0.09232200
H	-3.61828400	-1.35458000	-1.50712900	H	-6.08058200	-3.77170100	1.26084500
H	-4.86493400	-2.19953500	-0.58233300	H	-6.81153600	-3.06541500	-0.18776500
Rh	-3.86544900	-4.18664800	-4.94055100	H	-6.48789700	-4.80099300	-0.11974300
Cl	-2.99202900	-5.08338600	-2.90696700	C	0.42053500	-2.93465300	-9.04703700
C	-4.46393000	-3.64368800	-6.62391000	C	-0.41952000	-3.62290200	-9.58493500

C	2.41952500	-1.59058800	-10.75350900	H	-5.25936400	-9.77752700	-6.63946600
O	1.95944700	-1.37440000	-11.85109000	H	-4.79457600	-10.23306900	-4.99590200
O	3.42822000	-2.45480100	-10.51920300	H	-5.71371800	-7.72119200	-7.62879100
C	3.08779500	-0.20063500	-8.77328200	H	-6.27321800	-6.16861800	-6.94841400
O	3.26177500	-0.14145400	-7.57254100	H	-7.36784300	-7.18368300	-5.09748400
O	3.86179000	0.39690200	-9.68525000	H	-7.77186700	-8.26543100	-6.45544900
C	3.95791200	-3.11127000	-11.68329300	C	-1.41027300	-4.46566500	-10.28171000
H	4.35523200	-2.37691800	-12.38805900	C	-1.78423100	-5.67414000	-9.39172200
H	4.75187700	-3.76216100	-11.31785200	C	-2.67729900	-3.63325500	-10.58792500
H	3.17903200	-3.69506900	-12.17963600	C	-0.78907300	-4.96793100	-11.60748800
C	4.89408200	1.26279500	-9.17406400	H	-0.90021400	-6.27300200	-9.15259500
H	5.48127600	1.55806900	-10.04302800	H	-2.23915000	-5.34482400	-8.45225600
H	4.43169800	2.13366900	-8.70725800	H	-2.50352500	-6.31372100	-9.91564400
H	5.51366500	0.72982100	-8.44969300	H	-2.43722900	-2.77261600	-11.21927500
S	0.60342300	2.46578700	-8.33665000	H	-3.41341800	-4.25041200	-11.11477300
O	1.99957900	2.57187100	-8.80171500	H	-3.13823200	-3.26410100	-9.66709800
O	-0.42255800	3.36085000	-8.89628100	H	-1.51394400	-5.58140700	-12.15409700
C	0.58775500	2.67870500	-6.54880200	H	-0.49660200	-4.12752200	-12.24377900
C	1.63295200	2.15555100	-5.78260000	H	0.10058300	-5.57579600	-11.41611800
C	-0.45541100	3.40589200	-5.97409000	INT-1b⁴			
C	1.61655500	2.36277100	-4.40268000	C	1.50986500	-1.34195100	-9.57468300
H	2.43335800	1.59497900	-6.25423800	C	0.64148600	-0.05575300	-9.73411700
C	-0.45608500	3.60641500	-4.59237500	H	1.14884000	0.60672100	-10.43852900
H	-1.23444000	3.81423500	-6.60823800	H	-0.29411800	-0.36632500	-10.20310100
C	0.57628100	3.08423000	-3.80959600	C	0.88818200	-2.36732800	-8.58462200
H	2.42049200	1.96384700	-3.79139000	H	1.57773000	-3.21206400	-8.49234100
H	-1.25751400	4.17550600	-4.13078500	H	0.85379100	-1.89247900	-7.60035900
H	0.57359200	3.24406600	-2.73516600	C	0.29852100	0.71835300	-8.47272400
C	-3.17853000	0.00139200	-5.13221900	C	-0.76660200	0.55637200	-7.72795700
H	-4.14592400	0.10853400	-5.63402100	C	-1.85990500	0.47689300	-7.01356400
H	-3.35194700	-0.51214500	-4.18242800	H	-2.72111300	1.03878900	-7.38385100
H	-2.79062400	1.00163400	-4.91608900	C	-2.11143700	-0.34080800	-5.74961200
C	-0.83476800	-0.92659200	-5.27459800	C	-2.99679200	-1.54934600	-6.20455700
H	-0.12415600	-1.52056600	-5.85624400	H	-3.89104400	-1.17304400	-6.71940900
H	-0.38612500	0.05171300	-5.08418500	H	-2.43785400	-2.12932000	-6.94369200
H	-0.97633000	-1.43052300	-4.31437800	C	-3.45844600	-2.43692200	-5.11603600
Rh	-3.83672100	-5.04309100	-5.31105200	C	-4.08020200	-2.83254100	-4.10335200
Cl	-6.00291500	-4.05317300	-5.59807800	C	-4.91913400	-2.81929200	-2.88935300
C	-2.13517800	-5.77180900	-5.16024500	C	-6.17133800	-3.71359300	-2.97753300
O	-1.06750400	-6.20549100	-5.07223300	H	-5.21867900	-1.77681800	-2.70866400
C	-6.95257600	-7.88723700	-5.82430900	H	-4.31292800	-3.12261500	-2.02513000
C	-5.92990000	-7.17303300	-6.70371100	C	-7.02935800	-3.63965000	-1.70938500
C	-4.10918300	-8.26840100	-5.55454700	H	-6.76106600	-3.41957600	-3.85312500
C	-5.14087400	-9.39836500	-5.61253800	H	-5.85519800	-4.74719700	-3.16037500
O	-4.69886000	-7.01133200	-5.96903700	C	-8.26988600	-4.53576600	-1.78014700
O	-6.36978200	-8.96018400	-5.07214200	H	-6.42070100	-3.92423600	-0.83967300
H	-3.77293000	-8.12013500	-4.52582500	H	-7.33827400	-2.59934800	-1.53658400
H	-3.24116200	-8.48966900	-6.19017400	H	-8.86571400	-4.46532100	-0.86438900

H	-8.91353700	-4.25374700	-2.62064000	C	-3.83123200	-8.72676600	-6.18272500
H	-7.99072000	-5.58634800	-1.91744100	C	-3.12628000	-7.45187300	-6.64247000
C	-0.43566400	-2.84401200	-8.98716600	C	-1.72460600	-7.44624400	-4.68339800
C	-1.52162100	-3.24397800	-9.34562600	C	-1.82115600	-8.95082900	-4.95966100
C	-2.83425100	-3.72492800	-9.77266800	O	-2.68517600	-6.71458600	-5.48333600
H	-2.74128500	-4.61735000	-10.40202900	O	-3.17564100	-9.33706700	-5.06477200
H	-3.46439600	-3.98173600	-8.91279800	H	-1.98079600	-7.23619700	-3.64255400
H	-3.35914200	-2.96185800	-10.35831700	H	-0.71291900	-7.07133300	-4.88936500
C	1.63046100	-1.98562000	-10.96787200	H	-1.24913100	-9.22823600	-5.85856700
O	1.12203800	-1.56897000	-11.98275600	H	-1.39093400	-9.50076700	-4.11754800
O	2.37408300	-3.10999900	-10.90747500	H	-2.25752800	-7.65841600	-7.27967000
C	2.91446500	-0.97940800	-9.06790700	H	-3.81491700	-6.79723600	-7.17556200
O	3.27016900	-1.08603200	-7.91123500	H	-4.84898900	-8.49549600	-5.85576000
O	3.68485000	-0.52243400	-10.06063800	H	-3.88804100	-9.43208700	-7.02687700
C	2.55328600	-3.79523700	-12.15850400	INT-1a⁵			
H	3.06244000	-3.14904300	-12.87763300	C	1.05789000	-2.08054000	-9.56466800
H	3.16198600	-4.66986200	-11.92999700	C	0.26726700	-0.74310900	-9.69807000
H	1.58741900	-4.09502600	-12.57187200	H	0.75771100	-0.13758200	-10.46271700
C	4.97593300	-0.00959000	-9.67734200	H	-0.72378200	-0.99978300	-10.07735400
H	5.48349100	0.22496200	-10.61243600	C	0.39587100	-3.05988000	-8.55229500
H	4.83959700	0.89034400	-9.07600300	H	1.02662200	-3.95072600	-8.47280700
H	5.53173300	-0.76098900	-9.11220200	H	0.41406300	-2.57982300	-7.57086300
S	1.32642500	2.19514600	-8.11520200	C	0.09553500	0.08299400	-8.43475300
O	2.63090700	1.96209500	-8.76369700	C	-0.85605200	-0.03692000	-7.54354100
O	0.54714500	3.39715400	-8.45411500	C	-1.84211200	-0.07587000	-6.68364900
C	1.57240000	2.19948900	-6.33119000	H	-2.74488000	0.47686600	-6.95567300
C	2.48803200	1.31291100	-5.75817300	C	-1.91414500	-0.81204700	-5.34889500
C	0.86150800	3.12406600	-5.56474800	C	-2.90885400	-2.00338000	-5.57752000
C	2.68102700	1.35499200	-4.37682000	H	-3.87266200	-1.61986200	-5.93262200
H	3.02876100	0.60431200	-6.37692200	H	-2.51234400	-2.64983600	-6.36870800
C	1.06790400	3.15506800	-4.18438000	C	-3.16699700	-2.79393700	-4.36366500
H	0.17638600	3.80773300	-6.05355600	C	-3.27730600	-3.26808800	-3.23434000
C	1.97357100	2.27119500	-3.59291100	C	-3.28052000	-3.64687900	-1.81316000
H	3.38821600	0.67360900	-3.91349200	C	-4.59296400	-3.30453200	-1.07806700
H	0.52740300	3.87275800	-3.57440100	H	-2.43912600	-3.12418500	-1.33635600
H	2.13258000	2.29908000	-2.51870400	H	-3.06767300	-4.71862700	-1.71769900
C	-2.87827400	0.54848100	-4.75045300	C	-4.54803000	-3.70098200	0.40202300
H	-3.81369300	0.92104000	-5.18266000	H	-4.78611100	-2.22977500	-1.17551400
H	-3.12305700	-0.01662300	-3.84590800	H	-5.42489100	-3.80978500	-1.58108100
H	-2.27111000	1.41101500	-4.45865800	C	-5.84420500	-3.36140100	1.14446000
C	-0.80583200	-0.83823800	-5.11402000	H	-4.34992400	-4.77870300	0.48401200
H	-0.25551200	-1.49429700	-5.79399700	H	-3.70214200	-3.19779500	0.89079800
H	-0.15515600	-0.00067200	-4.84958000	H	-5.78794800	-3.65665700	2.19699100
H	-1.01854700	-1.40524000	-4.20329800	H	-6.05022700	-2.28598600	1.10970500
Rh	-3.19570300	-4.56927700	-5.03635100	H	-6.70187000	-3.87622300	0.69795100
Cl	-5.02142400	-4.72194400	-6.59883200	C	-0.96431300	-3.43961400	-8.93519400
C	-1.75225400	-4.39533800	-3.88697500	C	-2.07483200	-3.74052500	-9.31640400
O	-0.85372000	-4.25584600	-3.17265900	C	1.08989000	-2.73782200	-10.95565700

O	0.57444800	-2.29288700	-11.95526500	H	-3.91880900	-2.08257100	-10.46507900
O	1.75498400	-3.90994900	-10.91053600	H	-5.32065600	-3.13944800	-10.20740700
C	2.49111700	-1.79269300	-9.09461800	H	-4.44951500	-2.46798400	-8.81760300
O	2.84498600	-1.83856600	-7.93313400	H	-4.24105200	-4.91942400	-11.67212700
O	3.28233100	-1.46194500	-10.11985100	H	-2.80514800	-3.90246900	-11.91867200
C	1.84271200	-4.61591200	-12.16015800	H	-2.62686100	-5.54751100	-11.28472500
H	2.36261200	-4.00889400	-12.90513400	INT-1b⁵			
H	2.40391000	-5.52494800	-11.94518800	C	0.96821500	-2.10196500	-9.58327900
H	0.84453900	-4.85830300	-12.53250900	C	0.24340900	-0.72623300	-9.70486200
C	4.61089200	-1.01613000	-9.78322700	H	0.71649300	-0.16753700	-10.51490100
H	5.13358900	-0.91912700	-10.73420700	H	-0.78131200	-0.93814400	-10.01581400
H	4.54654700	-0.05067700	-9.27917500	C	0.35105300	-3.00558600	-8.47750900
H	5.10642500	-1.74686600	-9.14056600	H	0.93431700	-3.93017300	-8.42723500
S	1.18678700	1.55007700	-8.29352900	H	0.49642900	-2.49864200	-7.51967100
O	2.42833800	1.21435600	-9.01611000	C	0.18926800	0.14298800	-8.46022100
O	0.41489000	2.74103800	-8.68323600	C	-0.74202200	0.12752500	-7.54018300
C	1.57941100	1.70675500	-6.54365500	C	-1.70144600	0.19079600	-6.65226500
C	2.51850600	0.84610900	-5.96871900	H	-2.56520400	0.80664700	-6.91417400
C	0.96698200	2.72540000	-5.81259200	C	-1.79317800	-0.52592800	-5.30694700
C	2.83739900	1.01258200	-4.62051800	C	-2.73321300	-1.75678500	-5.54649500
H	2.97782600	0.06061400	-6.55972300	H	-3.68671000	-1.43038400	-5.97911900
C	1.29786100	2.87972200	-4.46497100	H	-2.27214700	-2.41191400	-6.29208700
H	0.26110100	3.38574100	-6.30405400	C	-3.04655400	-2.51522100	-4.32349600
C	2.22920900	2.02444100	-3.87143200	C	-3.33430300	-2.92635900	-3.20087300
H	3.56536700	0.35393700	-4.15645400	C	-3.66865400	-3.19066900	-1.79370800
H	0.83488800	3.67140400	-3.88352800	C	-5.13274000	-3.61900300	-1.56407600
H	2.48645800	2.14961100	-2.82352500	H	-3.46056100	-2.26692500	-1.23523700
C	-2.48196100	0.16813600	-4.30166400	H	-2.98971700	-3.95228800	-1.38999900
H	-3.46098600	0.55346900	-4.60507500	C	-5.44492000	-3.83816900	-0.07942300
H	-2.60260300	-0.32661600	-3.33357500	H	-5.79820200	-2.85542100	-1.98293200
H	-1.80424500	1.01708800	-4.17037900	H	-5.32614600	-4.53674200	-2.13150800
C	-0.54400300	-1.33316000	-4.89336200	C	-6.89497000	-4.26820700	0.16331100
H	-0.12215000	-2.04447100	-5.60878800	H	-4.76373100	-4.59825100	0.32758400
H	0.16629000	-0.51128800	-4.77595200	H	-5.23824100	-2.91394300	0.47790200
H	-0.63500100	-1.84560100	-3.93109900	H	-7.09118600	-4.41868400	1.22959200
Rh	-4.71966100	-4.54206000	-4.67369100	H	-7.59856500	-3.51245900	-0.20260600
Cl	-6.38061300	-2.83369100	-4.72908200	H	-7.12099000	-5.20713200	-0.35392600
C	-6.07760300	-5.70102700	-5.30575300	C	-1.06164900	-3.31468100	-8.70334400
O	-6.92025500	-6.37964400	-5.67994700	C	-2.22504400	-3.56701100	-8.92870600
C	-3.39003500	-5.87253500	-4.66697700	C	-3.62794200	-3.86918800	-9.20633000
O	-2.56418700	-6.67376300	-4.66040800	H	-3.73646500	-4.86789200	-9.64395100
C	-3.40913000	-4.11469200	-9.82327500	H	-4.23327500	-3.83608400	-8.29340200
C	-4.02056100	-5.21029400	-8.91908600	H	-4.04848100	-3.14876300	-9.91678000
C	-4.32900500	-2.87127800	-9.82735100	C	0.84184700	-2.80716900	-10.94577000
C	-3.25871000	-4.65425200	-11.26611900	O	0.27315300	-2.36383500	-11.91648600
H	-3.38240600	-6.09902300	-8.89374200	O	1.43821900	-4.01613900	-10.91031100
H	-4.14600700	-4.84759300	-7.89373300	C	2.45370800	-1.88713800	-9.25696900
H	-5.00487900	-5.50293800	-9.30086900	O	2.91708800	-1.94336200	-8.13521800

O	3.15873500	-1.61195300	-10.35883600	H	-4.31246700	-1.46447900	-2.66117200
C	1.37513700	-4.76863400	-12.13419500	C	-3.81800300	-2.18832700	-0.66082000
H	1.86171800	-4.22038200	-12.94439400	C	-5.04177700	-3.14468900	-0.48798700
H	1.89943500	-5.70232700	-11.93217500	H	-5.85803100	-2.79395000	-1.13472200
H	0.33572500	-4.96215600	-12.40951400	H	-4.75820700	-4.13433000	-0.85927400
C	4.53601500	-1.23817100	-10.15753800	C	-5.53212200	-3.26869300	0.88527600
H	4.96804400	-1.17525800	-11.15571500	C	-5.93818000	-3.38640900	2.02025600
H	4.57353300	-0.26819600	-9.65944700	C	-6.47349600	-3.52249500	3.37648400
H	5.05128400	-1.99159200	-9.55802600	C	-7.95385100	-3.10159800	3.49244600
S	1.39587400	1.52350600	-8.38597400	H	-5.86979000	-2.92077900	4.07011900
O	2.55621300	1.10412400	-9.19418700	H	-6.36465700	-4.56395800	3.71021800
O	0.68954500	2.77256500	-8.71334200	C	-8.50518900	-3.25639100	4.91471100
C	1.91507800	1.63353900	-6.66537400	H	-8.05427400	-2.05928600	3.16512300
C	2.83859500	0.71393900	-6.16124800	H	-8.55016300	-3.70235400	2.79450600
C	1.41026200	2.67465500	-5.88473700	C	-9.97404600	-2.83854500	5.03461100
C	3.25165300	0.84282300	-4.83467300	H	-8.39356700	-4.30117200	5.23542500
H	3.21827200	-0.08580500	-6.78841300	H	-7.89613900	-2.65926700	5.60724600
C	1.83470500	2.79077400	-4.55988200	H	-10.34068000	-2.95797300	6.05916000
H	0.71458900	3.38191100	-6.32252300	H	-10.11137700	-1.78870000	4.75193300
C	2.75158400	1.87585100	-4.03652300	H	-10.61237100	-3.44251000	4.37995500
H	3.96907700	0.13743500	-4.42622700	C	-1.36096000	-4.74525500	-2.48211000
H	1.45594600	3.59921400	-3.94161400	C	-2.25876000	-5.58196200	-2.32670300
H	3.08204200	1.97111800	-3.00613300	C	1.05246500	-4.41847400	-4.60950300
C	-2.42319000	0.44690700	-4.29044300	O	1.10063400	-4.16420900	-5.78717700
H	-3.41434700	0.77949200	-4.61742100	O	1.40611500	-5.60898000	-4.07804000
H	-2.53278400	-0.03142900	-3.31257400	C	1.91664600	-2.75116500	-2.96973500
H	-1.79065400	1.33112500	-4.16606600	O	2.15254300	-2.58629300	-1.78796200
C	-0.41808400	-0.99191100	-4.80614900	O	2.71961900	-2.35296600	-3.95686200
H	0.06818500	-1.65837500	-5.52413700	C	1.80173100	-6.60335500	-5.04281400
H	0.24407200	-0.13877300	-4.63924300	H	2.66881900	-6.25921000	-5.61129000
H	-0.52328200	-1.53497100	-3.86207800	H	2.04938400	-7.49226300	-4.46280700
Rh	-3.53425100	-4.78480600	-4.72619700	H	0.97859300	-6.80402600	-5.73199900
Cl	-5.58492000	-3.99253300	-5.66036600	C	3.84508400	-1.53952300	-3.56800000
C	-3.96973400	-6.45091500	-5.50963400	H	4.41788400	-1.38504000	-4.48132500
O	-4.26107700	-7.44756600	-5.99213500	H	3.48153100	-0.58779900	-3.17513600
C	-1.89286100	-5.38593500	-4.03561100	H	4.44500600	-2.05130200	-2.81277500
O	-0.88137900	-5.73528300	-3.61251200	S	-0.57607800	0.15863100	-2.85797100
INT-1a⁶				O	0.81863700	0.23118600	-3.33747400
C	0.63290500	-3.41637700	-3.51421000	O	-1.59764200	1.07283100	-3.39698300
C	-0.24273500	-2.31529500	-4.19927200	C	-0.52128400	0.42745900	-1.07416000
H	0.41388400	-1.63785100	-4.74330300	C	0.40355700	-0.26142700	-0.28358600
H	-0.87995600	-2.81927000	-4.92782600	C	-1.32630900	1.43865200	-0.54656900
C	-0.05391200	-4.09086900	-2.30036700	C	0.48808800	0.05222000	1.07356300
H	0.61563500	-4.86823500	-1.91950200	H	1.05393700	-1.01549900	-0.71415400
H	-0.13689000	-3.34542400	-1.50773700	C	-1.21927800	1.75032700	0.81042900
C	-1.13125400	-1.55721700	-3.23489200	H	-2.00710100	1.97234300	-1.20050000
C	-2.30097300	-2.02681000	-2.82976400	C	-0.31966600	1.05384100	1.61925700
C	-3.52907600	-2.04132700	-2.16585500	H	1.19763700	-0.47855400	1.70111500

H	-1.83671200	2.53796000	1.23163000	C	-6.71902300	1.05263400	1.83957100
H	-0.24025300	1.29755400	2.67473400	H	-4.62905200	0.53269700	2.10719200
C	-4.22081400	-0.78564600	-0.14829600	H	-5.72812500	-0.81590200	2.32621900
H	-5.08368400	-0.39494500	-0.69941700	C	-6.96165100	1.48537900	3.29003400
H	-4.49722000	-0.84566700	0.90830400	H	-6.52376700	1.93334500	1.21517200
H	-3.39897000	-0.07592700	-0.25150100	H	-7.62386900	0.58252800	1.43464900
C	-2.62210800	-2.71518700	0.14330300	C	-8.13296800	2.46205300	3.43480600
H	-2.30997100	-3.70168100	-0.20802300	H	-7.14666100	0.59606600	3.90802600
H	-1.77016700	-2.03378000	0.07702200	H	-6.04782300	1.94722400	3.68844400
H	-2.90090300	-2.80437300	1.19701500	H	-8.28162700	2.75479200	4.47913900
Rh	-3.27462400	-3.78618400	-3.57968000	H	-7.96103500	3.37538000	2.85425600
C	-3.89232700	-2.67863900	-4.98319000	H	-9.06792000	2.01543000	3.07816400
C	-5.03934700	-4.83376900	-3.51742600	C	-2.82956000	-4.64176400	-3.94977800
O	-4.25771000	-2.02693000	-5.84999400	C	-3.97638200	-4.83483300	-3.54481700
O	-6.13806500	-5.15111700	-3.57558800	C	-5.12819700	-5.51745300	-2.93297800
Cl	-2.40771500	-5.00200900	-5.65407400	H	-4.76576200	-6.34256000	-2.31029600
C	-2.77816800	-6.94484200	-1.98364000	H	-5.72179300	-4.84816600	-2.30419600
C	-3.93760200	-6.89041400	-0.96894300	H	-5.77221100	-5.93013300	-3.71508400
C	-3.20778100	-7.71261000	-3.25153800	C	-1.06047300	-5.98555000	-6.27280700
C	-1.57582100	-7.68008100	-1.33320200	O	-1.24171000	-6.04963200	-7.46313900
H	-3.65607600	-6.34293500	-0.06448100	O	-1.06861200	-7.05380700	-5.44674900
H	-4.82744700	-6.41985300	-1.39315800	C	0.78883700	-4.62914700	-5.29994700
H	-4.21217100	-7.90918000	-0.67716700	O	1.33068300	-4.34300300	-4.24970900
H	-2.40439700	-7.73478900	-3.99065800	O	1.44068100	-4.90238400	-6.43106300
H	-3.47085000	-8.73980600	-2.97675500	C	-1.36243500	-8.31055100	-6.08752800
H	-4.07587400	-7.25507900	-3.72949000	H	-0.61366900	-8.53250200	-6.85142200
H	-1.87153700	-8.69985200	-1.06557500	H	-1.33656500	-9.05690300	-5.29382300
H	-0.73222600	-7.73681500	-2.02668600	H	-2.34918200	-8.27211700	-6.55392400
H	-1.24514000	-7.16987200	-0.42356900	C	2.86442700	-4.67268300	-6.41102100
INT-1b⁶				H	3.22487600	-5.01330600	-7.38064200
C	-0.74136800	-4.68848600	-5.50099000	H	3.05325500	-3.60508800	-6.28203700
C	-1.17415900	-3.48533500	-6.40165600	H	3.33199400	-5.23607900	-5.60096700
H	-0.42663800	-3.35043500	-7.18250000	S	-0.07110800	-0.94057800	-5.81488200
H	-2.11103400	-3.76665500	-6.88553300	O	1.07242400	-1.66399900	-6.40591900
C	-1.36658500	-4.66355500	-4.08152700	O	-0.66218700	0.21414000	-6.51278200
H	-1.03248500	-5.55921400	-3.54845900	C	0.46977200	-0.35092000	-4.19706800
H	-0.94539900	-3.81331200	-3.54222500	C	1.15726000	-1.20225000	-3.32657600
C	-1.40216800	-2.19961000	-5.63390600	C	0.30079300	1.00537500	-3.91293500
C	-2.54848900	-1.93458300	-5.02569000	C	1.64865100	-0.67944400	-2.12952900
C	-3.47950400	-1.20427800	-4.27991100	H	1.31955800	-2.24520100	-3.57752200
H	-3.99596800	-0.42683800	-4.84611900	C	0.81107000	1.51591200	-2.71757900
C	-3.48007100	-0.88566000	-2.77191200	H	-0.20743900	1.63963800	-4.63081000
C	-4.92718300	-1.10495000	-2.22003300	C	1.47642800	0.67375600	-1.82505300
H	-5.63621600	-0.56664600	-2.86396600	H	2.17956600	-1.32988500	-1.44097900
H	-5.17316200	-2.16860800	-2.31427000	H	0.69009400	2.57027400	-2.48804300
C	-5.12322000	-0.68689800	-0.83122600	H	1.87039500	1.07333400	-0.89507900
C	-5.29399000	-0.35384500	0.32055200	C	-3.12957900	0.61430800	-2.63575500
C	-5.53839100	0.06792900	1.70135300	H	-3.84007400	1.23928100	-3.18856500

H	-3.17196700	0.90912500	-1.58344300	C	1.03001200	-2.27523100	-6.65427000
H	-2.12684300	0.81964900	-3.01356300	O	1.64503600	-2.41607300	-5.61585300
C	-2.48390700	-1.73014600	-1.96621500	O	1.55415400	-1.83776200	-7.80036400
H	-2.71096700	-2.79621500	-2.04513800	C	-0.07123200	-5.09766000	-9.49895200
H	-1.45860800	-1.56303200	-2.30512700	H	-0.09451300	-4.46602700	-10.38931000
H	-2.53909000	-1.45214900	-0.90996300	H	0.77874700	-5.77796200	-9.52353300
Rh	-4.33712200	-3.08436700	-5.14994100	H	-1.00098000	-5.66146600	-9.40939700
Cl	-4.69020300	-5.02392900	-6.76310100	C	2.93056700	-1.41201000	-7.75010600
C	-4.69835700	-2.14872000	-6.74799600	H	3.20926500	-1.21273000	-8.78425400
O	-4.92805000	-1.61249600	-7.73280500	H	3.00285400	-0.50456300	-7.14930800
C	-6.33959400	-3.18129200	-4.60000700	H	3.55537700	-2.19987900	-7.32448600
O	-7.46465400	-3.05949600	-4.43928700	S	-0.10647800	1.00869600	-5.46932600
INT-1a⁷				O	0.99101900	0.67042700	-6.39438600
C	-0.47168700	-2.56505600	-6.80644500	O	-0.85715300	2.26111300	-5.65460400
C	-1.28349300	-1.23349400	-6.80808700	C	0.54739100	1.01848300	-3.79068300
H	-0.90711100	-0.62429200	-7.63372600	C	1.45425200	0.03162800	-3.39353200
H	-2.31565700	-1.48788800	-7.05226200	C	0.16849200	2.05726800	-2.93927900
C	-0.88319000	-3.54084200	-5.66041200	C	1.97525100	0.08718100	-2.10009400
H	-0.18133300	-4.37785200	-5.65331800	H	1.74563200	-0.75940100	-4.07701200
H	-0.77439800	-3.02489700	-4.70275900	C	0.70503200	2.10245100	-1.65090900
C	-1.29868400	-0.39066400	-5.54435500	H	-0.52082400	2.81461000	-3.29563600
C	-2.21652300	-0.38972800	-4.60906700	C	1.60234900	1.11759500	-1.23207700
C	-3.13864800	-0.23980100	-3.69166800	H	2.67993400	-0.67181600	-1.77399300
H	-3.96219700	0.43185900	-3.94975600	H	0.42570000	2.90852300	-0.97905700
C	-3.20914500	-0.84092200	-2.29428000	H	2.01707400	1.15565800	-0.22890900
C	-4.58961600	-1.57205600	-2.18608400	C	-3.15982700	0.32471400	-1.28164400
H	-5.38305300	-0.86235700	-2.45896400	H	-3.95287500	1.05510200	-1.47745600
H	-4.61931200	-2.37173300	-2.93728200	H	-3.29728000	-0.05811700	-0.26630000
C	-4.87458500	-2.13220700	-0.86521900	H	-2.19863200	0.84325700	-1.33619400
C	-5.10413300	-2.59162700	0.23127900	C	-2.05963300	-1.82209200	-2.02927200
C	-5.41945700	-3.17226800	1.53792300	H	-2.08172300	-2.65587000	-2.73787800
C	-6.64411100	-4.11137300	1.50632100	H	-1.08949000	-1.32440100	-2.11517700
H	-5.59806600	-2.36718700	2.26433900	H	-2.14744700	-2.23809900	-1.02217100
H	-4.54767800	-3.72734900	1.91118300	Rh	-2.61927700	-6.19834300	-4.92865500
C	-6.95982800	-4.71894100	2.87790800	Cl	-1.65347100	-7.14130200	-6.89481300
H	-7.51280100	-3.55170700	1.13767500	C	-2.40598200	-7.92782500	-4.18042800
H	-6.46017500	-4.91064800	0.77772700	O	-2.26229100	-8.97950400	-3.75237800
C	-8.17515700	-5.65122000	2.85294800	C	-3.38376600	-5.48905800	-3.36775900
H	-6.08191900	-5.27054500	3.24117800	O	-3.86205700	-5.06637300	-2.41018100
H	-7.13207800	-3.91096700	3.60213400	C	-4.75221000	-4.30826500	-6.82353000
H	-8.37744700	-6.07032100	3.84384600	C	-5.84125300	-4.70676200	-5.80438800
H	-9.07584200	-5.11927800	2.52623900	C	-5.01475300	-2.86948200	-7.33771600
H	-8.01800900	-6.48820300	2.16325000	C	-4.75365100	-5.28983700	-8.01769700
C	-2.25459900	-4.05533200	-5.82854200	H	-5.68772700	-5.72718300	-5.44201600
C	-3.40530700	-4.29313800	-6.19592200	H	-5.85209000	-4.03057700	-4.94353500
C	-0.73274500	-3.27411600	-8.15311700	H	-6.82269100	-4.65896500	-6.28663700
O	-1.61992000	-2.98272700	-8.92741300	H	-4.25839700	-2.57804100	-8.07133000
O	0.12092600	-4.28926500	-8.31999200	H	-5.99709700	-2.83286800	-7.82007700

H	-5.00909900	-2.14697700	-6.51564400	H	0.07158100	-4.93669600	-10.06747500
H	-5.73940100	-5.27545300	-8.49487700	H	0.66624600	-6.25840700	-9.00466200
H	-4.00326700	-4.99651200	-8.75603200	H	-1.08574400	-5.89918800	-9.09476400
H	-4.53049200	-6.30899800	-7.69442800	C	3.08159200	-1.62777300	-7.72784200
INT-1b⁷				H	3.37802500	-1.51187500	-8.76961900
C	-0.35893400	-2.62935100	-6.75185100	H	3.15624000	-0.67795600	-7.19666800
C	-1.13972900	-1.28735800	-6.89453300	H	3.68971300	-2.38784100	-7.23304900
H	-0.70972500	-0.74828900	-7.74169500	S	0.02165500	1.01334100	-5.65148300
H	-2.16372000	-1.54093000	-7.17591100	O	1.14924200	0.59385400	-6.50470400
C	-0.80536300	-3.47829300	-5.52719200	O	-0.69242200	2.26625400	-5.94439700
H	-0.16212400	-4.35831200	-5.47065200	C	0.60093500	1.10943000	-3.94967100
H	-0.63004800	-2.89753700	-4.61729100	C	1.52656900	0.17373500	-3.47971000
C	-1.19408000	-0.36426600	-5.68994300	C	0.13494200	2.15247900	-3.14766600
C	-2.14201200	-0.31332500	-4.78702700	C	1.97868300	0.28621200	-2.16416500
C	-3.10036800	-0.14736200	-3.91109500	H	1.88321800	-0.62247700	-4.12504000
H	-3.92685200	0.49825400	-4.22048000	C	0.60047300	2.25328100	-1.83536700
C	-3.22853600	-0.73621500	-2.51173200	H	-0.56350700	2.87227600	-3.55972800
C	-4.48861800	-1.66749300	-2.53826700	C	1.51693600	1.32024400	-1.34467000
H	-5.35096500	-1.08303100	-2.88793100	H	2.69792200	-0.43194000	-1.78211300
H	-4.31839400	-2.44664500	-3.29266000	H	0.25290800	3.06339000	-1.20124200
C	-4.80996500	-2.28898200	-1.25335500	H	1.87722000	1.40216200	-0.32327400
C	-5.06353500	-2.80320000	-0.18669600	C	-3.45699800	0.42883000	-1.52582700
C	-5.40353900	-3.44359200	1.08549500	H	-4.32086500	1.03631400	-1.81841300
C	-6.65175100	-4.34749900	0.99937800	H	-3.64379800	0.03785100	-0.52156800
H	-5.56673400	-2.67209300	1.85086700	H	-2.57909400	1.08062800	-1.49029100
H	-4.54846000	-4.03895900	1.43412200	C	-1.98498900	-1.53597000	-2.10230000
C	-6.99434700	-5.01138100	2.33809000	H	-1.82005600	-2.38206700	-2.77554700
H	-7.50276000	-3.74869500	0.65166700	H	-1.09069000	-0.90697400	-2.11443200
H	-6.48251400	-5.11632300	0.23506300	H	-2.11439900	-1.93771800	-1.09409000
C	-8.23132100	-5.91155700	2.26008300	Rh	-2.68244800	-6.14304700	-4.92627200
H	-6.13306500	-5.60041700	2.68178500	Cl	-2.97217700	-6.92581000	-7.16275100
H	-7.15371800	-4.23419000	3.09807400	C	-2.57358400	-7.97089600	-4.45840900
H	-8.45253000	-6.37020100	3.22915300	O	-2.50753600	-9.08480000	-4.20332100
H	-9.11608500	-5.34364600	1.95097900	C	-2.51204800	-5.55776300	-3.14573000
H	-8.08805500	-6.72007100	1.53435200	O	-2.41546200	-5.20906900	-2.05395500
C	-2.21687200	-3.89159100	-5.60490600	INT-1a⁸			
C	-3.42447300	-4.03647900	-5.77583700	C	-0.52956700	-2.99857700	-5.93687400
C	-4.84757300	-4.01596400	-6.12471900	C	-1.74010600	-2.26991200	-6.61168700
H	-5.47902900	-4.19710600	-5.25003400	H	-1.33430100	-1.61479500	-7.38576800
H	-5.10424100	-3.03619800	-6.54254500	H	-2.32012700	-3.04251900	-7.12422000
H	-5.05492200	-4.78733300	-6.87142500	C	-0.97402700	-4.37613700	-5.34216300
C	-0.59718300	-3.44373500	-8.04247800	H	-0.17036400	-4.76160200	-4.70646100
O	-1.33342500	-3.11197000	-8.94298600	H	-1.84418800	-4.21773500	-4.69848700
O	0.10735100	-4.58463200	-8.00826600	C	-2.68723900	-1.46638900	-5.73983500
C	1.14770200	-2.36182700	-6.59637600	C	-3.88589000	-1.77428000	-5.29142500
O	1.74400000	-2.43146500	-5.54016600	C	-5.11248300	-1.67930900	-4.74491000
O	1.69993800	-2.03910200	-7.76717100	H	-5.89475800	-1.26501500	-5.38560800
C	-0.08055100	-5.47523500	-9.13013800	C	-5.53953700	-1.82729400	-3.28306200

C	-6.77607300	-2.78695100	-3.22184300	C	-5.99238200	-0.41112100	-2.84646800
H	-7.52595600	-2.44284700	-3.94881800	H	-6.77729300	-0.01722700	-3.50269700
H	-6.45897000	-3.78441800	-3.54184100	H	-6.40315400	-0.47123300	-1.83485000
C	-7.39149300	-2.87342700	-1.89761700	H	-5.15879600	0.29212300	-2.84514500
C	-7.89938900	-2.95328400	-0.80118400	C	-4.40737100	-2.32601400	-2.37569100
C	-8.54383200	-3.09006300	0.50654900	H	-4.08164000	-3.32610200	-2.66608700
C	-9.77067900	-4.02671000	0.48282400	H	-3.54621800	-1.65466500	-2.41746900
H	-8.85109800	-2.10036200	0.87258200	H	-4.76401700	-2.36465600	-1.34273300
H	-7.81450000	-3.46876900	1.23608200	Rh	-4.99688000	-3.67639600	-6.23326200
C	-10.43414700	-4.16789600	1.85759800	Cl	-4.45041100	-5.21748700	-4.49032100
H	-10.49762800	-3.64383700	-0.24432400	C	-5.51344200	-5.25074000	-7.15130900
H	-9.45820200	-5.01232800	0.11646100	O	-5.82683300	-6.21508000	-7.68206000
C	-11.65358700	-5.09500900	1.84019700	C	-5.44926900	-2.56027200	-7.68590100
H	-9.69654500	-4.54519000	2.57910800	O	-5.73292000	-1.89996200	-8.58215600
H	-10.73348800	-3.17488000	2.22034500	C	-1.64063700	-7.15744200	-8.34616800
H	-12.10665000	-5.17784400	2.83343300	C	-2.49863100	-8.32610300	-7.80650300
H	-12.42278100	-4.72448200	1.15318500	C	-2.34587900	-6.50454900	-9.55791400
H	-11.37893000	-6.10450000	1.51425400	C	-0.25691500	-7.69244500	-8.78675100
C	-1.27243600	-5.35481900	-6.38831900	H	-2.01346900	-8.80398100	-6.95043600
C	-1.45342600	-6.15452100	-7.28038500	H	-3.48256700	-7.97533400	-7.48372500
C	0.53312300	-3.24055600	-7.02893200	H	-2.64021100	-9.08061400	-8.58857100
O	0.49828200	-2.79160500	-8.15255500	H	-1.76474100	-5.66020900	-9.94049000
O	1.51129700	-4.04365000	-6.57348400	H	-2.46364300	-7.23701300	-10.36418100
C	0.06477500	-2.16607500	-4.79296600	H	-3.33979200	-6.13981700	-9.28329800
O	-0.48947600	-2.03537100	-3.71775500	H	-0.37657500	-8.45242000	-9.56703800
O	1.24733700	-1.62821300	-5.10204000	H	0.36380000	-6.88536100	-9.18826500
C	2.55782000	-4.33136600	-7.51383500	H	0.27386700	-8.14521200	-7.94409200
H	3.04073200	-3.40802300	-7.84271100	INT-1b⁸			
H	3.26477800	-4.96720100	-6.98128800	C	-0.39235600	-2.85658000	-6.06800000
H	2.15496900	-4.85250400	-8.38572700	C	-1.68764300	-2.17132500	-6.61030600
C	1.82106200	-0.74236900	-4.12388400	H	-1.37748800	-1.45234500	-7.37161000
H	2.82421200	-0.51986500	-4.48600400	H	-2.25063400	-2.95365200	-7.12627600
H	1.22365200	0.16963200	-4.07009100	C	-0.71719400	-4.21754600	-5.37255000
H	1.86003300	-1.22568800	-3.14535400	H	0.17626100	-4.56184300	-4.84224800
S	-2.22488000	0.32940300	-5.69652200	H	-1.49330200	-4.05859300	-4.61821500
O	-0.75496600	0.37301000	-5.78976500	C	-2.63943500	-1.46783000	-5.65713900
O	-3.03854200	0.97659000	-6.73981700	C	-3.80884800	-1.86963300	-5.19926800
C	-2.69567300	1.06225500	-4.12019200	C	-5.06549600	-1.79621900	-4.70721000
C	-2.07266300	0.65955200	-2.93486200	H	-5.80731400	-1.41671200	-5.41402700
C	-3.57848100	2.14345300	-4.15857500	C	-5.59536700	-1.87828200	-3.27418900
C	-2.36848300	1.35123700	-1.75975200	C	-6.72100100	-2.96688400	-3.20840500
H	-1.37953900	-0.17548300	-2.93170100	H	-7.43363000	-2.79142500	-4.02691600
C	-3.85184500	2.83287300	-2.97577900	H	-6.26601300	-3.94582600	-3.38831400
H	-4.02439300	2.43562700	-5.10264100	C	-7.44210400	-2.99040400	-1.93565900
C	-3.25087900	2.43537600	-1.77976000	C	-8.03433600	-3.01697300	-0.87969200
H	-1.90178500	1.04632200	-0.82805200	C	-8.77488800	-3.08520200	0.38163200
H	-4.53264700	3.67847500	-2.99133300	C	-9.98589200	-4.04091000	0.32599200
H	-3.46739900	2.97264700	-0.86103700	H	-9.12036400	-2.07979400	0.66050100

H	-8.09877900	-3.40584900	1.18631700	C	-4.49875600	-2.15854000	-2.23877300
C	-10.75043800	-4.10286000	1.65326300	H	-4.00743700	-3.11306900	-2.43245200
H	-10.65935900	-3.71726100	-0.47738400	H	-3.74625300	-1.36642500	-2.24416500
H	-9.63576800	-5.04318200	0.04994600	H	-4.94777400	-2.19665900	-1.24233800
C	-11.95513700	-5.04808400	1.60589400	Rh	-4.71004100	-3.88602300	-5.96256700
H	-10.06582800	-4.42041800	2.45164000	Cl	-3.99933200	-5.16251600	-4.06546600
H	-11.08709200	-3.09303700	1.92554000	C	-5.01812000	-5.61350200	-6.71150400
H	-12.48290800	-5.07092600	2.56482800	O	-5.19091700	-6.66081100	-7.13732500
H	-12.67248000	-4.73672400	0.83819500	C	-5.29838000	-2.98903900	-7.51157700
H	-11.64567700	-6.07290700	1.37180800	O	-5.66623300	-2.45784700	-8.46193500
C	-1.13211400	-5.24080400	-6.33338200	INT-1a⁹			
C	-1.41572200	-6.07938900	-7.15953600	C	1.10018100	-2.89454500	-5.49646800
C	-1.74365400	-7.11381600	-8.13741500	C	0.47948600	-1.80971600	-6.42893600
H	-1.00683300	-7.92466000	-8.11493200	H	1.20706200	-1.58309600	-7.21093900
H	-2.72685400	-7.55460900	-7.93991900	H	-0.38277100	-2.26895200	-6.91623500
H	-1.75750500	-6.70678800	-9.15492300	C	0.13487100	-3.31872500	-4.35260300
C	0.52240200	-3.12184300	-7.28117600	H	0.65733400	-4.03660100	-3.71280900
O	0.30832500	-2.75825600	-8.41541500	H	-0.05157100	-2.43558400	-3.73672900
O	1.59806700	-3.84303800	-6.91469000	C	0.02282100	-0.51676200	-5.77593900
C	0.33274500	-1.96200900	-5.05676100	C	-1.16201100	-0.26842300	-5.27713000
O	0.00934700	-1.88835200	-3.88675800	C	-2.35800600	0.04845900	-4.85077000
O	1.34785900	-1.28906700	-5.60450600	H	-3.06480500	0.39886000	-5.60746000
C	2.51333300	-4.16280500	-7.97470400	C	-2.91514800	-0.02309900	-3.43150000
H	2.89842200	-3.25018800	-8.43591000	C	-3.97913500	-1.17296300	-3.45939700
H	3.31944600	-4.72725200	-7.50647100	H	-4.73788200	-0.93409900	-4.21418800
H	2.01571800	-4.76552000	-8.73832500	H	-3.47803200	-2.09460000	-3.78335400
C	2.00723700	-0.32742200	-4.75995100	C	-4.65471500	-1.44785600	-2.17047900
H	2.87774800	0.00589900	-5.32386300	C	-4.93132900	-2.10360400	-1.12566200
H	1.33097700	0.50833900	-4.57181500	C	-4.89236200	-3.23673800	-0.17400100
H	2.30831500	-0.78928900	-3.81736100	C	-6.01029200	-4.27147900	-0.41942000
S	-2.33549400	0.36269200	-5.56102100	H	-4.96031400	-2.86281400	0.85406000
O	-0.90879900	0.54678500	-5.88328600	H	-3.91132600	-3.72207500	-0.27233300
O	-3.36245300	0.99631300	-6.40638800	C	-5.94136500	-5.45047900	0.55907500
C	-2.59734100	0.95434900	-3.87784800	H	-6.98340600	-3.77325000	-0.33023200
C	-1.80291800	0.49168800	-2.82489200	H	-5.93907100	-4.63897800	-1.45088300
C	-3.51510200	1.99309100	-3.70673400	C	-7.05249300	-6.47901800	0.32687600
C	-1.95952300	1.07537900	-1.56700100	H	-4.96217800	-5.94023600	0.47036800
H	-1.08474900	-0.30606900	-2.98197800	H	-6.00154900	-5.07046600	1.58767700
C	-3.64841000	2.57448500	-2.44437300	H	-6.98071700	-7.30728400	1.03864700
H	-4.09815400	2.33584400	-4.55417300	H	-8.04278700	-6.02496000	0.44260900
C	-2.87588200	2.11331800	-1.37683900	H	-6.99761700	-6.90153200	-0.68264300
H	-1.35774800	0.72075200	-0.73576800	C	-1.11427500	-3.90479900	-4.84026100
H	-4.35492700	3.38588500	-2.29823600	C	-2.11746000	-4.42124600	-5.28278900
H	-2.98460500	2.56564100	-0.39540800	C	1.42073600	-4.12155000	-6.36813600
C	-6.23644500	-0.49139400	-3.01063800	O	1.19444900	-4.22141200	-7.55209300
H	-7.02222300	-0.26436700	-3.74037900	O	1.97004400	-5.10188500	-5.62260400
H	-6.69452900	-0.50005000	-2.01802000	C	2.39441700	-2.36579400	-4.85865900
H	-5.49117100	0.30547000	-3.04484900	O	2.45442000	-1.88814500	-3.74348600

O	3.43039800	-2.48468000	-5.69441400	INT-1b⁹			
C	2.30940900	-6.30205700	-6.33837900	C	1.20265800	-2.89605500	-5.52644700
H	3.03204300	-6.08330900	-7.12804300	C	0.53969300	-1.83300900	-6.45509800
H	2.74117100	-6.97410600	-5.59716900	H	1.25222700	-1.58691000	-7.24507100
H	1.41632800	-6.74459000	-6.78602200	H	-0.31274900	-2.31987300	-6.93253800
C	4.66880100	-1.88574100	-5.26311800	C	0.27679100	-3.32579800	-4.35335000
H	5.40649200	-2.17664400	-6.01018100	H	0.81809700	-4.05220800	-3.73940100
H	4.55226400	-0.80142300	-5.23792400	H	0.11872000	-2.44743500	-3.72254800
H	4.94832200	-2.25913900	-4.27565300	C	0.04807800	-0.55219700	-5.80369600
S	1.16065900	0.91337100	-5.94441800	C	-1.14664000	-0.33234300	-5.31500700
O	2.52074500	0.35175800	-6.04559800	C	-2.35181600	-0.03894800	-4.89820100
O	0.64857100	1.78428300	-7.01448900	H	-3.05953500	0.29867800	-5.65985900
C	1.03502100	1.82295600	-4.39657200	C	-2.91401900	-0.11210600	-3.48148800
C	1.69294400	1.34416800	-3.26006400	C	-4.01056500	-1.23050400	-3.52170400
C	0.30842200	3.01436000	-4.38178900	H	-4.75431400	-0.96999700	-4.28397000
C	1.60262100	2.08068100	-2.07813700	H	-3.53099100	-2.16588000	-3.83870900
H	2.25332200	0.41581300	-3.29922800	C	-4.70528300	-1.48317200	-2.23845600
C	0.22917000	3.74017100	-3.19170400	C	-5.00376100	-2.12037000	-1.18854000
H	-0.16645200	3.36229700	-5.29238600	C	-4.99428300	-3.24230900	-0.22312200
C	0.87244800	3.27241900	-2.04330200	C	-6.14536800	-4.24487200	-0.44816900
H	2.10739400	1.72500300	-1.18497600	H	-5.04413700	-2.85386300	0.80060700
H	-0.32750900	4.67207600	-3.16458500	H	-4.02925600	-3.75887500	-0.32106800
H	0.80923500	3.84055100	-1.11974600	C	-6.10033200	-5.41835700	0.53829500
C	-3.57631200	1.33452400	-3.11891700	H	-7.10183100	-3.71676900	-0.35161700
H	-4.35106900	1.58447300	-3.85133600	H	-6.09758900	-4.62164600	-1.47764200
H	-4.04591800	1.32693600	-2.12894200	C	-7.24421500	-6.41493100	0.32654500
H	-2.82768600	2.13235000	-3.12667000	H	-5.13727400	-5.93779000	0.44216100
C	-1.82678400	-0.32929300	-2.39339200	H	-6.13718800	-5.02936300	1.56461200
H	-1.37673700	-1.31153500	-2.56173400	H	-7.18900900	-7.23971500	1.04379500
H	-1.03254400	0.42028400	-2.42734800	H	-8.21917800	-5.93071600	0.44981800
H	-2.25312100	-0.32822300	-1.38580300	H	-7.21355100	-6.84638300	-0.68024100
Rh	-6.16874800	-0.40018300	-1.13770700	C	-0.99568000	-3.89812200	-4.79449400
Cl	-7.22911000	1.45727100	-0.19756600	C	-2.02846100	-4.39511300	-5.18482800
C	-7.63985400	-1.07102700	-1.92546300	C	-3.26398800	-5.01099000	-5.66351800
O	-8.56247400	-1.53072400	-2.44386200	H	-3.60139500	-5.80367700	-4.98628000
C	-3.31110100	-5.08540500	-5.84130100	H	-4.07372700	-4.27742600	-5.74767700
C	-4.26877700	-5.48303800	-4.69346600	H	-3.12022900	-5.45909000	-6.65286300
C	-4.03331900	-4.12353100	-6.81362300	C	1.52881200	-4.12391300	-6.39549800
C	-2.86477700	-6.35374200	-6.60758700	O	1.28384100	-4.23602000	-7.57441400
H	-3.77621400	-6.16067000	-3.98970600	O	2.11184000	-5.08789900	-5.65384600
H	-4.60674900	-4.60170200	-4.13891300	C	2.50403200	-2.33974900	-4.92624300
H	-5.15119900	-5.98966100	-5.09906400	O	2.58951800	-1.86779900	-3.81035400
H	-3.37604800	-3.83556800	-7.63922700	O	3.51505300	-2.42963300	-5.79539600
H	-4.92040400	-4.60982900	-7.23382000	C	2.46665200	-6.28420600	-6.36891900
H	-4.35380000	-3.21187400	-6.30034600	H	3.17565700	-6.05403100	-7.16766200
H	-3.73559700	-6.85651000	-7.04270200	H	2.92046700	-6.94432800	-5.63018300
H	-2.17407400	-6.09647800	-7.41590600	H	1.57774800	-6.74648100	-6.80463100
H	-2.36014400	-7.05726100	-5.93855900	C	4.75148000	-1.80225600	-5.40019700

H	5.46764000	-2.05793400	-6.18033900	C	-6.69777300	-7.49971700	-8.50235900
H	4.60503600	-0.72250200	-5.34951500	H	-7.77039800	-5.74939900	-7.80022500
H	5.07987600	-2.18521400	-4.43155000	H	-7.47998500	-6.94960700	-6.55438500
S	1.14751100	0.90916400	-5.96373200	C	-7.93952600	-8.27663300	-8.95432900
O	2.51979300	0.38344200	-6.08900600	H	-6.23963300	-6.99542200	-9.36219100
O	0.60095300	1.78315000	-7.01402300	H	-5.94301600	-8.19551800	-8.11538600
C	1.01713600	1.79318600	-4.40111700	C	-7.63251200	-9.32167700	-10.03155600
C	1.69354800	1.31138700	-3.27672700	H	-8.39528000	-8.76933600	-8.08445000
C	0.26736800	2.96964200	-4.36332500	H	-8.69178300	-7.57067100	-9.33210200
C	1.59751600	2.02870800	-2.08341900	H	-8.53585400	-9.86212500	-10.33215100
H	2.27374500	0.39613700	-3.33362000	H	-7.21054600	-8.85430200	-10.92837200
C	0.18371500	3.67695100	-3.16238900	H	-6.90688100	-10.05994400	-9.67198000
H	-0.22175700	3.32077400	-5.26510200	C	-1.99382600	-4.40934000	-1.92093700
C	0.84458600	3.20524100	-2.02566100	C	-1.94785600	-5.49096900	-2.50681500
H	2.11644200	1.67030100	-1.19949600	C	-0.17733400	-2.99250000	0.21628600
H	-0.39052600	4.59745600	-3.11772400	O	0.98132600	-2.87797900	-0.10345700
H	0.77753900	3.75868200	-1.09350100	O	-0.60290400	-3.72945800	1.26361500
C	-3.53616500	1.26087900	-3.15501200	C	-2.07547000	-1.40050800	0.50940700
H	-4.30359600	1.54054900	-3.88434900	O	-3.27503700	-1.36780800	0.69801200
H	-4.00523500	1.25670600	-2.16464400	O	-1.19302700	-0.61003300	1.12771000
H	-2.76510400	2.03692300	-3.15494800	C	0.43624100	-4.38904100	2.01243600
C	-1.83617800	-0.46417800	-2.44709500	H	1.13230300	-3.65443100	2.42360100
H	-1.42020900	-1.45873000	-2.63038000	H	-0.07454500	-4.92560100	2.81148800
H	-1.01811800	0.26005700	-2.47195700	H	0.98629900	-5.08076900	1.37057600
H	-2.26181300	-0.46175300	-1.43920600	C	-1.75080000	0.43842900	1.94639000
Rh	-6.20925700	-0.39359900	-1.23342100	H	-0.89580100	0.93033800	2.40825500
Cl	-7.24468700	1.49472900	-0.32837400	H	-2.30107000	1.13569900	1.31164900
C	-7.68506600	-1.04910100	-2.02493100	H	-2.41505600	0.01875600	2.70460600
O	-8.61128700	-1.49920300	-2.54538100	S	-2.54965100	0.48749600	-2.77852900
INT-1a¹⁰				O	-2.20929300	1.05590600	-1.45870000
C	-1.37249700	-2.33033300	-0.49708100	O	-2.10808700	1.15832200	-4.01273300
C	-0.82268100	-1.47682100	-1.67951700	C	-4.34792900	0.36876700	-2.86003800
H	-0.42175500	-0.54442000	-1.28091900	C	-5.07021300	-0.15915000	-1.78525700
H	0.01212500	-2.02822200	-2.11720400	C	-4.98774900	0.92861500	-3.96729500
C	-2.41140700	-3.39402100	-0.93575200	C	-6.46425600	-0.15436400	-1.84943900
H	-2.73754200	-3.93829700	-0.04444400	H	-4.56349400	-0.55028900	-0.90902700
H	-3.29145700	-2.86970900	-1.31404800	C	-6.38362700	0.93892600	-4.00934000
C	-1.83276600	-1.19881100	-2.77358100	H	-4.39248800	1.35819700	-4.76543500
C	-2.05275400	-2.04295400	-3.76904000	C	-7.11937800	0.39175300	-2.95675500
C	-2.55023500	-2.52674500	-4.95907900	H	-7.03807400	-0.56528200	-1.02428200
H	-2.06752100	-2.12393600	-5.85082200	H	-6.89256800	1.37662100	-4.86281100
C	-3.91329600	-3.14672400	-5.28820400	H	-8.20484000	0.39907500	-2.99380200
C	-3.64116000	-4.38741300	-6.20021000	C	-4.69856900	-2.09770700	-6.11056000
H	-3.08175200	-4.05230300	-7.08464200	H	-4.13078300	-1.77160900	-6.98907700
H	-2.97135700	-5.06916000	-5.66558100	H	-5.63503300	-2.54150300	-6.46185300
C	-4.84280700	-5.10405600	-6.62652300	H	-4.93589200	-1.21821900	-5.50913800
C	-5.83793000	-5.70243000	-6.97112200	C	-4.72186300	-3.53906500	-4.04555900
C	-7.01583800	-6.44996300	-7.41618400	H	-4.20089200	-4.29058400	-3.44856800

H	-4.91598200	-2.66603100	-3.41579900	H	-6.92403000	-9.44638500	-10.41397100
H	-5.68473000	-3.95710500	-4.35096100	H	-7.01561100	-10.38563100	-8.91937000
Rh	-0.89680700	-3.79703300	-4.01322700	C	-2.06858500	-4.37410700	-1.86905800
C	0.23390900	-3.01093700	-5.27896500	C	-2.07676700	-5.41118900	-2.52539200
O	0.94745200	-2.53556400	-6.04103600	C	-2.17907100	-6.77811000	-3.04503400
Cl	0.96815200	-5.30694000	-3.79784600	H	-2.87785800	-6.83658500	-3.88510100
C	-2.04903700	-6.96357800	-2.74425600	H	-1.19895100	-7.12910100	-3.37483300
C	-3.44066600	-7.38005300	-2.19747300	H	-2.54606800	-7.43333700	-2.24683600
C	-1.94504300	-7.37557500	-4.22510600	C	-0.16245000	-3.00956500	0.24650600
C	-0.94235600	-7.66824300	-1.92266600	O	0.99005500	-2.92507900	-0.10370100
H	-3.54597000	-7.12556400	-1.13864900	O	-0.57944500	-3.73194800	1.30656800
H	-4.24895600	-6.89585200	-2.75323700	C	-2.02509600	-1.38206000	0.58079600
H	-3.55649600	-8.46411600	-2.30129000	O	-3.21880700	-1.33348900	0.79963800
H	-0.99863700	-7.04975600	-4.65914500	O	-1.11666100	-0.60224800	1.17441200
H	-2.00156100	-8.46698500	-4.29282800	C	0.46041500	-4.42060300	2.02841800
H	-2.77183200	-6.96669400	-4.81239500	H	1.18600100	-3.70542700	2.42239500
H	-1.04910000	-8.75312700	-2.03057600	H	-0.04454300	-4.94436200	2.83949100
H	0.04592300	-7.36962400	-2.27458300	H	0.97471000	-5.12590500	1.37191800
H	-1.02615200	-7.41847800	-0.86048300	C	-1.63954200	0.45425100	2.00598200
INT-1b¹⁰				H	-0.76662300	0.93484000	2.44565500
C	-1.35960700	-2.32276100	-0.44144000	H	-2.19630600	1.15853500	1.38473700
C	-0.81699300	-1.47616700	-1.63318500	H	-2.29009600	0.04388600	2.78093100
H	-0.40801600	-0.54465700	-1.24048000	S	-2.55393200	0.48847700	-2.72377200
H	0.01225300	-2.03307200	-2.07386200	O	-2.19891800	1.06183200	-1.40997200
C	-2.42805900	-3.36735500	-0.85535500	O	-2.13758200	1.15850300	-3.96703000
H	-2.73168900	-3.91672200	0.04095500	C	-4.35146100	0.35120100	-2.77880400
H	-3.31306000	-2.82560800	-1.19703000	C	-5.05447200	-0.13427100	-1.67173100
C	-1.82803000	-1.19382300	-2.72546400	C	-5.01060900	0.84376100	-3.90642400
C	-2.04257800	-2.03235300	-3.72659400	C	-6.44894100	-0.15570900	-1.72209500
C	-2.52931900	-2.51800500	-4.92195300	H	-4.53213200	-0.47389700	-0.78331000
H	-2.04073800	-2.11151800	-5.80871500	C	-6.40663400	0.82712900	-3.93583500
C	-3.89239600	-3.13831400	-5.26105100	H	-4.42954100	1.24594400	-4.72898000
C	-3.62353100	-4.44003700	-6.08692100	C	-7.12320300	0.32166200	-2.84956100
H	-2.98861200	-4.18444900	-6.94631100	H	-7.00825700	-0.53339700	-0.87150400
H	-3.02784000	-5.12620200	-5.47337200	H	-6.93089700	1.21263300	-4.80504000
C	-4.83118900	-5.11762200	-6.55920200	H	-8.20889800	0.30841600	-2.87646400
C	-5.83097100	-5.67847700	-6.94996600	C	-4.62625900	-2.12200000	-6.16755500
C	-7.01022800	-6.38769200	-7.45089900	H	-4.03058800	-1.87215600	-7.05258000
C	-6.65932600	-7.66899100	-8.23719600	H	-5.57075400	-2.55497200	-6.50966400
H	-7.59423400	-5.71614100	-8.09550500	H	-4.84358800	-1.19837100	-5.62735300
H	-7.66883900	-6.64657700	-6.61019400	C	-4.75098000	-3.44111800	-4.02624500
C	-7.89967100	-8.39640400	-8.76853100	H	-4.26489000	-4.16172800	-3.36492700
H	-5.99671800	-7.40428300	-9.07051600	H	-4.95318700	-2.52924500	-3.45768300
H	-6.08359500	-8.33952500	-7.58708000	H	-5.70855300	-3.86436000	-4.34118700
C	-7.55723800	-9.66988900	-9.54798800	Rh	-0.91905700	-3.80112700	-3.97278500
H	-8.56168700	-8.64765600	-7.92838600	C	0.26397400	-3.05452700	-5.21343500
H	-8.47178000	-7.71474800	-9.41276900	O	1.00968400	-2.60514200	-5.96004900
H	-8.46033700	-10.16736000	-9.91592300	Cl	0.82183800	-5.45284000	-3.78745100

INT-1a^{II}				O	2.45858200	0.61247000	-6.06354400
C	1.39367900	-2.73747000	-5.70408100	O	0.43261000	2.06142300	-6.60964100
C	0.59317400	-1.67952300	-6.52571300	C	1.02312300	1.64629900	-4.06651600
H	1.23232200	-1.34434500	-7.34633400	C	1.79537800	1.02035700	-3.08401200
H	-0.25470400	-2.19563100	-6.97648700	C	0.21651300	2.74896700	-3.77929600
C	0.67431000	-3.19466100	-4.40271300	C	1.73777600	1.51038300	-1.77845700
H	1.38819800	-3.75568400	-3.79554100	H	2.42550500	0.17250600	-3.33240700
H	0.42043100	-2.30711300	-3.81735900	C	0.17378700	3.22913900	-2.46920000
C	0.04741700	-0.46891700	-5.78805100	H	-0.34751100	3.22090500	-4.57598700
C	-1.17876600	-0.32783600	-5.34724800	C	0.92926300	2.60841400	-1.47152600
C	-2.40797700	-0.10107400	-4.95963500	H	2.33057700	1.03623000	-1.00216300
H	-3.08847400	0.29688200	-5.71717700	H	-0.44356700	4.09010700	-2.23095100
C	-3.02911900	-0.34621800	-3.59011300	H	0.89266500	2.98445100	-0.45322900
C	-4.14867100	-1.41947900	-3.81455000	C	-3.66023900	0.97241800	-3.09702500
H	-4.87812300	-1.02076400	-4.53326600	H	-4.36164400	1.37976300	-3.83376300
H	-3.68759100	-2.29108900	-4.29806000	H	-4.21000300	0.79687200	-2.16751700
C	-4.83287600	-1.85072100	-2.59655200	H	-2.88778400	1.72426800	-2.90959000
C	-5.37200200	-2.23554200	-1.58269800	C	-2.00077800	-0.85115400	-2.56986900
C	-6.01399300	-2.75673000	-0.37467300	H	-1.56903300	-1.80647300	-2.88442800
C	-6.12032400	-4.29733800	-0.36553000	H	-1.18673700	-0.13199600	-2.44119700
H	-7.01592900	-2.31734900	-0.27043300	H	-2.48127900	-1.01021900	-1.60165500
H	-5.44575000	-2.42805700	0.50645600	Rh	-1.41032700	-5.29774400	-3.16125200
C	-6.76778600	-4.83490300	0.91568900	Cl	-2.25894300	-5.92953600	-1.07580100
H	-6.70318700	-4.61738200	-1.23871500	C	-0.32756300	-6.72147600	-3.33118400
H	-5.11788300	-4.72495000	-0.48631700	O	0.37778900	-7.62297100	-3.47813500
C	-6.88777600	-6.36210500	0.92486000	C	-2.37070300	-5.12878200	-6.28291500
H	-6.17734400	-4.50936100	1.78310000	C	-3.78154900	-5.42749400	-5.73182500
H	-7.76366500	-4.38632400	1.03913100	C	-2.45025100	-4.03594500	-7.37437700
H	-7.34736100	-6.72087100	1.85173600	C	-1.76448500	-6.41607600	-6.89128100
H	-7.50343400	-6.71534400	0.08967700	H	-3.74916100	-6.20103400	-4.95899400
H	-5.90404800	-6.83489100	0.83302000	H	-4.23895800	-4.53213700	-5.29896200
C	-0.53037300	-4.03152000	-4.61214800	H	-4.42758300	-5.77912300	-6.54279900
C	-1.47156400	-4.64840200	-5.18597900	H	-1.46992800	-3.86520000	-7.82606600
C	1.61656200	-3.97036300	-6.60060700	H	-3.13804900	-4.36048300	-8.16247800
O	1.10968200	-4.15683800	-7.68556500	H	-2.82411900	-3.09226400	-6.96512700
O	2.43058400	-4.84985500	-5.99014600	H	-2.41265200	-6.77859900	-7.69602300
C	2.77258800	-2.17991200	-5.30245600	H	-0.77530700	-6.21668700	-7.31239100
O	3.07880700	-1.85923200	-4.17309900	H	-1.67998800	-7.20801600	-6.14115700
O	3.58016000	-2.10680200	-6.36430200	INT-1b^{II}			
C	2.72576200	-6.05430300	-6.72308100	C	1.43740800	-2.79687000	-5.61248500
H	3.12283600	-5.81041200	-7.71051900	C	0.60599200	-1.80852200	-6.48876600
H	3.46701500	-6.58395600	-6.12605000	H	1.23690100	-1.49932600	-7.32580300
H	1.82449900	-6.66154200	-6.83578000	H	-0.22219900	-2.37660700	-6.91569600
C	4.85900300	-1.47661100	-6.14361700	C	0.75497700	-3.15980500	-4.26307000
H	5.39651400	-1.57592600	-7.08591300	H	1.46731400	-3.71299500	-3.64750100
H	4.70224500	-0.42607200	-5.89593400	H	0.53572900	-2.23774000	-3.71751200
H	5.39478700	-1.97945200	-5.33576500	C	0.02362700	-0.57670800	-5.81807400
S	1.08193600	1.04820300	-5.76324700	C	-1.21245100	-0.44210300	-5.40376600

C	-2.45190700	-0.23035500	-5.04111200	H	2.47460500	0.19307000	-3.42459900
H	-3.13405400	0.11659700	-5.82176800	C	0.10582300	3.15946000	-2.56057300
C	-3.08146400	-0.43910700	-3.66884500	H	-0.46092200	3.09193300	-4.65405800
C	-4.12794900	-1.59216900	-3.84850300	C	0.91082600	2.59101100	-1.57033400
H	-4.86952700	-1.27920800	-4.59655800	H	2.39302900	1.09284500	-1.10795300
H	-3.60630300	-2.45781300	-4.27735900	H	-0.54357900	3.99661300	-2.32266400
C	-4.80250600	-2.00033300	-2.61708100	H	0.88062600	2.98362700	-0.55810500
C	-5.33194400	-2.36674600	-1.59130700	C	-3.80193800	0.86100100	-3.25709500
C	-5.96341000	-2.86631700	-0.36858100	H	-4.51585500	1.18227000	-4.02374600
C	-6.09381500	-4.40496500	-0.34256300	H	-4.35419200	0.70126300	-2.32625800
H	-6.95671900	-2.41040600	-0.25358300	H	-3.08225400	1.67037700	-3.10128800
H	-5.37686800	-2.53819600	0.50071800	C	-2.03992300	-0.82094000	-2.60852400
C	-6.72673200	-4.91971500	0.95518400	H	-1.54184000	-1.76076100	-2.86517300
H	-6.69676100	-4.72409000	-1.20226800	H	-1.27756600	-0.04299700	-2.50851200
H	-5.10074200	-4.85015900	-0.47676100	H	-2.52611700	-0.95843700	-1.63969900
C	-6.86821300	-6.44484900	0.98318300	Rh	-1.40033800	-5.33927000	-3.13888100
H	-6.11696700	-4.59345700	1.80887800	Cl	-2.27869900	-6.15066600	-1.13165000
H	-7.71389500	-4.45565300	1.09071900	C	-0.39761500	-6.79305300	-3.47813000
H	-7.31796400	-6.78667900	1.92121000	O	0.26016100	-7.70397000	-3.73982400
H	-7.50201400	-6.79840800	0.16187500	INT-1a¹²			
H	-5.89295200	-6.93282500	0.88118700	C	-0.40638200	-2.57298800	-6.24323500
C	-0.47887300	-3.95985400	-4.43509600	C	-1.73159500	-1.91924800	-6.74164500
C	-1.44599400	-4.48157700	-5.06026600	H	-1.46532500	-1.13491900	-7.45390900
C	-2.31643100	-4.77218000	-6.21771400	H	-2.25549500	-2.69446200	-7.30576400
H	-3.24665200	-5.26182800	-5.92088400	C	-0.65847300	-3.75239600	-5.25382700
H	-2.56279300	-3.84025200	-6.73869200	H	0.27701200	-3.96849900	-4.72963100
H	-1.78683900	-5.42017400	-6.92424300	H	-1.36879100	-3.41847700	-4.48996300
C	1.62364200	-4.09714800	-6.42184300	C	-2.71845400	-1.34201500	-5.73788600
O	1.06338600	-4.36656000	-7.46087500	C	-3.88089800	-1.88058800	-5.39097300
O	2.46658000	-4.92884000	-5.78297100	C	-5.17704100	-1.81661700	-4.89060400
C	2.82764700	-2.21531300	-5.29888200	H	-5.87538500	-1.25992600	-5.52876500
O	3.18407900	-1.84683500	-4.19922800	C	-5.69030200	-1.94781300	-3.45088700
O	3.58487200	-2.18227200	-6.39955700	C	-6.92172400	-2.91482100	-3.44542200
C	2.70892600	-6.19515700	-6.42655000	H	-7.63714500	-2.57904800	-4.20875800
H	3.07986600	-6.04015100	-7.44178800	H	-6.59742200	-3.91354400	-3.75924500
H	3.45630200	-6.69564500	-5.81236400	C	-7.59747700	-3.01224800	-2.15163100
H	1.78976300	-6.78447200	-6.46398200	C	-8.15167600	-3.09796400	-1.07837900
C	4.86525200	-1.53149300	-6.26590400	C	-8.85334800	-3.23007400	0.19997600
H	5.35921200	-1.66479200	-7.22765300	C	-10.08789200	-4.15396800	0.12501400
H	4.70878900	-0.47283800	-6.05444900	H	-9.16517700	-2.23644900	0.55074000
H	5.44444600	-1.99450000	-5.46424600	H	-8.15948100	-3.61445200	0.96043600
S	1.03270700	0.95787900	-5.83604900	C	-10.80970700	-4.28299500	1.47125500
O	2.41179400	0.53631600	-6.14545100	H	-10.77898900	-3.76535400	-0.63314600
O	0.35461800	1.94444200	-6.69100200	H	-9.77120000	-5.14423200	-0.22497900
C	0.98858700	1.58697000	-4.15022700	C	-12.03610400	-5.19873000	1.40642500
C	1.81074000	1.01459000	-3.17567400	H	-10.10646900	-4.66354200	2.22471100
C	0.14045900	2.65836100	-3.86291200	H	-11.11445000	-3.28546900	1.81648700
C	1.76101700	1.52528800	-1.87764800	H	-12.53257900	-5.27018100	2.37949600

H	-12.77094100	-4.82566400	0.68419900	H	-1.25801000	-6.16717100	-9.25218100
H	-11.75758200	-6.21311400	1.09955400	H	-2.22763400	-7.64815200	-9.41528500
C	-1.13008500	-4.96071800	-5.93407600	H	-2.97793600	-6.15279800	-8.82314500
C	-1.42399000	-5.95367100	-6.56476100	H	-0.63085800	-8.96476100	-7.95014500
C	0.32302000	-3.11800400	-7.48974400	H	0.40540300	-7.53222900	-7.80047000
O	-0.09480100	-3.08363900	-8.62353200	H	-0.17162800	-8.36163700	-6.34465700
O	1.50309800	-3.66164500	-7.13427300	C	-4.35921100	-4.76118200	-4.99478600
C	0.51502900	-1.54277400	-5.57690200	O	-4.07681400	-5.57484100	-4.23145100
O	0.66996500	-1.43627900	-4.37571800	Cl	-5.63662800	-5.03517300	-7.80722100
O	1.13063400	-0.78317700	-6.48659700	INT-1b¹²			
C	2.27283400	-4.22371200	-8.21050500	C	-0.26081000	-2.53831000	-6.12231200
H	2.49522400	-3.46079900	-8.96025600	C	-1.61019600	-1.97139100	-6.65887500
H	3.19002400	-4.59390700	-7.75322400	H	-1.37317700	-1.20895300	-7.40456900
H	1.72325200	-5.04031900	-8.68491000	H	-2.09170900	-2.79446700	-7.19153100
C	1.92123800	0.30784700	-5.97572800	C	-0.45980000	-3.64133200	-5.04157400
H	2.40704200	0.74557000	-6.84698800	H	0.50566100	-3.83603600	-4.56575600
H	1.26351400	1.03471800	-5.49688700	H	-1.11498200	-3.24388300	-4.25902000
H	2.66108200	-0.05979600	-5.26157500	C	-2.63670300	-1.39645100	-5.69488800
S	-2.54002600	0.46310300	-5.37644200	C	-3.78448100	-1.96944700	-5.35298600
O	-1.23797400	0.85869100	-5.94454400	C	-5.09826900	-1.94280400	-4.89859500
O	-3.77175100	1.11906500	-5.85137500	H	-5.79653700	-1.44277300	-5.58148800
C	-2.47694800	0.72356500	-3.58947200	C	-5.64870500	-2.02934700	-3.46902700
C	-1.59144700	0.01177100	-2.77680700	C	-6.84006700	-3.04485000	-3.44889300
C	-3.26861400	1.75659100	-3.08003300	H	-7.54517400	-2.77581000	-4.24738500
C	-1.52518700	0.33083900	-1.41915400	H	-6.46811600	-4.04368600	-3.70303100
H	-0.95241900	-0.76142400	-3.18779200	C	-7.54944600	-3.10619200	-2.17091800
C	-3.18026800	2.07150300	-1.72334800	C	-8.13121000	-3.16010700	-1.11025800
H	-3.93687100	2.29477400	-3.74301200	C	-8.86584000	-3.25257100	0.15296200
C	-2.31454500	1.35640600	-0.89347000	C	-10.08990400	-4.19041000	0.07944500
H	-0.84516700	-0.21918600	-0.77583300	H	-9.19584700	-2.24972400	0.45799400
H	-3.78963600	2.87323600	-1.31735100	H	-8.18961500	-3.60164100	0.94562200
H	-2.25143300	1.60109800	0.16281600	C	-10.85045800	-4.27160200	1.40795900
C	-6.17465200	-0.53685800	-3.03698600	H	-10.76132700	-3.83920300	-0.71382000
H	-6.95135200	-0.16871300	-3.71612400	H	-9.75483600	-5.19097200	-0.22057800
H	-6.60100000	-0.58178300	-2.03119100	C	-12.06670400	-5.20090100	1.34443700
H	-5.35221800	0.17968900	-3.03741800	H	-10.16706900	-4.61438100	2.19695500
C	-4.61267900	-2.43381200	-2.47133200	H	-11.17378300	-3.26379800	1.70271000
H	-4.24719100	-3.43325200	-2.72008200	H	-12.59192800	-5.23688600	2.30428200
H	-3.75967000	-1.75124000	-2.45204400	H	-12.78225400	-4.86499000	0.58555300
H	-5.03368400	-2.48305300	-1.46369100	H	-11.77058600	-6.22440500	1.08847300
Rh	-4.86777800	-3.52564500	-6.21197600	C	-0.99889300	-4.88212900	-5.59952200
C	-1.71048400	-7.16749300	-7.35478800	C	-1.39308800	-5.90629500	-6.11224200
C	-2.89094500	-7.94841700	-6.73239700	C	0.47709400	-3.15027300	-7.33218700
C	-2.06511700	-6.75385600	-8.80327200	O	0.05961000	-3.19136600	-8.46555200
C	-0.44608900	-8.06040600	-7.36022900	O	1.66525300	-3.65438400	-6.94548600
H	-2.68035800	-8.22083000	-5.69360400	C	0.63038600	-1.43000700	-5.54481300
H	-3.81006400	-7.35753500	-6.75990900	O	0.80377200	-1.23890900	-4.35691900
H	-3.06392900	-8.86915500	-7.30026400	O	1.19872600	-0.70999500	-6.51564600

C	2.44083500	-4.27093000	-7.98812100	C	-2.14829400	-2.46737300	-4.93364100
H	2.66497700	-3.54723200	-8.77528400	H	-1.68879700	-2.06117400	-5.83577100
H	3.35679200	-4.61452200	-7.50820700	C	-3.47353200	-3.16697700	-5.16075900
H	1.89409800	-5.11160300	-8.42149700	C	-3.39160700	-4.19217900	-6.31503800
C	1.95311000	0.44315400	-6.09338800	H	-3.14959800	-3.66612100	-7.24884500
H	2.40842200	0.83891100	-7.00045600	H	-2.55038200	-4.87253000	-6.12810700
H	1.27415900	1.17468400	-5.65264300	C	-4.62689300	-4.95808000	-6.47799800
H	2.71706400	0.15366500	-5.36882400	C	-5.65566100	-5.58798300	-6.58182300
S	-2.53054300	0.42531500	-5.39692200	C	-6.88707600	-6.36191200	-6.75183900
O	-1.23759700	0.84762200	-5.96690300	C	-6.87882300	-7.25324100	-8.01199700
O	-3.78122200	1.01840800	-5.90365500	H	-7.74511600	-5.67675500	-6.79781200
C	-2.49238600	0.74686900	-3.61952200	H	-7.05124300	-6.98972600	-5.86496200
C	-1.55137800	0.13438100	-2.78798600	C	-8.17467200	-8.05555200	-8.17734800
C	-3.36615500	1.72550600	-3.13838900	H	-6.71618400	-6.62138200	-8.89395300
C	-1.51537300	0.49413000	-1.43953800	H	-6.02159900	-7.93589800	-7.95992000
H	-0.84613300	-0.59100100	-3.17783700	C	-8.17254500	-8.94439300	-9.42496400
C	-3.30814200	2.08276800	-1.79050900	H	-8.33352900	-8.67645600	-7.28497200
H	-4.07146900	2.19223100	-3.81694700	H	-9.02674700	-7.36341900	-8.22133100
C	-2.38922000	1.46364400	-0.94129800	H	-9.10885700	-9.50396700	-9.51771200
H	-0.79251100	0.02118100	-0.78178700	H	-8.04941200	-8.34809900	-10.33604000
H	-3.98174400	2.84311800	-1.40702700	H	-7.35257700	-9.67060100	-9.39256300
H	-2.34937200	1.74052800	0.10814900	C	-2.06314700	-4.28060400	-2.01906700
C	-6.20183400	-0.62237600	-3.13613500	C	-2.06258800	-5.27326000	-2.74223900
H	-6.97322600	-0.31921600	-3.85243600	C	-0.36693200	-3.01912600	0.37077000
H	-6.65374200	-0.63755700	-2.14069900	O	0.81843500	-2.91916300	0.16223800
H	-5.40917800	0.12661000	-3.14974700	O	-0.90114400	-3.79366100	1.33650700
C	-4.57898700	-2.42141000	-2.43967100	C	-2.26629800	-1.40968200	0.57199100
H	-4.16029700	-3.41207500	-2.63394200	O	-3.47472000	-1.40694900	0.68550400
H	-3.75893200	-1.69914300	-2.42894800	O	-1.44092400	-0.62468700	1.27259000
H	-5.02586900	-2.44644200	-1.44231300	C	0.05022300	-4.52365500	2.13625300
Rh	-4.65940100	-3.69669300	-6.12907700	H	0.71454600	-3.83238200	2.65973700
C	-1.88688100	-7.13831900	-6.72137500	H	-0.54464900	-5.09832400	2.84541400
C	-4.20805700	-4.86269800	-4.82365800	H	0.64785400	-5.18477700	1.50502900
O	-3.97788000	-5.64329900	-4.00962200	C	-2.07635200	0.37377000	2.09735500
Cl	-5.24300600	-5.33119000	-7.68451000	H	-1.26320200	0.88462200	2.61131000
H	-1.17924500	-7.51980400	-7.46552500	H	-2.63021600	1.06800200	1.46234500
H	-2.03305000	-7.91925100	-5.96689700	H	-2.75398800	-0.09688800	2.81264400
H	-2.84541000	-6.96564100	-7.22351900	S	-2.56442800	0.46417900	-2.76413200
INT-1b^{10H}				O	-2.51099100	1.00322300	-1.39130800
C	-1.47812000	-2.29463000	-0.41675700	O	-2.05015000	1.25001100	-3.89735100
C	-0.80077200	-1.38173000	-1.48979900	C	-4.27973700	0.05659800	-3.13525300
H	-0.50215100	-0.44696800	-1.01408000	C	-5.10507600	-0.45154700	-2.12755400
H	0.11072400	-1.88602000	-1.81659100	C	-4.75995100	0.30806700	-4.42177400
C	-2.49768100	-3.31485300	-0.99222700	C	-6.43578100	-0.73825300	-2.43538500
H	-2.88569300	-3.90432200	-0.15620000	H	-4.72071800	-0.60838000	-1.12454300
H	-3.34698300	-2.74996500	-1.38343200	C	-6.09550400	0.02224400	-4.71174200
C	-1.65832100	-1.11865900	-2.70461000	H	-4.09631800	0.73670500	-5.16477500
C	-1.71627700	-1.95235000	-3.72732200	C	-6.92844000	-0.50567200	-3.72236800

H	-7.09024000	-1.13372600	-1.66450500	O	-2.07249700	-7.18483300	-5.26371000
H	-6.48519700	0.21889000	-5.70603500	C	-0.42178300	-4.95697600	-6.40865500
H	-7.96658000	-0.72746000	-3.95188300	O	0.56137200	-4.36528700	-6.01034300
Rh	-0.61443700	-3.71311100	-3.91117100	O	-0.43837800	-5.71417600	-7.51493500
C	0.71344800	-2.95492100	-4.99511500	C	-2.75941200	-8.45008600	-5.38236300
O	1.54211300	-2.50266500	-5.64538400	H	-2.73452000	-8.79782600	-6.41744300
Cl	1.01082100	-5.44523200	-3.56076200	H	-2.21667700	-9.13518200	-4.73160200
C	-2.20282900	-6.58560200	-3.38099400	H	-3.79393700	-8.33244000	-5.05362500
H	-4.22770800	-2.40799700	-5.40724900	C	0.80114500	-5.78785400	-8.24678400
H	-3.80799100	-3.65936100	-4.24545500	H	0.59613500	-6.43328600	-9.09972300
H	-1.22245900	-6.97311200	-3.66675200	H	1.10464000	-4.79276200	-8.57960600
H	-2.84097900	-6.52860200	-4.26850400	H	1.58810000	-6.21243700	-7.61960200
H	-2.66561800	-7.27891800	-2.66939300	S	-2.63216700	-0.88070000	-6.34269300
TS1a				O	-2.31535800	-1.13476300	-7.76019500
C	-1.81121400	-4.86984200	-5.75638600	O	-3.75189700	0.01208500	-5.98747100
C	-2.57467800	-3.69952400	-6.46839700	C	-1.14936300	-0.21361100	-5.55987000
H	-2.00434800	-3.33327800	-7.32296700	C	0.02281300	-0.97353900	-5.50844300
H	-3.48741400	-4.12518500	-6.89098600	C	-1.18851800	1.09947700	-5.08802900
C	-1.59679600	-4.61983500	-4.24516000	C	1.16743300	-0.40700300	-4.94762200
H	-1.07213500	-5.47812900	-3.81649400	H	0.05737800	-1.98984500	-5.88671700
H	-0.94180700	-3.74938300	-4.14419700	C	-0.03181600	1.65754900	-4.54080300
C	-2.93746800	-2.52282100	-5.59472100	H	-2.11084800	1.66517300	-5.15712000
C	-3.58324700	-2.55679600	-4.42954800	C	1.14148700	0.90489200	-4.46637500
C	-4.36552500	-1.83007300	-3.51831800	H	2.07973900	-0.99289700	-4.89275300
H	-5.17331500	-1.30202900	-4.02289900	H	-0.05054200	2.67863000	-4.17199100
C	-3.89248400	-1.07120300	-2.25720000	H	2.03780300	1.34042600	-4.03454500
C	-4.77269600	-1.48094600	-1.03476100	C	-4.12675400	0.43174100	-2.54106000
H	-5.82728000	-1.32198200	-1.29650300	H	-5.18906200	0.63932900	-2.71350800
H	-4.65933800	-2.55641500	-0.87112700	H	-3.80313000	1.02680800	-1.68218700
C	-4.47369200	-0.76508200	0.20661000	H	-3.57760300	0.75295500	-3.42769100
C	-4.23041500	-0.18738700	1.24306100	C	-2.40215900	-1.29431000	-1.95113100
C	-3.96607300	0.52595300	2.49403200	H	-2.17614500	-2.34689800	-1.77867200
C	-4.73649500	1.85760700	2.61927900	H	-1.77867400	-0.94180500	-2.77751400
H	-2.88814700	0.72075800	2.58352800	H	-2.12362000	-0.73421600	-1.05384900
H	-4.22441400	-0.12242200	3.34299100	Rh	-5.00475400	-3.94867000	-3.64523700
C	-4.44976000	2.58320500	3.93859200	Cl	-5.65302700	-6.34201100	-3.94292800
H	-4.47242700	2.50394000	1.77284700	C	-6.70062100	-3.76371000	-2.63672300
H	-5.81140400	1.65712700	2.52990400	O	-7.64809400	-3.65033600	-2.00313600
C	-5.20875100	3.90737200	4.07142200	C	-6.58761800	-3.80238200	-8.04924000
H	-4.71097500	1.92476600	4.77832700	C	-6.50723300	-4.43373400	-6.66606100
H	-3.37023100	2.76921200	4.02319400	C	-7.27441100	-2.39899500	-5.73065000
H	-4.98502400	4.40270300	5.02178000	C	-7.33696200	-1.78854600	-7.12549200
H	-4.94207300	4.59937600	3.26457800	O	-6.24404500	-3.40042000	-5.68651000
H	-6.29222600	3.74955000	4.02559000	O	-7.59109900	-2.79203500	-8.09779700
C	-2.85231100	-4.41119300	-3.48635400	H	-7.02428500	-1.64266300	-4.98297900
C	-3.51486300	-4.67450300	-2.41859900	H	-8.23891400	-2.85919300	-5.47019000
C	-2.57160500	-6.19123100	-6.01232300	H	-8.15633900	-1.06546000	-7.18873000
O	-3.48212300	-6.32313100	-6.79929600	H	-6.38894800	-1.26861700	-7.33630500

H	-7.45161400	-4.93109800	-6.41052100	C	1.19415400	-1.67400900	0.57488900
H	-5.69739200	-5.15926400	-6.59058300	C	0.30553700	-2.45570100	1.24034200
H	-5.60901000	-3.37681800	-8.32418400	C	1.38407600	-2.87582400	-2.08320000
H	-6.85996000	-4.55775200	-8.79244600	O	0.41913500	-2.47438900	-2.69568800
C	-3.44260800	-5.41241300	-1.10118100	O	1.62364200	-4.16549300	-1.80354100
C	-2.46089100	-4.68537200	-0.15159300	C	3.84641000	-2.40821100	-2.08343600
C	-4.81670800	-5.54669400	-0.41894700	O	4.84756200	-2.62011000	-1.43704200
C	-2.89831500	-6.83121400	-1.40748200	O	3.78571100	-2.48173400	-3.42719400
H	-1.47016700	-4.58114900	-0.60523500	C	0.61942100	-5.10271900	-2.26138300
H	-2.81872100	-3.68936700	0.12294800	H	0.50107500	-5.02342500	-3.34427500
H	-2.35024100	-5.26585200	0.77090300	H	0.99985200	-6.08601900	-1.98668900
H	-5.52052200	-6.07575100	-1.06529500	H	-0.33330600	-4.89894800	-1.76730900
H	-4.70447400	-6.11249400	0.51199200	C	5.00863700	-2.86123900	-4.08561000
H	-5.23948500	-4.57083500	-0.16210900	H	4.77530100	-2.87599700	-5.14963500
H	-2.82527200	-7.40352700	-0.47568500	H	5.79781500	-2.13607200	-3.87324600
H	-3.56618500	-7.35498400	-2.09456600	H	5.33240300	-3.84827100	-3.74748300
H	-1.90025500	-6.78712100	-1.85463900	S	0.62076000	1.72180500	-1.76671900
INT-2a				O	0.12053600	1.38093700	-3.11304800
C	2.49424100	-1.97825200	-1.50045900	O	-0.24669500	2.47830900	-0.84176200
C	2.22819000	-0.50575400	-1.89079700	C	2.12054200	2.69864200	-2.00968300
H	3.17495900	0.04745800	-1.83907500	C	2.68462000	2.76199100	-3.28521100
H	1.89270600	-0.47820700	-2.93031300	C	2.67019100	3.40071200	-0.93373200
C	2.52895100	-2.12260200	0.04242100	C	3.82907200	3.53689700	-3.48164200
H	2.75765000	-3.15272100	0.31345900	H	2.21612100	2.22553900	-4.10307100
H	3.33889500	-1.48925900	0.42214800	C	3.81568100	4.16800500	-1.14200600
C	1.19566600	0.18633900	-1.01553200	H	2.20123700	3.35735700	0.04261100
C	0.69411100	-0.34389100	0.13792100	C	4.39483600	4.23425600	-2.41244300
C	-0.44789000	0.15091300	0.98547200	H	4.27369600	3.59934900	-4.47031500
H	-1.05189000	0.86722900	0.43353900	H	4.25119700	4.72057200	-0.31498200
C	-0.14702900	0.76130800	2.38655500	H	5.28487000	4.83650600	-2.56954500
C	-1.49532900	1.36123200	2.90749100	C	0.85173700	1.93150900	2.20579700
H	-1.86768800	2.06956600	2.15481100	H	0.47892900	2.65412500	1.47624400
H	-2.24447900	0.56341700	2.97553800	H	0.99769600	2.44242200	3.16210900
C	-1.41627400	2.04062800	4.20145500	H	1.82364100	1.56136700	1.86349100
C	-1.36462200	2.59816100	5.27524200	C	0.43615000	-0.19739300	3.43816900
C	-1.31675000	3.30115200	6.55889900	H	-0.22986300	-1.03858500	3.64741000
C	-1.33472700	4.83774000	6.41795800	H	1.40176300	-0.60080300	3.12411000
H	-0.41497600	2.99757600	7.10894200	H	0.58381500	0.34527000	4.37627100
H	-2.16651000	2.98369300	7.17934800	Rh	-1.43898500	-1.70529800	0.67913400
C	-1.29301900	5.55795600	7.77042600	Cl	-2.35027000	-3.88354200	-0.11369800
H	-0.48105500	5.14917100	5.80293500	C	-2.31201200	-1.88147000	2.26327000
H	-2.23545700	5.13381100	5.86591500	O	-2.87839300	-2.07511800	3.24755000
C	-1.31135400	7.08390200	7.63673400	C	0.49714700	-3.74098600	1.96315300
H	-2.14692000	5.23326100	8.38074600	H	-0.18086200	-4.50489500	1.57179300
H	-0.39288600	5.24851400	8.31927000	H	1.53286300	-4.09160400	1.89454200
H	-1.28219100	7.57125500	8.61667100	H	0.26397700	-3.60862900	3.02719500
H	-0.45006200	7.44174800	7.06125200	C	-3.15097100	-0.21179400	-3.27586900
H	-2.21656400	7.42536900	7.12199800	C	-2.98981800	-1.27508800	-2.20000600

C	-3.82121900	0.28981900	-0.59787900	C	-2.33716300	5.36035800	-1.36783100
C	-3.96794700	1.31872300	-1.71252500	H	-0.85278500	4.74314000	0.08913500
O	-2.75633200	-0.62762600	-0.91902800	C	-3.94388300	3.66058300	-1.99698400
O	-4.22124400	0.67697800	-2.95299900	H	-3.72873700	1.74173800	-1.02987500
H	-3.55273400	0.76544500	0.34852800	C	-3.44613300	4.96109700	-2.11653000
H	-4.75241000	-0.27945300	-0.47038700	H	-1.95481600	6.37308700	-1.45508500
H	-4.82078700	1.97404500	-1.50730800	H	-4.80985900	3.35310400	-2.57565200
H	-3.05403000	1.92967200	-1.76794100	H	-3.92572900	5.66460800	-2.79103700
H	-3.88711400	-1.89869300	-2.11541400	C	1.11367300	1.54665500	-2.69567100
H	-2.12475900	-1.91195300	-2.38730300	C	2.58671800	2.00618700	-2.58201800
H	-2.21146400	0.34541700	-3.39718600	C	1.00901400	0.38256100	-3.68605800
H	-3.40944700	-0.68577100	-4.22776700	H	1.73613800	-0.40159100	-3.47100600
TS2a				H	0.01269400	-0.06797300	-3.67706900
C	-0.03690000	0.16547600	-0.70952000	H	1.19521200	0.75747700	-4.69910700
C	0.14861800	-1.26773500	-1.10945900	C	0.13101400	2.65377700	-3.09023700
Rh	2.20745000	-0.35391700	0.26451200	H	0.33284700	2.98431600	-4.11586700
Cl	3.22485500	-1.97146700	1.72177000	H	-0.90428600	2.30146500	-3.05246400
C	-1.12731300	-1.98774800	-1.51269000	H	0.21340200	3.52304400	-2.43241200
C	-1.14473700	0.45663200	0.03741200	C	2.93675800	1.09620500	-1.45907800
H	-1.44113700	-1.60442400	-2.49234800	C	3.76388300	0.36591800	-0.80001200
H	-0.96833500	-3.05702200	-1.62117200	C	5.21220800	0.07924700	-0.62745200
H	-5.98980200	-2.07646300	-2.20005800	C	6.10610600	0.80295300	-1.65101000
C	-5.13341200	-2.33631500	-2.82652100	H	5.36642900	-1.00330700	-0.68014800
O	-3.95729000	-2.52200900	-2.01819000	H	5.49657700	0.36374900	0.39427300
H	-5.29751900	-3.29000800	-3.32698300	C	7.59515300	0.49763300	-1.44303200
H	-4.97312400	-1.54074300	-3.55822000	H	5.80926600	0.50588800	-2.66569100
C	-3.57137900	-1.45684100	-1.28872700	H	5.93946300	1.88597900	-1.58039900
C	-2.29773200	-1.78173900	-0.49620800	C	8.49952600	1.21012900	-2.45342400
O	-4.15536400	-0.39476400	-1.30537700	H	7.88380800	0.78660700	-0.42364200
C	-2.56194300	-3.08993800	0.27641700	H	7.75297200	-0.58701900	-1.50796600
O	-1.91591500	-4.11035800	0.20076500	H	9.55385900	0.97298000	-2.27919200
O	-3.62736100	-2.94006800	1.08742200	H	8.25771700	0.91438900	-3.48066100
C	-3.97482700	-4.09103900	1.88049900	H	8.38839100	2.29845100	-2.38738700
H	-3.15267400	-4.35453500	2.54968700	H	3.20237500	1.86880300	-3.47775000
H	-4.85429300	-3.79667300	2.45198100	H	2.65594200	3.05730700	-2.27285400
H	-4.19799900	-4.94411400	1.23560100	C	2.54841700	0.95697400	1.84107500
C	1.41699800	-1.75192100	-1.01735400	O	2.71257000	1.56659000	2.79043000
C	0.98982600	1.15827300	-1.17760200	C	-0.35733000	0.45546600	4.24911900
H	0.93540700	2.07196000	-0.58999800	C	-1.63125100	-0.03349200	4.92574600
C	-2.01529900	-0.66807300	0.55115700	C	-0.92973400	-2.25523000	4.63778800
H	-1.48518300	-1.10960100	1.40447700	C	0.34629900	-1.76622600	3.96265600
H	-2.95751500	-0.28640400	0.93875000	O	-1.41966000	-1.29273900	5.56302400
S	-1.47088400	2.05533600	0.81335900	O	0.10430300	-0.51889900	3.30651800
O	-0.18446800	2.67809100	1.20455300	H	-1.69408500	-2.46596400	3.86884200
O	-2.48172700	1.80484000	1.85808600	H	-0.74401800	-3.17388200	5.20436900
C	-2.22233300	3.16142800	-0.39899500	H	1.14001700	-1.64169100	4.71498000
C	-1.71537700	4.45802100	-0.50307300	H	0.70278100	-2.46304300	3.20091400
C	-3.34057300	2.75011300	-1.12823500	H	-1.95085400	0.66368300	5.70668600

H	-2.43344300	-0.11048600	4.17540500	O	3.56258000	2.33677300	-2.66890200
H	-0.53712400	1.37761500	3.69433700	C	2.93791900	3.55605500	-0.39649400
H	0.42399700	0.63143700	5.00513800	C	2.51796100	4.88807300	-0.36718900
C	1.96929500	-3.08712200	-1.52120600	C	3.81428700	3.04853800	0.56582700
C	1.45996800	-3.41553800	-2.94937600	C	2.98668200	5.72644900	0.64544100
C	3.51098500	-3.04179500	-1.60826500	H	1.83350700	5.24782400	-1.12714900
C	1.56339300	-4.22828700	-0.55305900	C	4.26737000	3.89592300	1.57727600
H	0.37916300	-3.55450500	-3.00324300	H	4.10581800	2.00505900	0.56427800
H	1.73665300	-2.63282000	-3.66300200	C	3.86021100	5.23178200	1.61584900
H	1.92389100	-4.34816300	-3.28907800	H	2.66703400	6.76389800	0.67543900
H	3.95328400	-2.86788900	-0.62704000	H	4.93802000	3.50775100	2.33792800
H	3.88436000	-3.99757200	-1.99295600	H	4.22041100	5.88549700	2.40497300
H	3.84259300	-2.25378600	-2.29364900	C	-0.77862500	1.70898600	0.90342400
H	1.98078400	-5.17618000	-0.91426000	C	-1.29047600	0.38742100	1.53874400
H	1.95954400	-4.03648900	0.44599400	C	0.46374000	2.19090100	1.67909300
H	0.47908000	-4.33979900	-0.47889100	H	1.28725400	1.47508800	1.63072800
TS2aa				H	0.82362600	3.14738400	1.29288700
C	0.67760500	0.50888800	-0.86855900	H	0.20423600	2.33966300	2.73398700
C	0.33276100	-0.92832400	-0.76066500	C	-1.85461000	2.80432000	1.00673700
Rh	-2.00181200	0.37609900	-1.66909900	H	-2.05014200	3.05408600	2.05559400
Cl	-3.65651200	-0.78578700	-3.23985100	H	-1.51659500	3.71595100	0.50323300
C	1.46921400	-1.92131900	-0.94446800	H	-2.79889000	2.50016800	0.54856800
C	1.94242500	0.89185900	-1.22458500	C	-2.17769400	-0.19796200	0.49994300
H	1.29861400	-2.84737300	-0.40495100	C	-3.29294800	0.11484900	-0.05929500
H	1.52855200	-2.20004400	-2.00209400	C	-4.76100600	0.25185800	-0.01055800
H	3.88056900	-1.93404900	3.29276300	C	-5.35421800	0.02181800	1.39173500
C	2.83619400	-2.13762900	3.04538700	H	-5.18789200	-0.45132100	-0.73767100
O	2.66744600	-2.22592700	1.61855100	H	-5.03714400	1.24787100	-0.38311100
H	2.52861300	-3.10648900	3.43723200	C	-6.88195400	0.16120200	1.40480000
H	2.21189900	-1.34047700	3.45572800	H	-5.07210600	-0.97862100	1.74355400
C	3.01832300	-1.12682300	0.92033700	H	-4.91312500	0.73777100	2.09771900
C	2.85821300	-1.36863500	-0.58615700	C	-7.49008600	-0.06969900	2.79158700
O	3.41899800	-0.10905300	1.44378800	H	-7.15717800	1.16120900	1.04380900
C	3.91888400	-2.39849100	-1.01762500	H	-7.31414500	-0.55061700	0.68936600
O	3.72969600	-3.30559900	-1.79588600	H	-8.57937900	0.03502900	2.76971200
O	5.11058400	-2.12849900	-0.45150000	H	-7.25987900	-1.07470300	3.16281600
C	6.19287300	-2.99923900	-0.83397700	H	-7.10122500	0.65002300	3.52095100
H	6.35949700	-2.94706200	-1.91216300	H	-0.45989900	-0.27823800	1.78611900
H	7.06519200	-2.63616200	-0.29183400	H	-1.86517600	0.58589000	2.45146200
H	5.96664600	-4.03158500	-0.55741700	C	-2.97194000	1.98455500	-2.34620500
C	-1.00414300	-1.28825300	-0.73971800	O	-3.63197200	2.86800600	-2.65370100
C	-0.46866100	1.44343300	-0.61367400	C	-0.65196100	1.65147500	-4.44364000
H	-0.31636200	2.39662700	-1.11217000	C	0.50235400	1.70576900	-5.43572800
C	3.09877600	-0.07521800	-1.38533100	C	0.70510400	-0.61205300	-5.37739200
H	3.23673700	-0.33747500	-2.44144100	C	-0.45105900	-0.71210400	-4.39152100
H	4.03540000	0.38438800	-1.06776500	O	0.56021500	0.51998800	-6.22100900
S	2.39214200	2.54832700	-1.79568100	O	-0.52383300	0.49023200	-3.59101900
O	1.21650200	3.24973800	-2.36031600	H	1.66252600	-0.56044900	-4.83187000

H	0.72006500	-1.49619300	-6.02277500	H	-11.04253600	-5.18754300	4.63217300
H	-1.40614100	-0.85280400	-4.90829700	H	-9.38696700	-4.60704400	4.85606400
H	-0.30494200	-1.53828200	-3.69497500	H	-10.59809300	-3.55692500	4.11065700
H	0.35738600	2.54134100	-6.12741500	C	-4.27485600	-4.23863700	-1.36415900
H	1.44844500	1.85822900	-4.89582700	C	-5.03328400	-5.34895500	-1.22169500
H	-0.61966000	2.52153200	-3.78827000	C	-2.07822900	-5.13479200	-3.74633300
H	-1.61353400	1.59534000	-4.97126700	O	-2.72249300	-5.64733700	-4.63513400
C	-1.52613800	-2.75167600	-0.60659400	O	-0.95862600	-5.68194300	-3.23122000
C	-1.01020500	-3.38229900	0.71740000	C	-1.18672500	-2.89467500	-3.10546600
C	-3.06685200	-2.88934100	-0.54513000	O	-0.76495500	-2.20114500	-2.20697100
C	-1.09379700	-3.59568600	-1.83541900	O	-0.65374700	-2.92387200	-4.34269100
H	0.07508100	-3.41179500	0.82005100	C	-0.53072600	-6.91479800	-3.83964700
H	-1.40830400	-2.82965400	1.57500100	H	-0.35204000	-6.76947300	-4.90746500
H	-1.37608200	-4.41235400	0.79253300	H	0.39130200	-7.18826400	-3.32764800
H	-3.55209100	-2.38544000	-1.38125100	H	-1.28830500	-7.69044000	-3.70661800
H	-3.31546700	-3.95475100	-0.60154500	C	0.50994600	-2.10019600	-4.54421900
H	-3.47546500	-2.51349100	0.39438000	H	0.81768000	-2.27843800	-5.57424900
H	-1.44332700	-4.62537400	-1.70347000	H	0.26350700	-1.04758600	-4.39270700
H	-1.56569200	-3.20111200	-2.73956500	H	1.30274300	-2.38875700	-3.85005300
H	-0.01602200	-3.64234100	-1.99115700	S	-4.95236700	-0.70880200	-3.47210300
INT-3a				O	-5.64364100	-0.99121200	-4.74825700
C	-2.41539100	-3.81811400	-3.02604800	O	-5.61676800	0.11303700	-2.44695000
C	-3.62319600	-3.14124800	-3.75570900	C	-3.40830000	0.12402800	-3.89556700
H	-3.26787000	-2.55948200	-4.60766400	C	-3.10362900	0.32734700	-5.24294900
H	-4.23905500	-3.95184400	-4.15949600	C	-2.59841700	0.63383000	-2.87771600
C	-2.76139000	-4.09882300	-1.53532700	C	-1.96054000	1.05673700	-5.57464900
H	-2.20474300	-4.96013800	-1.18835600	H	-3.76827800	-0.06486900	-6.00484400
H	-2.41181700	-3.23527600	-0.96565800	C	-1.45526200	1.35406400	-3.22141300
C	-4.47564500	-2.32500800	-2.81506700	H	-2.85992200	0.47839400	-1.83697400
C	-4.90862400	-2.87977900	-1.64183200	C	-1.13983600	1.56867800	-4.56659400
C	-5.75442200	-2.18819500	-0.58710700	H	-1.71764000	1.23150100	-6.61842300
H	-6.31816200	-1.38670700	-1.06784100	H	-0.81666800	1.75356200	-2.43994700
C	-5.16975100	-1.57142600	0.77116900	H	-0.25542700	2.14235100	-4.82861000
C	-6.45136400	-2.11861100	1.48787200	C	-5.00918800	-0.05367500	0.77979000
H	-6.28402000	-2.61684200	2.44689900	H	-5.89948500	0.44978100	0.39332100
H	-7.21652900	-1.34481200	1.62682200	H	-4.82857600	0.30116600	1.80213100
C	-6.70886900	-3.00613400	0.27393500	H	-4.16037800	0.26370500	0.16467100
C	-7.36071100	-4.11654300	-0.04154700	C	-3.91086900	-2.25750400	1.30203600
C	-8.38409400	-4.89911900	0.73264800	H	-4.00499200	-3.34718700	1.28309700
C	-8.75110100	-4.32714800	2.11435700	H	-3.02469600	-1.97627100	0.72311400
H	-8.04995600	-5.93444700	0.84900900	H	-3.73306600	-1.95189800	2.33990200
H	-9.29438600	-4.97015300	0.12280000	Rh	-6.84164900	-4.62561300	-1.95007200
C	-9.86587000	-5.13499300	2.79261800	Cl	-8.11297700	-6.62725500	-2.04878600
H	-7.86616500	-4.32251200	2.76275800	C	-8.51838800	-3.65087400	-2.60842700
H	-9.07013600	-3.28187400	2.01398400	O	-9.51988600	-3.14621000	-2.82733200
C	-10.24529900	-4.59273500	4.17435100	C	-6.36730900	-4.27609900	-6.81919000
H	-10.75251500	-5.14153400	2.14445700	C	-6.90358800	-4.04148800	-5.41680400
H	-9.54969600	-6.18292800	2.88344200	C	-6.12316800	-6.29676900	-5.03474400

C	-6.97141300	-6.51699600	-6.27697900	C	-1.05671300	-1.35181600	-0.29691800
O	-6.31395800	-4.96802300	-4.48347400	C	-0.59351000	1.46758000	-0.53023800
O	-6.67919400	-5.58046900	-7.31006900	H	-0.41182400	2.43283800	-0.99054000
H	-6.41045400	-7.00707500	-4.25807600	C	2.96720500	-0.01359700	-1.38122500
H	-5.05945900	-6.41381700	-5.26690000	H	3.09352400	-0.21501200	-2.45202000
H	-6.76560900	-7.51357000	-6.68182200	H	3.90112500	0.44404300	-1.05237000
H	-8.03876400	-6.48294200	-6.01069300	S	2.21728000	2.59451200	-1.73093800
H	-6.64547600	-3.03738000	-5.07496500	O	1.03726300	3.29414300	-2.28779800
H	-7.99691600	-4.14853500	-5.40936100	O	3.39258500	2.41452000	-2.60518500
H	-6.80626000	-3.54461500	-7.50810100	C	2.74211400	3.57620100	-0.30569500
H	-5.27672200	-4.12825000	-6.81923600	C	2.33353400	4.91149400	-0.26708400
C	-4.63826300	-6.75611800	-0.76291600	C	3.59154000	3.04632800	0.66866700
C	-3.21293000	-6.87157000	-0.16399300	C	2.78763100	5.73124300	0.76715600
C	-5.61168500	-7.20095000	0.35706600	H	1.66788400	5.28827400	-1.03549300
C	-4.73682300	-7.75743000	-1.93728900	C	4.03036800	3.87575400	1.70125300
H	-2.42987200	-6.83288800	-0.92580500	H	3.87454200	2.00020900	0.65883800
H	-3.01499700	-6.10078300	0.58741600	C	3.63501100	5.21476700	1.74939200
H	-3.12009600	-7.84447600	0.33027400	H	2.47639100	6.77096400	0.80512500
H	-6.63661400	-7.23668700	-0.00802300	H	4.68044400	3.47077500	2.47095000
H	-5.33455600	-8.20296300	0.70392500	H	3.98372200	5.85406000	2.55530500
H	-5.56029600	-6.52054400	1.21357200	C	-0.98558100	1.68533700	0.97393700
H	-4.42290200	-8.75226900	-1.59962000	C	-1.46547200	0.34327000	1.62171800
H	-5.76104300	-7.83228400	-2.30355700	C	0.22394600	2.21155900	1.77734700
H	-4.08706200	-7.45827500	-2.76626600	H	1.07142100	1.52201100	1.74227000
INT-3aa				H	0.56225900	3.18212000	1.40571000
C	0.55539600	0.53715900	-0.73430200	H	-0.06291200	2.34117900	2.82790400
C	0.23809700	-0.91339400	-0.58948500	C	-2.09311400	2.75115400	1.04400700
Rh	-1.99316400	0.33321400	-1.79974700	H	-2.34626900	2.97924900	2.08545000
Cl	-3.40254100	-1.16758100	-3.22021200	H	-1.75464700	3.67890900	0.57038300
C	1.34840200	-1.87063700	-0.97365000	H	-3.00570700	2.43875700	0.53420800
C	1.79845300	0.92388000	-1.16430300	C	-2.04175400	-0.47646800	0.48736600
H	1.22021900	-2.84217700	-0.51113200	C	-3.10586700	0.01202700	-0.18524100
H	1.32960900	-2.04069100	-2.05523000	C	-4.52842900	0.35209500	0.05177100
H	3.98172800	-2.10217700	3.14394200	C	-5.02860300	0.20723000	1.50081600
C	2.93650700	-2.33281100	2.92572000	H	-5.09727400	-0.33270100	-0.59793200
O	2.71382600	-2.34383500	1.50314800	H	-4.75797300	1.35272300	-0.33795400
H	2.68246600	-3.33479100	3.26938000	C	-6.54985800	0.37959600	1.60509800
H	2.29934500	-1.58706600	3.40653100	H	-4.74075200	-0.77844100	1.88662700
C	2.97783600	-1.18766100	0.86146200	H	-4.53479200	0.95026700	2.13941600
C	2.75622100	-1.34585700	-0.64919800	C	-7.06831200	0.25004500	3.04077700
O	3.35072600	-0.18335200	1.42877400	H	-6.83268100	1.36005700	1.19923100
C	3.78713700	-2.35755900	-1.18061200	H	-7.04100200	-0.36726400	0.96755800
O	3.54758800	-3.24433600	-1.96829300	H	-8.15508100	0.37340200	3.08311400
O	5.01256300	-2.09543600	-0.68848500	H	-6.82850400	-0.73308100	3.46130200
C	6.07108600	-2.94873100	-1.16575600	H	-6.62213000	1.00787300	3.69485400
H	6.16740500	-2.86383200	-2.25042200	H	-0.62414200	-0.19374700	2.07403700
H	6.97528900	-2.59678500	-0.67063000	H	-2.20272800	0.54275000	2.40638200
H	5.86665500	-3.98984400	-0.90572600	C	-2.96162000	1.77776500	-2.51689200

O	-3.62960400	2.62847900	-2.90390500	C	4.99039900	-3.48220300	3.73087200
C	-0.38992100	1.59587500	-4.61446600	H	5.70285800	-2.96434300	3.08497200
C	0.79364200	1.63620400	-5.57157800	H	5.13550300	-3.19466300	4.77146500
C	0.93918200	-0.69400500	-5.52545900	H	5.11238000	-4.56059000	3.60569400
C	-0.24262000	-0.76245100	-4.56606100	C	-0.86747800	-3.31233700	-0.78805800
O	0.85208800	0.45103300	-6.36058200	C	-1.37993300	-0.73417100	-0.26961800
O	-0.29602800	0.43380500	-3.76498900	H	-1.27556700	0.34352800	-0.30478400
H	1.88375400	-0.67879500	-4.95522900	C	1.88595700	-1.28777900	1.84793400
H	0.94435300	-1.57058700	-6.18131100	H	2.73871100	-0.98806300	1.22295500
H	-1.18671300	-0.87623800	-5.11151900	H	2.08103400	-0.89158100	2.84386800
H	-0.14469400	-1.60139700	-3.87354800	S	0.43992700	1.07414400	1.69225100
H	0.69092800	2.47559900	-6.26623700	O	-0.02407800	1.85373600	0.52239400
H	1.72562600	1.76541200	-4.99998300	O	1.70764200	1.46183700	2.33862100
H	-0.37500900	2.46437600	-3.95570300	C	-0.86696200	1.20715800	2.93192800
H	-1.33357900	1.55196000	-5.17725500	C	-1.82203400	2.21181800	2.76094600
C	-1.48955600	-2.86506300	-0.30325200	C	-0.85161300	0.39833800	4.07103700
C	-3.01891900	-3.04237900	-0.13553300	C	-2.78592900	2.40552900	3.75219000
C	-1.13028300	-3.61584700	-1.60934600	H	-1.79732000	2.82624100	1.86795400
C	-0.84993700	-3.54592800	0.94002400	C	-1.82815700	0.59742100	5.04776400
H	-3.37867700	-2.66484300	0.82385000	H	-0.11826000	-0.39154600	4.18471600
H	-3.57150700	-2.55837400	-0.94340700	C	-2.78990800	1.59921700	4.89204400
H	-3.24252100	-4.11364800	-0.17422800	H	-3.53134300	3.18589600	3.63171700
H	-0.06295800	-3.70799700	-1.80372600	H	-1.83355900	-0.03168600	5.93275900
H	-1.52654300	-4.63501100	-1.54900200	H	-3.54300700	1.75084500	5.65991600
H	-1.60873800	-3.12522900	-2.46115400	C	-2.85013600	-1.11945400	0.15172700
H	-1.15716800	-4.59691300	0.97514200	C	-3.18455500	-2.12158200	-0.97166700
H	0.24128600	-3.51910900	0.95348700	C	-2.94784700	-1.74350500	1.55364600
H	-1.20486600	-3.06681400	1.85921200	H	-2.33848200	-2.64651000	1.64369000
TS3aa				H	-2.62648500	-1.04235300	2.32822300
C	-0.19114300	-1.33337800	0.39330900	H	-3.98864100	-2.01829200	1.76048300
C	0.04419800	-2.74921300	0.05434000	C	-3.75677600	0.11850700	0.07889000
Rh	-0.74435300	-0.38203600	-2.56376800	H	-4.80355400	-0.16562000	0.23661200
Cl	0.10400700	-0.07147300	-4.84372400	H	-3.48531400	0.84866200	0.84784000
C	1.31729700	-3.38894400	0.56052600	H	-3.68553700	0.60788600	-0.89745900
C	0.63124400	-0.68156100	1.25786200	C	-1.77331700	-2.34150400	-1.53528600
H	1.26756300	-4.47139500	0.61209500	C	-1.45326500	-2.05790300	-2.90756100
H	2.10530600	-3.16797400	-0.17001100	C	-1.74330800	-2.73731500	-4.20822000
H	0.53953400	-4.86178100	5.16951000	C	-3.21798500	-2.58832400	-4.65732200
C	0.13959800	-5.20259500	4.21188600	H	-1.49826700	-3.80489800	-4.13494900
O	0.89982500	-4.64393400	3.12457900	H	-1.09873600	-2.29630700	-4.97170800
H	0.23981900	-6.28305500	4.11460900	C	-3.46956800	-3.24658500	-6.01993400
H	-0.90881400	-4.90482100	4.13712100	H	-3.89393500	-3.02414300	-3.90891500
C	0.94082300	-3.29607800	3.07294200	H	-3.45412200	-1.51931100	-4.71510100
C	1.81953500	-2.82806900	1.90449400	C	-4.91496900	-3.08315400	-6.50083400
O	0.36088100	-2.58623500	3.86492700	H	-2.78431600	-2.81070000	-6.75771800
C	3.24559700	-3.35672900	2.14852500	H	-3.21964300	-4.31490600	-5.96089700
O	3.93687800	-3.90463200	1.32022700	H	-5.06579000	-3.55792500	-7.47578000
O	3.64321600	-3.08810500	3.40584100	H	-5.62313000	-3.53632000	-5.79731100

H	-5.17967300	-2.02479700	-6.60201700	O	3.02206000	-3.23747800	-2.40141100
H	-3.65487100	-3.04882100	-0.63149200	O	4.26975700	-1.35508900	-2.41386500
H	-3.82865500	-1.67310500	-1.73290700	C	5.08298500	-1.92706400	-3.45529100
C	2.50778600	-0.70864200	-2.38752300	H	4.47716700	-2.13893300	-4.33940300
C	3.95208900	-0.31899200	-2.02608400	H	5.84121700	-1.17747400	-3.67921000
C	3.31780400	1.63123400	-0.88890900	H	5.54600400	-2.85482800	-3.11126700
C	2.12073100	1.57243400	-1.86057200	C	-0.24992300	-2.28122100	1.69311700
O	3.96983600	0.36087900	-0.78213600	C	-0.92205600	0.06570200	1.42830800
O	1.57685800	0.24723000	-1.84490000	H	-1.75546800	0.62500300	1.00832100
H	4.03257700	2.39838000	-1.22997100	C	1.66560100	-0.24859800	-1.56082800
H	2.99122500	1.88179700	0.12210300	H	1.17250800	-0.62617700	-2.46528700
H	1.32681300	2.23925000	-1.52559100	H	2.37807300	0.51773000	-1.87398900
H	2.40316200	1.84034200	-2.88707900	S	0.02016600	1.95071900	-1.14132100
H	4.57296600	-1.21338700	-1.91947500	O	-0.85358200	2.50246600	-0.08716100
H	4.40210700	0.30575100	-2.81379900	O	-0.48338000	1.78388800	-2.51739100
H	2.36807000	-0.78409300	-3.47282400	C	1.46381800	3.02774400	-1.25177700
H	2.23387000	-1.66346600	-1.93074600	C	2.07475500	3.21475400	-2.49354100
C	-1.49507500	1.46341100	-2.68193000	C	1.91671700	3.69435500	-0.11166600
O	-2.18273500	2.33903800	-2.97178400	C	3.17345100	4.07029400	-2.58654600
C	-1.01057700	-4.83490500	-1.07692200	H	1.67363900	2.71256400	-3.36712000
C	-2.34472100	-5.19243100	-1.77948300	C	3.01477700	4.54708100	-0.21633500
C	0.15850200	-5.31056200	-1.97722700	H	1.40116300	3.56364200	0.83272900
C	-1.03887300	-5.65953800	0.23795700	C	3.64474200	4.73042500	-1.44993000
H	-3.19918000	-5.06700100	-1.10867700	H	3.65466000	4.22662600	-3.54737600
H	-2.53765600	-4.61464200	-2.68129600	H	3.37451100	5.07274500	0.66295700
H	-2.31671900	-6.24815700	-2.06723300	H	4.49914800	5.39663600	-1.52661600
H	1.13114900	-5.15153800	-1.50637100	C	-0.41748700	0.69380000	2.79673700
H	0.05785900	-6.38235300	-2.18288200	C	-0.87450400	-0.59219300	3.54670500
H	0.16602000	-4.78370900	-2.93554800	C	1.08902500	0.94073600	2.90106500
H	-1.23177300	-6.71033100	-0.00496800	H	1.66939700	0.04426500	2.67033100
H	-0.11587100	-5.62583800	0.81383100	H	1.42099500	1.73009300	2.22192100
H	-1.85017500	-5.31554700	0.88778300	H	1.33780000	1.24765600	3.92406900
INT-4aa				C	-1.18666700	1.96244500	3.17645400
C	0.08700200	-0.35178200	0.39440600	H	-0.93499400	2.27043400	4.19819900
C	0.46969500	-1.74412800	0.66773400	H	-0.94045000	2.77822300	2.49148100
C	1.47067900	-2.40962400	-0.24212800	H	-2.27026100	1.81450500	3.12972900
C	0.63020500	0.34398900	-0.63075300	C	-1.29192100	-1.28369100	2.19468600
H	2.04195700	-3.18963900	0.25756200	C	-2.73271700	-1.61146100	1.91814300
H	0.93240800	-2.89931600	-1.06182900	C	-3.77486100	-0.89663200	2.72881000
H	5.84281700	-0.77354400	1.23522700	C	-5.00790900	-0.36788900	1.96748400
C	5.10630400	-1.43327500	1.69986900	H	-3.34416700	-0.07881300	3.31385900
O	4.11977500	-1.84209600	0.73554000	H	-4.11786600	-1.66074700	3.44889000
H	5.57674000	-2.35293500	2.04643200	C	-5.99477800	0.34271400	2.90241900
H	4.63305100	-0.90641600	2.53178900	H	-4.67711000	0.32467600	1.18266100
C	3.43162300	-0.83812600	0.14698000	H	-5.50788300	-1.20103500	1.46452700
C	2.44582800	-1.40214100	-0.89013600	C	-7.21501300	0.89968300	2.16266100
O	3.59324000	0.33005100	0.41523700	H	-6.32425600	-0.36057400	3.67869400
C	3.26084600	-2.13217500	-1.97140300	H	-5.48101700	1.16067000	3.42668100

H	-7.90296400	1.40167900	2.85071700	C	-4.42919600	-0.95578400	-1.23504200
H	-6.91793400	1.62713300	1.39872000	C	-4.05179700	-1.48242500	0.16111500
H	-7.77130200	0.10004400	1.66077900	O	-4.69031900	0.19104400	-1.51405000
H	-0.06484600	-1.12097200	4.05373400	C	-5.17606800	-2.41841200	0.63786300
H	-1.67846000	-0.44373500	4.26914800	O	-5.01086600	-3.49428900	1.16750400
Rh	-3.40000500	-2.84724400	0.63551300	O	-6.38520700	-1.86252000	0.42868000
C	-2.33798500	-2.25672500	-0.78494300	C	-7.51247800	-2.63678900	0.87905900
O	-1.74429700	-2.01375900	-1.74561000	H	-7.45475200	-2.80266500	1.95733400
Cl	-4.74012800	-4.03682600	2.26722700	H	-8.39218800	-2.04545700	0.62747100
C	-4.61802700	-6.45170500	-1.94669300	H	-7.53830500	-3.60388300	0.37157200
C	-3.88037400	-5.62459700	-0.90619300	C	-0.29690600	-1.72581200	-0.58801500
C	-5.81752000	-4.16907100	-1.07094600	C	-0.29104200	0.65688400	-0.07284800
C	-6.49917800	-5.50442200	-0.82110100	H	0.10332300	1.33128900	0.68469600
O	-4.37656900	-4.26794600	-0.90120500	C	-3.94713400	-0.30221400	1.15241800
O	-6.02023700	-6.52430300	-1.69521300	H	-3.93990800	-0.69069900	2.17862200
H	-6.00595800	-3.82227400	-2.09389500	H	-4.84027200	0.31831000	1.05052100
H	-6.17618900	-3.42289600	-0.35895900	S	-2.75879000	2.15597400	1.64003700
H	-6.36746600	-5.78896500	0.23110100	O	-1.55128600	2.91275000	1.26729200
H	-7.57231500	-5.40292700	-1.01268100	O	-3.10682800	1.94099200	3.05830200
H	-3.98597600	-6.05324100	0.09681700	C	-4.16668100	2.99999700	0.88945500
H	-2.81714400	-5.55952200	-1.15087900	C	-5.38769600	3.01787700	1.56632200
H	-4.44135900	-6.02126300	-2.94431500	C	-3.99998600	3.66578200	-0.32656300
H	-4.22001600	-7.47394000	-1.94764000	C	-6.46638600	3.69989100	1.00112700
C	-0.03339500	-3.65005100	2.36466700	H	-5.47131600	2.52448800	2.52852700
C	-1.05187100	-3.91914800	3.49553800	C	-5.08439300	4.34296400	-0.88232200
C	-0.17249900	-4.80323100	1.34034100	H	-3.03158500	3.66909500	-0.81363900
C	1.38352200	-3.68588200	2.99933400	C	-6.31583300	4.35610500	-0.22206100
H	-1.00002800	-3.16792800	4.28893300	H	-7.41996400	3.72504200	1.52015200
H	-2.07902500	-3.96902800	3.12582200	H	-4.96647500	4.86646000	-1.82627200
H	-0.82531100	-4.88694800	3.95539100	H	-7.15695600	4.88744100	-0.65802200
H	0.56460300	-4.74969100	0.53659600	C	-0.14047100	1.28690400	-1.52555100
H	-0.03848600	-5.76325100	1.85122000	C	0.92815100	0.20000200	-1.84966700
H	-1.17162500	-4.79028000	0.89516400	C	-1.37336200	1.20954100	-2.42848300
H	1.56076000	-4.66907900	3.44935500	H	-1.74904100	0.18682300	-2.52374700
H	2.17958600	-3.50077200	2.27444500	H	-2.19497300	1.82880700	-2.05724900
H	1.47691500	-2.93736900	3.79337000	H	-1.11265600	1.56156900	-3.43402000
TS4aa				C	0.41334600	2.71323800	-1.48225000
C	-1.59314900	0.01466800	0.31570900	H	0.68454200	3.04952000	-2.49095200
C	-1.52421300	-1.39901700	-0.08992900	H	-0.32687200	3.40546300	-1.06973900
C	-2.72987900	-2.28009600	0.13141400	H	1.30345100	2.77067800	-0.84804700
C	-2.70222900	0.52226900	0.90276900	C	0.65487900	-0.52593400	-0.49217000
H	-2.81118400	-3.07051700	-0.61255200	C	1.86439200	-0.72299300	0.45400300
H	-2.64761600	-2.78358300	1.10146200	C	1.65523400	-1.44185600	1.62264700
H	-5.84052800	-1.15656700	-3.46314700	C	2.66136300	-1.71855700	2.69686200
C	-4.83983000	-1.59490300	-3.46811500	H	0.65551500	-1.85089700	1.80393300
O	-4.44844100	-1.96610600	-2.13369700	H	1.84567800	0.08368400	1.39541200
H	-4.82623600	-2.51874300	-4.04571700	C	3.04225300	-3.21716500	2.71459500
H	-4.13706000	-0.86970900	-3.88477100	H	3.55592100	-1.11099300	2.52990000

H	2.23320700	-1.44937800	3.67174100	H	1.83711900	-3.95813200	0.40119200
C	4.02281500	-3.54373400	3.84524400	H	-0.05474300	-4.77201100	5.81894000
H	2.13777800	-3.82986400	2.82381700	C	-0.53862700	-5.08150500	4.88973700
H	3.48757600	-3.48254000	1.74851000	O	0.30597600	-4.78349000	3.76247100
H	4.28672700	-4.60582800	3.83962000	H	-0.68210400	-6.16130100	4.87049800
H	4.94876000	-2.96782900	3.74253100	H	-1.49581600	-4.56360200	4.79658200
H	3.59120400	-3.31011200	4.82462300	C	0.63197400	-3.48337100	3.60736000
H	0.73699400	-0.39420100	-2.74831600	C	1.58111000	-3.29971300	2.41262000
H	1.94824000	0.59207900	-1.89450900	O	0.22893500	-2.60786700	4.34101200
Rh	3.68716600	0.21299400	0.09001100	C	2.91653300	-3.98279500	2.76178900
C	4.30678700	-1.12667000	-1.00309600	O	3.57095500	-4.66047500	2.00223700
O	4.75906600	-1.96105400	-1.67182200	O	3.29232000	-3.68599800	4.02015400
Cl	2.90363800	1.88795500	1.70942400	C	4.56135400	-4.22622900	4.43566400
C	6.70086700	3.34858600	-1.13575500	H	5.36279900	-3.84850000	3.79679000
C	5.40447400	2.55786700	-1.06867900	H	4.69876200	-3.89124700	5.46306200
C	6.37636200	1.68730900	0.98251600	H	4.54677200	-5.31725800	4.38220100
C	6.50347400	3.17974200	1.23820300	C	-1.14229900	-3.62565300	-0.28898300
O	5.55821200	1.42014000	-0.19029200	C	-1.50441700	-1.26061200	0.16560000
O	7.09163000	3.86588900	0.13434600	H	-1.36033300	-0.29328100	-0.31258800
H	7.36092200	1.23705700	0.80794300	C	1.86470200	-1.79723600	2.18088000
H	5.89308300	1.19509900	1.82802900	H	2.74684000	-1.70122400	1.53521600
H	5.51537700	3.59309300	1.48058700	H	2.13017600	-1.32466900	3.12710400
H	7.15883700	3.34460100	2.09960000	S	0.73904100	0.70112900	1.66044000
H	4.57576100	3.18159900	-0.71500500	O	0.26469900	1.28018200	0.38571100
H	5.14471500	2.15059800	-2.04879200	O	2.09544500	1.02111700	2.14146700
H	7.49812800	2.70580900	-1.54005800	C	-0.43306600	1.23569100	2.92549900
H	6.57482100	4.19581600	-1.82053000	C	-1.19291400	2.37692000	2.65902200
C	0.09588900	-3.07417100	-1.22343800	C	-0.49765000	0.58812800	4.16200700
C	1.59384400	-3.14017900	-1.58632000	C	-2.03531900	2.87844600	3.65266400
C	-0.18814800	-4.26318600	-0.27105900	H	-1.12080100	2.85121500	1.68653400
C	-0.70373900	-3.26389000	-2.54096900	C	-1.35353100	1.09459400	5.14152600
H	1.89926800	-2.32771400	-2.24832100	H	0.07858000	-0.31044700	4.35310000
H	2.23211300	-3.11276800	-0.70111300	C	-2.11622500	2.23808900	4.89097200
H	1.79936800	-4.08163100	-2.10637800	H	-2.62960000	3.76589600	3.45641700
H	-1.24518000	-4.37989200	-0.02892400	H	-1.42137200	0.59311600	6.10230100
H	0.14539100	-5.19454800	-0.74188300	H	-2.77609400	2.62833900	5.66046200
H	0.36279800	-4.15573700	0.66914600	C	-2.92185700	-1.33029800	0.88795300
H	-0.46110800	-4.23582000	-2.98549800	C	-3.40668100	-2.31308100	-0.21999000
H	-1.78477300	-3.22340900	-2.38932100	C	-2.92739900	-1.94086500	2.29167700
H	-0.44127400	-2.48996300	-3.26912800	H	-2.43235100	-2.91543800	2.31706400
INT-5aa				H	-2.42885000	-1.28986100	3.01598800
C	-0.25273700	-1.75441800	0.82167300	H	-3.96243900	-2.08481400	2.62462200
C	-0.15139800	-3.19403000	0.54926300	C	-3.65692300	0.01224700	0.88545100
Rh	-2.30836300	-2.79285900	-4.18197600	H	-4.70142300	-0.12723500	1.18922500
Cl	-3.99398700	-1.05153900	-4.22593700	H	-3.19578700	0.72080600	1.58027700
C	1.01824900	-3.95240100	1.12975600	H	-3.65953700	0.46581100	-0.11119000
C	0.68076400	-1.09565100	1.54837400	C	-1.95668100	-2.42865800	-0.79545600
H	0.78966900	-4.99660100	1.33104100	C	-1.76624900	-1.87566200	-2.20263400

C	-0.62766000	-1.89828000	-3.01405800	C	0.80147400	-1.13084800	1.96541300
C	-0.12675800	-0.70481400	-3.80114400	H	0.80452400	-5.01785100	1.53749300
H	0.13848200	-2.63782000	-2.77747500	H	1.97871900	-3.96663600	0.78644900
H	-2.38934500	-0.99371400	-2.32794800	H	-0.53361100	-5.02578200	5.89599000
C	0.99175900	0.04488500	-3.04418600	C	-0.94608400	-5.21710200	4.90253700
H	0.26746400	-1.03888100	-4.76935900	O	0.02425400	-4.89933900	3.88816900
H	-0.95933600	-0.02555200	-4.01287600	H	-1.16741200	-6.27627500	4.77477300
C	1.53839100	1.22932400	-3.84770600	H	-1.84842700	-4.61572500	4.77059500
H	0.61878500	0.39944300	-2.07681900	C	0.44761400	-3.61761400	3.87107300
H	1.80884700	-0.65549700	-2.82326400	C	1.52731000	-3.41385500	2.79599000
H	2.32623800	1.74791900	-3.29279400	O	0.02896800	-2.77316300	4.63188500
H	1.96003100	0.90301900	-4.80571900	C	2.78965000	-4.17058300	3.24893900
H	0.74914200	1.95824800	-4.06289200	O	3.49927700	-4.83451900	2.52755800
H	-3.84741100	-3.24116000	0.14841000	O	3.03411900	-3.96166400	4.55701100
H	-4.10052300	-1.86067400	-0.93416600	C	4.22703200	-4.58081000	5.07367900
C	-3.33539200	-2.85392300	-7.14575000	H	5.10807400	-4.20783700	4.54657600
C	-4.14140600	-3.51413900	-8.25209300	H	4.26494500	-4.30726300	6.12748200
C	-5.81404700	-3.43782500	-6.54989200	H	4.17484400	-5.66584000	4.95674100
C	-4.79172600	-4.12084300	-5.65636200	C	-0.89963300	-3.48701300	-0.17882100
O	-5.52769900	-3.62732700	-7.93209300	C	-1.23419500	-1.13746300	0.34941400
O	-3.44217800	-3.63321200	-5.92806500	H	-1.00095800	-0.17152200	-0.09468300
H	-6.79910500	-3.87970200	-6.36906100	C	1.88634300	-1.91422000	2.67933100
H	-5.86691400	-2.37199500	-6.29267700	H	2.83436800	-1.82172500	2.13480000
H	-5.00900300	-3.91542700	-4.60681100	H	2.06780600	-1.50437500	3.67341900
H	-4.78069500	-5.20285700	-5.82993800	S	0.93331900	0.65227800	2.16365400
H	-4.04715800	-2.91981900	-9.16963000	O	0.58814700	1.31403600	0.88979900
H	-3.73026400	-4.51438300	-8.45516200	O	2.25887800	0.88493700	2.76701100
H	-2.27245700	-2.83783400	-7.39820900	C	-0.30714600	1.18225400	3.36566500
H	-3.66852800	-1.83130700	-6.94458800	C	-1.00873500	2.35844400	3.09259500
C	-1.11838400	-4.18812500	-4.41160700	C	-0.48190600	0.49310600	4.56864900
O	-0.39367900	-5.04851600	-4.68221700	C	-1.90279800	2.85337500	4.04370000
C	-1.48162300	-5.10487500	-0.57383700	H	-0.85000300	2.86504400	2.14697800
C	-0.28782900	-5.83052400	-1.24392900	C	-1.38753000	0.99352300	5.50552400
C	-1.82381900	-5.81933000	0.76321000	H	0.04684400	-0.43339300	4.76372100
C	-2.72220300	-5.27974500	-1.47891600	C	-2.09225100	2.17217900	5.24776500
H	-0.02277000	-5.37470500	-2.19946500	H	-2.45156800	3.76850500	3.84148800
H	0.60587000	-5.83446700	-0.61790300	H	-1.53989800	0.45967500	6.43882900
H	-0.55614800	-6.87445700	-1.44037400	H	-2.79136900	2.55757500	5.98441400
H	-2.68901800	-5.35019200	1.24277500	C	-2.69751000	-1.16160700	0.98010600
H	-2.08213500	-6.86534300	0.56223700	C	-3.13826100	-2.14143100	-0.14978400
H	-1.00193600	-5.81168600	1.48110700	C	-2.82473300	-1.76385200	2.38122700
H	-2.81786800	-6.33522900	-1.75567100	H	-2.36381400	-2.75382600	2.44017500
H	-3.64483500	-4.99500500	-0.96752400	H	-2.36075300	-1.12919500	3.14132500
H	-2.65937400	-4.69385900	-2.39825900	H	-3.88560800	-1.87572800	2.63677600
PI^A				C	-3.39043800	0.20143400	0.91378300
C	-0.07938800	-1.71314600	1.11762300	H	-4.45795800	0.10086900	1.14543900
C	0.00278400	-3.14224500	0.78413800	H	-2.95450100	0.90340000	1.63150900
C	1.08760800	-3.97283600	1.42429300	H	-3.30478800	0.64355900	-0.08471700

C	-1.66409900	-2.24860600	-0.66024900	C	6.91079300	-3.80284700	-1.18287400
C	-1.45268400	-1.93132200	-2.12930000	H	6.97519300	-3.71727300	-2.26987600
C	-0.33852100	-1.40012200	-2.64292300	H	7.85957600	-3.53733300	-0.71832100
C	-0.13396800	-1.04737200	-4.09027900	H	6.62405000	-4.82396600	-0.92168100
H	0.49540000	-1.17177000	-1.97622900	C	-0.03343300	-1.28804200	-0.24209200
H	-2.29053200	-2.14110800	-2.79460000	C	0.65626600	1.04839100	-0.19368500
C	0.12753900	0.45487600	-4.31402300	H	0.64037600	1.90009800	-0.86384300
H	0.72572200	-1.61059500	-4.48473000	C	4.15016000	-0.56891900	-1.11716800
H	-1.00657500	-1.36206800	-4.67768700	H	4.25865900	-0.66422400	-2.20491500
C	0.39618000	0.80085500	-5.78161900	H	5.12110500	-0.26036700	-0.72305100
H	-0.73518900	1.02463200	-3.94704900	S	3.67532900	2.15419300	-1.12619900
H	0.98112800	0.76732200	-3.69864400	O	2.62701300	3.11535600	-0.74189900
H	0.57796900	1.87267500	-5.91089400	O	4.20365500	2.13112400	-2.50201500
H	1.27502900	0.26651200	-6.16069800	C	5.07825500	2.40446000	-0.02459600
H	-0.45456100	0.52894800	-6.41720200	C	6.36838100	2.32962300	-0.55309600
H	-3.59897500	-3.07227600	0.19397800	C	4.85694100	2.70966500	1.32035900
H	-3.80294600	-1.67902700	-0.88725000	C	7.45799400	2.55531300	0.28939800
C	-1.14532000	-4.89988900	-0.73572100	H	6.50193400	2.11880600	-1.60851600
C	0.16194500	-5.50157200	-1.30911400	C	5.95334300	2.92938800	2.15225000
C	-1.69542700	-5.80575600	0.39803700	H	3.84642900	2.78868200	1.70491800
C	-2.18537500	-4.92333900	-1.87882500	C	7.25049500	2.85009300	1.63820700
H	0.57831700	-4.84917700	-2.08294100	H	8.46647100	2.50639400	-0.10992000
H	0.92950100	-5.65702400	-0.54941300	H	5.79532200	3.16821800	3.19938700
H	-0.04979000	-6.47483000	-1.76647100	H	8.10097400	3.02532500	2.29046600
H	-2.67506300	-5.45162000	0.73596100	C	0.33401600	1.48627100	1.29157300
H	-1.82025200	-6.83024000	0.02904800	C	-1.15310100	0.98796700	1.34444600
H	-1.03865600	-5.83998800	1.26991000	C	1.15876100	0.73684800	2.34863200
H	-2.39286600	-5.96361600	-2.15160400	H	1.06959100	-0.34834400	2.24728200
H	-3.13439700	-4.46452000	-1.58866400	H	2.22069200	0.99118800	2.28897100
H	-1.81719000	-4.41476400	-2.77209400	H	0.79832400	1.00380500	3.34816000
TS4cc				C	0.44353800	2.99717000	1.53822500
C	1.82594900	0.17160600	-0.48848500	H	0.08184600	3.22776200	2.54690200
C	1.33100800	-1.21058300	-0.47974200	H	1.47634600	3.33876600	1.44699300
C	2.30988000	-2.29288800	-0.85578500	H	-0.15273700	3.57642900	0.82982700
C	3.10423400	0.47381700	-0.80924500	C	-0.55975800	0.11269100	-0.31093400
H	2.08182400	-3.25107300	-0.41177500	C	-1.85110000	0.74902700	-0.29339300
H	2.25790500	-2.44314700	-1.94193500	C	-1.92194700	2.15051200	-0.96237900
H	4.91713500	-3.02774900	3.22675500	C	-3.03563200	3.09156900	-0.48101400
C	3.86602200	-3.19647100	2.98213400	H	-2.07545100	1.94810300	-2.03027100
O	3.66110300	-3.08952400	1.55976800	H	-0.98312200	2.70482900	-0.90302800
H	3.56597500	-4.20995900	3.24541900	C	-3.02092200	4.43242100	-1.22881900
H	3.25457300	-2.46284700	3.51221600	H	-4.00644600	2.60089000	-0.60800100
C	3.99049000	-1.90178300	1.01238300	H	-2.93597000	3.27992700	0.59649000
C	3.77065200	-1.93157800	-0.51229800	C	-4.13007100	5.38283200	-0.76671300
O	4.40235100	-0.95823600	1.64777600	H	-2.04456400	4.92012300	-1.09804900
C	4.68944700	-3.01134900	-1.11027100	H	-3.12365100	4.24777900	-2.30702400
O	4.34446700	-3.85718900	-1.90327400	H	-4.09840500	6.33108300	-1.31342500
O	5.94980600	-2.86352200	-0.66159700	H	-5.12018600	4.94019100	-0.92390400

H	-4.03755900	5.61009000	0.30143100	O	3.14889000	-1.77566600	0.53655200
H	-1.33016000	0.12817200	1.98243700	C	3.55887300	-1.04310600	-2.67187100
H	-1.89883100	1.74171700	1.60261600	O	3.38873400	-1.08895500	-3.87010600
Rh	-3.76601700	-0.03491100	-0.28503700	O	4.76820500	-1.09654100	-2.08395700
C	-3.66752300	-0.23114500	-2.10444000	C	5.88990800	-1.20796200	-2.97861500
O	-3.64945800	-0.31662700	-3.26521000	H	5.93738900	-0.34024500	-3.64089300
Cl	-4.21212000	0.38862300	2.10197000	H	6.77029800	-1.25160400	-2.33844000
C	-7.62780100	-2.38709800	0.27577400	H	5.80685500	-2.11312500	-3.58481500
C	-6.15283600	-2.02237300	0.33856100	C	-1.34350200	-1.26298600	-1.47761900
C	-6.95423600	0.23393200	-0.05274400	C	-1.38097600	0.75184000	-0.11481100
C	-7.82452200	-0.16518000	1.12761800	H	-1.63777200	1.37923200	-0.99020100
O	-5.92330800	-0.75654600	-0.31362900	C	2.55569800	0.51104800	-0.99533000
O	-8.45970500	-1.42702700	0.92494500	H	2.77367300	1.25172600	-1.77443800
H	-7.55727500	0.32861900	-0.96426000	H	3.40626300	0.51304700	-0.31104100
H	-6.44856700	1.17896400	0.15286600	S	1.74679400	2.36055700	0.76858700
H	-7.21644500	-0.16803200	2.04128900	O	0.61086500	2.86450700	1.55476400
H	-8.62419600	0.57229500	1.25249100	O	2.48021800	3.29391000	-0.10812000
H	-5.79361300	-1.96698600	1.37216000	C	2.92731600	1.66822800	1.94350000
H	-5.55189000	-2.75562200	-0.20541700	C	4.16098100	2.30456600	2.08530700
H	-7.93253100	-2.48832500	-0.77741200	C	2.56525800	0.57501300	2.73346400
H	-7.78379100	-3.35765200	0.76375400	C	5.05058100	1.83997200	3.05500700
C	-0.85577100	-2.58538600	-0.04656200	H	4.40629500	3.14355100	1.44307400
C	-1.83953500	-2.41866400	1.13335700	C	3.46951300	0.11688400	3.69094000
C	-1.61420300	-2.92098100	-1.35208000	H	1.61428300	0.07076300	2.58917400
C	-0.01660900	-3.83691100	0.31681700	C	4.70430300	0.74944500	3.85559300
H	-1.30041100	-2.27736100	2.07731400	H	6.01312000	2.32692100	3.18087200
H	-2.53601100	-1.59108300	0.99631800	H	3.21038100	-0.74198600	4.30229600
H	-2.43680200	-3.33093400	1.23200700	H	5.40177100	0.38631400	4.60515700
H	-0.91692000	-3.05088200	-2.18716600	C	-2.16320300	1.47808700	1.03966100
H	-2.16226700	-3.86148300	-1.22373200	C	-3.58887300	0.91973600	0.75320000
H	-2.33360100	-2.14612800	-1.60761100	C	-1.74770900	1.16491400	2.48540200
H	-0.70958200	-4.60889200	0.66404500	H	-1.81223800	0.09684600	2.70703200
H	0.51288700	-4.26461700	-0.53708100	H	-0.73357000	1.50372500	2.68834300
H	0.69394800	-3.65123100	1.12830300	H	-2.42626100	1.69110400	3.16786600
INT-5cc				C	-2.23707500	3.00867500	0.84006700
C	0.06612300	0.40637600	-0.46797300	H	-3.00274000	3.42245000	1.50713700
C	-0.08243300	-0.70979100	-1.45101800	H	-1.29267500	3.49995700	1.05645200
C	1.09013800	-1.01173900	-2.34379600	H	-2.53413800	3.25462900	-0.18716300
C	1.29348400	0.95164000	-0.26924300	C	-2.15788900	-0.52915700	-0.47487400
H	1.03857500	-1.99180500	-2.78921700	C	-3.48780500	-0.38765700	-0.02511300
H	1.10062900	-0.29380500	-3.17446600	C	-4.78586000	-0.75965600	-0.74638100
H	3.45861300	-4.33253600	0.26378200	C	-6.10035000	-0.43889000	-0.00810000
C	2.41722500	-4.25130000	-0.05638200	H	-4.79966900	-1.79911700	-1.07534300
O	2.26423300	-3.17366900	-0.99994900	H	-4.79044400	-0.15814200	-1.66804200
H	2.10648300	-5.15098600	-0.58770400	C	-7.32284600	-1.00395700	-0.74386800
H	1.78098100	-4.07006000	0.81241100	H	-6.08360600	-0.83359400	1.01256400
C	2.65218000	-1.96315400	-0.54848300	H	-6.21373200	0.64727300	0.08843600
C	2.43952700	-0.88072900	-1.62555400	C	-8.64855200	-0.63462800	-0.07132900

H	-7.32426100	-0.64146500	-1.78121700	H	0.55997600	-5.20052300	0.34680500
H	-7.23338200	-2.09689000	-0.80133500	H	0.23497400	-3.74797300	1.35010300
H	-9.50151200	-1.05471200	-0.61393700	C	1.84413200	-2.27246500	-0.16466800
H	-8.68905700	-1.01314800	0.95619900	C	2.19386900	-1.54359300	-1.47301400
H	-8.78362200	0.45221900	-0.02939100	O	2.02550100	-1.85333400	0.95794400
H	-4.18427700	0.82311000	1.66588800	C	3.32576100	-2.32555100	-2.16268800
H	-4.13233500	1.62862600	0.10941100	O	3.37332600	-2.58950700	-3.34259600
Rh	-2.57907500	-1.97490700	1.46097200	O	4.29300700	-2.64574300	-1.28093900
C	-4.30274500	-2.61291700	1.43041700	C	5.43263100	-3.33344400	-1.83010700
O	-5.29485600	-3.21031400	1.49173300	H	5.92382700	-2.71399400	-2.58399300
Cl	-0.15423100	-1.94727500	1.71836100	H	6.09913500	-3.51352400	-0.98738800
C	-1.91325800	-5.48925400	4.24072100	H	5.12491100	-4.27596100	-2.28893500
C	-1.92011200	-4.67397800	2.95808400	C	-1.43742400	-0.54974900	-2.20966100
C	-2.00931700	-2.78162000	4.49337600	C	-1.01425000	1.26002900	-0.63214000
C	-0.81185800	-3.53243700	5.05119700	H	-0.98843100	2.23795300	-1.13178600
O	-2.44024900	-3.34791800	3.22043700	C	2.70281600	-0.11885900	-1.17753100
O	-1.08769500	-4.91669700	5.25216800	H	3.18433700	0.28281700	-2.07646400
H	-2.86343900	-2.83956700	5.17789100	H	3.48053800	-0.16236500	-0.41171500
H	-1.75328600	-1.73710400	4.31280300	S	2.17692700	2.40732600	-0.20940500
H	0.04567600	-3.39161300	4.38075800	O	1.13473800	3.42575000	-0.43468400
H	-0.55246000	-3.11590500	6.02996400	O	3.48253800	2.57155600	-0.87800500
H	-0.91955600	-4.58246600	2.52423100	C	2.50122800	2.35326500	1.56773500
H	-2.59000400	-5.12130300	2.21987200	C	2.63033400	3.58853800	2.21113500
H	-2.94412800	-5.58952600	4.61339200	C	2.68387700	1.15314100	2.25637600
H	-1.53651700	-6.49661700	4.02535400	C	2.95290300	3.61865700	3.56645300
C	-1.89150100	-2.35816800	-2.42689700	H	2.46500300	4.50633300	1.65676300
C	-2.64298300	-3.45903600	-1.64272900	C	3.00172100	1.19991900	3.61687600
C	-2.82898200	-1.67689300	-3.45835100	H	2.56446000	0.19518600	1.76094100
C	-0.84504600	-3.13516400	-3.26270700	C	3.14020900	2.42519000	4.26968300
H	-1.94815100	-4.00714300	-0.99935100	H	3.05279000	4.57338500	4.07433000
H	-3.43569700	-3.07691200	-1.00691900	H	3.13864000	0.27136900	4.16314300
H	-3.08961200	-4.16841200	-2.34835100	H	3.38859800	2.45230600	5.32676200
H	-2.27117000	-0.94877500	-4.05658800	C	-1.56035500	1.47990000	0.82368600
H	-3.23898800	-2.42812800	-4.14283100	C	-3.08459200	1.50928400	0.51004000
H	-3.66745500	-1.15710300	-2.99754400	C	-1.23765000	0.27350200	1.72384400
H	-1.37186700	-3.93120900	-3.79964000	H	-1.59163500	-0.66393400	1.28216700
H	-0.35900200	-2.51849800	-4.02123600	H	-0.16131900	0.18188200	1.89329300
H	-0.08447500	-3.61178500	-2.63882800	H	-1.72168100	0.38890900	2.70032800
P2^A				C	-1.14449600	2.77826900	1.52414800
C	0.26885100	0.52443800	-0.98202700	H	-1.77858900	2.92991300	2.40670000
C	-0.09715300	-0.57337800	-1.89524000	H	-0.10960700	2.75435600	1.86495400
C	0.98341700	-1.48137500	-2.42689700	H	-1.25614400	3.64523500	0.86749200
C	1.57725000	0.79924000	-0.73926500	C	-2.09086000	0.38196000	-1.27349300
H	0.61294200	-2.49319200	-2.58231000	C	-3.27696800	0.52872300	-0.63475000
H	1.35984700	-1.13458900	-3.39474400	C	-4.62626100	-0.12182200	-0.78956000
H	1.86325200	-4.46385400	1.33724000	C	-4.93716000	-1.17240400	0.30085200
C	0.97217500	-4.26984600	0.73559400	H	-4.74827400	-0.59085200	-1.76741700
O	1.30928200	-3.48294800	-0.42105900	H	-5.39485000	0.66376200	-0.73393200

C	-6.34188900	-1.77388600	0.16598500	H	-5.90617900	1.65801500	2.49239400
H	-4.18739300	-1.97345900	0.25312400	C	-5.28361600	3.89792100	4.03951000
H	-4.83166800	-0.71876800	1.29434400	H	-4.87853200	1.90586800	4.77869100
C	-6.65558500	-2.81711400	1.24325200	H	-3.48398600	2.69845600	4.06609800
H	-7.08580000	-0.96680900	0.20904600	H	-5.07624200	4.39448800	4.99292700
H	-6.44802900	-2.23034000	-0.82771500	H	-4.96625100	4.57304100	3.23669800
H	-7.66366000	-3.22679200	1.12186300	H	-6.36954900	3.77582600	3.95738800
H	-5.94948500	-3.65440200	1.20216000	C	-2.77328400	-4.40586400	-3.53822800
H	-6.59223900	-2.38173800	2.24702600	C	-3.42381900	-4.65369400	-2.46380700
H	-3.68560400	1.25557200	1.39236000	C	-2.50828400	-6.16374200	-6.07517500
H	-3.39341800	2.52322800	0.20843200	O	-3.43417300	-6.30400300	-6.84263500
C	-2.15734500	-1.30645600	-3.33738300	O	-1.97536800	-7.15440100	-5.34687400
C	-2.87429900	-2.55579700	-2.76969400	C	-0.39077800	-4.88399800	-6.50517100
C	-3.16198800	-0.34211600	-4.01924500	O	0.59355600	-4.28915900	-6.11442900
C	-1.22057200	-1.78016200	-4.47474900	O	-0.42263800	-5.61520600	-7.62835700
H	-2.14613600	-3.25253400	-2.34091000	C	-2.65060200	-8.42780500	-5.44666700
H	-3.59464500	-2.30854300	-1.98908200	H	-2.66822200	-8.76621800	-6.48488600
H	-3.40929700	-3.07951200	-3.57025500	H	-2.07026400	-9.11090800	-4.82698400
H	-2.62253600	0.45460300	-4.54239000	H	-3.66998600	-8.32573500	-5.06887600
H	-3.75455400	-0.88704100	-4.76209600	C	0.80048700	-5.65413900	-8.38993800
H	-3.84531600	0.13699700	-3.32052300	H	0.58559000	-6.28527500	-9.25109600
H	-1.83486300	-2.11062500	-5.31902700	H	1.08033400	-4.64767200	-8.70904100
H	-0.57835300	-0.97027700	-4.83305600	H	1.60845100	-6.07856300	-7.78999900
H	-0.58998600	-2.62444100	-4.19441200	S	-2.62159600	-0.84514400	-6.32477100
TS1b				O	-2.30066800	-1.07328900	-7.74572300
C	-1.76619600	-4.83117400	-5.82126500	O	-3.74826300	0.03241300	-5.95534400
C	-2.56973100	-3.66564200	-6.49936400	C	-1.14393600	-0.18185300	-5.52904000
H	-2.03278800	-3.28559700	-7.36938800	C	0.03505300	-0.93215400	-5.49489000
H	-3.49063800	-4.10127500	-6.89274900	C	-1.19288600	1.12251500	-5.03449600
C	-1.52554500	-4.59905100	-4.31115600	C	1.17603500	-0.36595400	-4.92616600
H	-0.99022300	-5.45937100	-3.89974200	H	0.07829600	-1.93975100	-5.89506700
H	-0.87628400	-3.72455700	-4.20937200	C	-0.03986800	1.68050400	-4.47940900
C	-2.91934800	-2.49987600	-5.60491500	H	-2.11990200	1.68175300	-5.09346200
C	-3.54695800	-2.55746600	-4.43031700	C	1.13986000	0.93659400	-4.42075700
C	-4.32812700	-1.86798200	-3.49032400	H	2.09384300	-0.94434700	-4.88508500
H	-5.14123600	-1.32602600	-3.97182400	H	-0.06623100	2.69495200	-4.09316100
C	-3.86678800	-1.15286300	-2.19897700	H	2.03350700	1.37206600	-3.98337900
C	-4.81671300	-1.53573000	-1.01938800	C	-4.02109700	0.36355400	-2.46993700
H	-5.85255500	-1.34465600	-1.33016500	H	-5.06037000	0.61974300	-2.70443100
H	-4.74551500	-2.61452400	-0.84793800	H	-3.72632200	0.93037400	-1.58219300
C	-4.55337700	-0.82605900	0.23378000	H	-3.40387800	0.67608100	-3.31327600
C	-4.33804200	-0.24944700	1.27679900	C	-2.40375700	-1.44257800	-1.82489700
C	-4.10203900	0.46231500	2.53436700	H	-2.23998200	-2.49674500	-1.59648000
C	-4.82887300	1.82120000	2.62054400	H	-1.72988000	-1.16272300	-2.64025700
H	-3.02251400	0.61955900	2.66801000	H	-2.13074900	-0.85731200	-0.94232100
H	-4.41819000	-0.17103600	3.37506300	Rh	-4.93986000	-3.98969500	-3.66371000
C	-4.56549000	2.54801600	3.94404900	Cl	-5.52880300	-6.40056900	-3.88315600
H	-4.51071500	2.45044500	1.77983200	C	-6.61613100	-3.86945900	-2.61224100

O	-7.53788000	-3.82480400	-1.93391800	H	-0.45006200	7.44174800	7.06125200
C	-3.42917200	-5.28983500	-1.13062200	H	-2.21656400	7.42536900	7.12199800
H	-4.14899200	-6.11380700	-1.12516300	C	1.19415400	-1.67400900	0.57488900
H	-2.43418800	-5.68143000	-0.88904500	C	0.30553700	-2.45570100	1.24034200
H	-3.71656300	-4.58169800	-0.34542800	C	1.38407600	-2.87582400	-2.08320000
C	-6.62658400	-3.98278400	-8.03109200	O	0.41913500	-2.47438900	-2.69568800
C	-6.50640800	-4.56094900	-6.62790600	O	1.62364200	-4.16549300	-1.80354100
C	-7.21941700	-2.48015500	-5.74833200	C	3.84641000	-2.40821100	-2.08343600
C	-7.32059200	-1.92482400	-7.16352100	O	4.84756200	-2.62011000	-1.43704200
O	-6.20206500	-3.49416400	-5.69694600	O	3.78571100	-2.48173400	-3.42719400
O	-7.61891000	-2.96188900	-8.08665600	C	0.61942100	-5.10271900	-2.26138300
H	-6.93379600	-1.69810400	-5.04117700	H	0.50107500	-5.02342500	-3.34427500
H	-8.18097200	-2.91500100	-5.43800700	H	0.99985200	-6.08601900	-1.98668900
H	-8.13203000	-1.19310500	-7.22901800	H	-0.33330600	-4.89894800	-1.76730900
H	-6.37360100	-1.42639500	-7.42519800	C	5.00863700	-2.86123900	-4.08561000
H	-7.44603800	-5.03930700	-6.32304500	H	4.77530100	-2.87599700	-5.14963500
H	-5.69867400	-5.28875600	-6.55232400	H	5.79781500	-2.13607200	-3.87324600
H	-5.65272700	-3.58177000	-8.35497600	H	5.33240300	-3.84827100	-3.74748300
H	-6.93239800	-4.76301500	-8.73449800	S	0.62076000	1.72180500	-1.76671900
INT-2b				O	0.12053600	1.38093700	-3.11304800
C	2.49424100	-1.97825200	-1.50045900	O	-0.24669500	2.47830900	-0.84176200
C	2.22819000	-0.50575400	-1.89079700	C	2.12054200	2.69864200	-2.00968300
H	3.17495900	0.04745800	-1.83907500	C	2.68462000	2.76199100	-3.28521100
H	1.89270600	-0.47820700	-2.93031300	C	2.67019100	3.40071200	-0.93373200
C	2.52895100	-2.12260200	0.04242100	C	3.82907200	3.53689700	-3.48164200
H	2.75765000	-3.15272100	0.31345900	H	2.21612100	2.22553900	-4.10307100
H	3.33889500	-1.48925900	0.42214800	C	3.81568100	4.16800500	-1.14200600
C	1.19566600	0.18633900	-1.01553200	H	2.20123700	3.35735700	0.04261100
C	0.69411100	-0.34389100	0.13792100	C	4.39483600	4.23425600	-2.41244300
C	-0.44789000	0.15091300	0.98547200	H	4.27369600	3.59934900	-4.47031500
H	-1.05189000	0.86722900	0.43353900	H	4.25119700	4.72057200	-0.31498200
C	-0.14702900	0.76130800	2.38655500	H	5.28487000	4.83650600	-2.56954500
C	-1.49532900	1.36123200	2.90749100	C	0.85173700	1.93150900	2.20579700
H	-1.86768800	2.06956600	2.15481100	H	0.47892900	2.65412500	1.47624400
H	-2.24447900	0.56341700	2.97553800	H	0.99769600	2.44242200	3.16210900
C	-1.41627400	2.04062800	4.20145500	H	1.82364100	1.56136700	1.86349100
C	-1.36462200	2.59816100	5.27524200	C	0.43615000	-0.19739300	3.43816900
C	-1.31675000	3.30115200	6.55889900	H	-0.22986300	-1.03858500	3.64741000
C	-1.33472700	4.83774000	6.41795800	H	1.40176300	-0.60080300	3.12411000
H	-0.41497600	2.99757600	7.10894200	H	0.58381500	0.34527000	4.37627100
H	-2.16651000	2.98369300	7.17934800	Rh	-1.43898500	-1.70529800	0.67913400
C	-1.29301900	5.55795600	7.77042600	Cl	-2.35027000	-3.88354200	-0.11369800
H	-0.48105500	5.14917100	5.80293500	C	-2.31201200	-1.88147000	2.26327000
H	-2.23545700	5.13381100	5.86591500	O	-2.87839300	-2.07511800	3.24755000
C	-1.31135400	7.08390200	7.63673400	C	0.49714700	-3.74098600	1.96315300
H	-2.14692000	5.23326100	8.38074600	H	-0.18086200	-4.50489500	1.57179300
H	-0.39288600	5.24851400	8.31927000	H	1.53286300	-4.09160400	1.89454200
H	-1.28219100	7.57125500	8.61667100	H	0.26397700	-3.60862900	3.02719500

C	-3.15097100	-0.21179400	-3.27586900	C	2.45332800	4.82506200	-0.39208600
C	-2.98981800	-1.27508800	-2.20000600	C	3.88341100	3.07605800	0.52024900
C	-3.82121900	0.28981900	-0.59787900	C	2.86324600	5.68577500	0.62776800
C	-3.96794700	1.31872300	-1.71252500	H	1.74786300	5.14198900	-1.15191700
O	-2.75633200	-0.62762600	-0.91902800	C	4.27723500	3.94380100	1.53885000
O	-4.22124400	0.67697800	-2.95299900	H	4.25363200	2.05803000	0.49744100
H	-3.55273400	0.76544500	0.34852800	C	3.77267800	5.24594200	1.59168600
H	-4.75241000	-0.27945300	-0.47038700	H	2.47214800	6.69817500	0.66716600
H	-4.82078700	1.97404500	-1.50730800	H	4.97937700	3.59988400	2.29236300
H	-3.05403000	1.92967200	-1.76794100	H	4.08735400	5.91700900	2.38574900
H	-3.88711400	-1.89869300	-2.11541400	C	-0.75977500	1.73760200	0.90368800
H	-2.12475900	-1.91195300	-2.38730300	C	-1.26639700	0.40575900	1.53086300
H	-2.21146400	0.34541700	-3.39718600	C	0.47518600	2.21808100	1.69467300
H	-3.40944700	-0.68577100	-4.22776700	H	1.30747100	1.51330700	1.63019900
TS2bb				H	0.82528000	3.18623200	1.32859600
C	0.71476800	0.54655800	-0.84585000	H	0.21359500	2.34091800	2.75239300
C	0.34131700	-0.86632800	-0.70387900	C	-1.84573300	2.82204500	1.01741000
Rh	-2.01222300	0.43523800	-1.65650900	H	-2.03745900	3.06586400	2.06841800
Cl	-3.63490300	-0.98782100	-2.97397700	H	-1.52017700	3.73925800	0.51570000
C	1.38852600	-1.95567800	-0.72013800	H	-2.78950200	2.50985000	0.56393500
C	1.98967500	0.85825000	-1.22631800	C	-1.51334100	-2.58199200	-0.80862800
H	1.15445200	-2.72285900	0.02356800	H	-1.09037400	-3.12494300	-1.66249900
H	1.38120600	-2.47266700	-1.68746800	H	-1.23454500	-3.13435300	0.09922200
H	4.11091200	-1.76140300	3.32222100	H	-2.59743400	-2.60202800	-0.91737400
C	3.04168400	-1.92575000	3.16949000	C	-2.15322000	-0.19271800	0.49645100
O	2.75878600	-2.11372800	1.77119900	C	-3.29225600	0.08400800	-0.03163100
H	2.71925000	-2.84384100	3.65969100	C	-4.76121500	0.18807900	0.05027200
H	2.49133200	-1.06652700	3.55996900	C	-5.31845700	-0.09838600	1.45691600
C	3.09655400	-1.08648100	0.96543800	H	-5.18793100	-0.49988800	-0.69050100
C	2.82066400	-1.43250200	-0.50575500	H	-5.06284800	1.19124100	-0.28235700
O	3.56965700	-0.04960100	1.37869700	C	-6.84814200	0.00793700	1.50415600
C	3.81832300	-2.52718700	-0.93081600	H	-5.00715400	-1.10336600	1.76897800
O	3.56350200	-3.44835400	-1.67320600	H	-4.87810100	0.60413600	2.17673800
O	5.03869800	-2.29716900	-0.41068400	C	-7.42404700	-0.27006700	2.89594800
C	6.06635900	-3.23018200	-0.79622300	H	-7.15144100	1.01084000	1.17475900
H	6.20140000	-3.22020700	-1.88002300	H	-7.27980800	-0.69422900	0.77897100
H	6.97127700	-2.89208800	-0.29271800	H	-8.51558700	-0.18878100	2.89719400
H	5.80102900	-4.24128600	-0.47890100	H	-7.16516300	-1.27838700	3.23826000
C	-0.99581300	-1.17057100	-0.77271300	H	-7.03679100	0.44027800	3.63531700
C	-0.43091900	1.49679200	-0.61388700	H	-0.43080700	-0.25635100	1.77377600
H	-0.25911400	2.45450600	-1.09985700	H	-1.83754500	0.60154700	2.44596300
C	3.06356000	-0.19936900	-1.40760900	C	-3.04088700	2.01508300	-2.31235200
H	3.09095200	-0.53986900	-2.45100200	O	-3.72366500	2.88510200	-2.61002700
H	4.05002500	0.21584200	-1.20164200	C	-0.70053200	1.64624500	-4.42905000
S	2.50182900	2.47804700	-1.82764900	C	0.44365000	1.64929300	-5.43399000
O	1.36245000	3.16050400	-2.48329700	C	0.59773500	-0.67073300	-5.32234600
O	3.72487800	2.22951300	-2.61403300	C	-0.55156600	-0.72651900	-4.32560700
C	2.96733700	3.52741300	-0.43271500	O	0.46460500	0.44404700	-6.19070400

O	-0.59332900	0.49863300	-3.55492100	H	3.91155800	2.00138600	0.68307800
H	1.56039500	-0.62386000	-4.78607800	C	3.72258200	5.21216900	1.79757500
H	0.59062900	-1.56978800	-5.94680500	H	2.59196100	6.79396600	0.86182600
H	-1.51312900	-0.86259600	-4.83074900	H	4.73854000	3.44655500	2.50857200
H	-0.41738200	-1.53666500	-3.60735400	H	4.08094800	5.84037000	2.60799400
H	0.31096200	2.47145600	-6.14390400	C	-1.03451700	1.79296400	0.95257800
H	1.39672900	1.79298000	-4.90538900	C	-1.49178200	0.46394100	1.64501800
H	-0.63907700	2.52669300	-3.78978100	C	0.15479500	2.37220300	1.75029900
H	-1.66926200	1.60584200	-4.94527500	H	1.01619900	1.69896500	1.74401300
INT-3bb				H	0.47640200	3.33595200	1.34711700
C	0.55877200	0.62508300	-0.70168100	H	-0.14275400	2.53125800	2.79369700
C	0.23820900	-0.80650700	-0.52809400	C	-2.17114400	2.82917700	0.97677900
Rh	-2.02949200	0.31418200	-1.74308600	H	-2.43843000	3.08806700	2.00742000
Cl	-3.39276800	-1.41157200	-2.90375800	H	-1.85754200	3.74809700	0.47008100
C	1.28830800	-1.83905600	-0.86155200	H	-3.07003600	2.46879500	0.47356700
C	1.80923500	0.97977400	-1.13564400	C	-1.45356900	-2.67993000	-0.39053200
H	1.12425100	-2.75244300	-0.28814500	H	-0.99266300	-3.16415000	-1.25374800
H	1.21648600	-2.12562400	-1.91745800	H	-1.15534800	-3.23065000	0.51273400
H	4.11423100	-2.07169200	3.11298700	H	-2.53471400	-2.76796300	-0.49770300
C	3.05343200	-2.27481400	2.94883100	C	-2.06780200	-0.39993200	0.54587100
O	2.76106000	-2.30074800	1.53980200	C	-3.15843000	0.01602600	-0.13407300
H	2.78862800	-3.26386500	3.32116300	C	-4.59538800	0.29166500	0.08873700
H	2.46236300	-1.50356300	3.44824200	C	-5.09334600	0.08610700	1.53069400
C	3.02136200	-1.16168800	0.86863200	H	-5.12841400	-0.39578700	-0.58682700
C	2.72201200	-1.33467000	-0.62818900	H	-4.85593400	1.29537300	-0.27407100
O	3.44321400	-0.15809100	1.40197300	C	-6.61975300	0.19903600	1.63758500
C	3.70951400	-2.36568000	-1.20352800	H	-4.76835600	-0.90074200	1.88338900
O	3.42665700	-3.21775200	-2.01488900	H	-4.62644000	0.82540600	2.19394000
O	4.95128000	-2.16035100	-0.72647100	C	-7.13464400	-0.00156400	3.06625100
C	5.97276900	-3.03059100	-1.25143700	H	-6.93862300	1.18235700	1.26669400
H	6.05272500	-2.91206400	-2.33427600	H	-7.08192100	-0.54208900	0.97230700
H	6.89649400	-2.72463200	-0.76182000	H	-8.22532400	0.07934500	3.11034300
H	5.73904700	-4.07277300	-1.02232000	H	-6.85843000	-0.98964600	3.45138100
C	-1.06302100	-1.22084300	-0.26301900	H	-6.71784200	0.74813700	3.74846700
C	-0.61591600	1.53927000	-0.53900900	H	-0.63926500	-0.04838000	2.10600800
H	-0.45201900	2.49277000	-1.03030000	H	-2.22526400	0.68049000	2.42827000
C	2.93078500	-0.00965500	-1.38534100	C	-3.02974900	1.68626200	-2.57026300
H	2.99492000	-0.22927200	-2.45840100	O	-3.71620400	2.48932200	-3.02162100
H	3.89562700	0.41719900	-1.10941600	C	-0.23911000	1.45839200	-4.54372000
S	2.26579800	2.63532800	-1.69748200	C	0.98704000	1.34402500	-5.43986600
O	1.09628800	3.35688200	-2.25041000	C	0.80329700	-0.98776200	-5.42187100
O	3.43861300	2.43642200	-2.57154200	C	-0.42748400	-0.89579200	-4.52934200
C	2.80470400	3.60225800	-0.26841700	O	0.92866300	0.16669200	-6.24005400
C	2.41869600	4.94403400	-0.22239800	O	-0.34845500	0.28626000	-3.70998900
C	3.64425800	3.05164600	0.70267800	H	1.70605600	-1.11681000	-4.80032700
C	2.88538600	5.74931000	0.81755200	H	0.72096400	-1.84857200	-6.09320900
H	1.76037600	5.33675100	-0.98913500	H	-1.34344600	-0.85912100	-5.13166300
C	4.09562600	3.86710000	1.74116800	H	-0.50355700	-1.74800000	-3.85169100

H	1.03369200	2.19386200	-6.12759900	C	-0.83262400	1.42892000	1.71630400
H	1.89869100	1.34777100	-4.82218800	C	-2.01782200	0.50549900	1.90638200
H	-0.14628700	2.31461700	-3.87508600	C	0.35826300	0.94561400	2.56530800
H	-1.14807400	1.54804500	-5.15690800	H	0.66052300	-0.07073000	2.29677800
TS3b				H	1.22546800	1.59616500	2.43810100
C	0.58299300	0.66783900	-0.35302900	H	0.08860100	0.94809600	3.62851000
C	0.37727900	-0.79865100	-0.51815300	C	-1.27518500	2.82779000	2.20255200
Rh	-2.21099100	0.44135100	-0.61744800	H	-1.59268900	2.79966600	3.25119700
Cl	-4.03621200	-1.00276700	-1.51699100	H	-0.44278900	3.53284400	2.11920800
C	1.40278800	-1.52059000	-1.37545100	H	-2.10614800	3.21141500	1.60168700
C	1.71120500	1.23501600	-0.88498800	C	-1.00237500	-2.90365100	-0.75862300
H	1.39868700	-2.58953400	-1.18014800	H	-0.47136500	-3.06451000	-1.69500300
H	1.15383000	-1.38008500	-2.43403800	H	-0.73670400	-3.70649600	-0.05921500
H	4.75231500	-2.54796300	2.05707000	H	-2.07197800	-2.96809400	-0.97185700
C	3.71742100	-2.86904600	1.91840400	C	-1.75030400	-1.29854800	0.91052100
O	3.25906500	-2.52868400	0.59749200	C	-2.64293400	-2.01007700	1.43209800
H	3.63789300	-3.95357400	1.98579800	C	-3.81551000	-2.56477200	2.07441000
H	3.09228400	-2.38961100	2.67557900	C	-3.85686300	-2.41888000	3.61461000
C	3.30695600	-1.21883300	0.28197800	H	-3.87761000	-3.63317700	1.81350800
C	2.83014500	-0.99574900	-1.16279300	H	-4.69709000	-2.10046200	1.60549700
O	3.68343100	-0.36079200	1.05038500	C	-5.11073400	-3.06369800	4.21831500
C	3.78161000	-1.75507500	-2.10276800	H	-2.95699100	-2.87482200	4.04551200
O	3.43675400	-2.48990800	-2.99962000	H	-3.82999600	-1.35510900	3.88058700
O	5.06424200	-1.45784000	-1.81921800	C	-5.17801900	-2.91899900	5.74149800
C	6.04860200	-2.07249300	-2.67258900	H	-6.00289800	-2.61256000	3.76488100
H	5.89153700	-1.77270700	-3.71107900	H	-5.13473300	-4.12757500	3.94690200
H	7.01226600	-1.71597500	-2.31080000	H	-6.08081500	-3.38903600	6.14349600
H	5.98691000	-3.16101600	-2.60244400	H	-4.31431300	-3.38968400	6.22451600
C	-0.73309400	-1.53444200	-0.13800700	H	-5.19145100	-1.86475500	6.04006200
C	-0.55915400	1.46779300	0.18353600	C	-3.16700500	2.00541800	-0.88653300
H	-0.49464900	2.49247900	-0.16491500	O	-3.79766200	2.95460500	-1.06700600
C	2.86890800	0.49366700	-1.51327000	C	-0.85505000	1.56648500	-3.98493200
H	2.83645000	0.60477900	-2.60461000	C	-0.10675300	1.39394800	-5.30121800
H	3.81736700	0.92859700	-1.19749500	C	-1.09499900	-0.71315600	-5.58922800
S	1.95698200	3.02929600	-1.06308800	C	-1.84643900	-0.54294300	-4.27443500
O	0.72519400	3.68179100	-1.55692000	O	-0.82828700	0.54920200	-6.19135500
O	3.19473700	3.17970500	-1.84980600	O	-1.08629000	0.28522300	-3.38518600
C	2.29358800	3.69660800	0.57865100	H	-0.15035200	-1.25486300	-5.40972000
C	1.68591500	4.90203600	0.93344700	H	-1.69255500	-1.28505600	-6.30651800
C	3.23557700	3.07991200	1.40760200	H	-2.82951000	-0.08632300	-4.45302600
C	2.02520300	5.49980100	2.14922000	H	-2.00635800	-1.49541100	-3.76496800
H	0.96369500	5.35425700	0.26229700	H	0.01817700	2.35637500	-5.80709300
C	3.55797400	3.68468700	2.62313300	H	0.89294000	0.97103500	-5.10262900
H	3.68902700	2.13386400	1.12871800	H	-0.28308800	2.16348300	-3.27100300
C	2.95826500	4.89228600	2.99176000	H	-1.81940600	2.06353100	-4.17114100
H	1.56055900	6.43871900	2.43512100	H	-1.97659300	-0.07812900	2.81746300
H	4.28113800	3.21175900	3.28073000	H	-3.00241400	0.93965100	1.76231600
H	3.21904200	5.35933700	3.93702700				

INT-3b

C	0.88646400	0.40749000	-0.17134400	H	0.10262400	0.33125100	3.94397100
C	0.82415000	-1.06815800	-0.06855300	C	0.31495000	2.63473600	2.63003400
Rh	-2.20721700	1.03144500	0.12300400	H	0.08488300	2.73607200	3.69732100
Cl	-4.72309600	1.45485400	-0.03228400	H	1.40328100	2.64606900	2.51278500
C	2.05319800	-1.91275900	-0.35503800	H	-0.08408500	3.51656200	2.11905400
C	1.89981400	0.92061100	-0.93672200	C	-0.36312300	-3.26394000	0.22297800
H	2.22771500	-2.61471300	0.46586700	H	-0.03596100	-3.69858000	-0.72890300
H	1.87497100	-2.53516000	-1.23943900	H	0.30662100	-3.65299300	0.99883300
H	5.89838600	-0.96360200	2.51184200	H	-1.36870200	-3.62998300	0.43090400
C	4.90880300	-1.37287900	2.72764600	C	-1.61196300	-1.13764200	0.39067200
O	4.21885900	-1.68611400	1.50385800	C	-2.81935700	-1.13656600	0.68127100
H	4.99067200	-2.31583600	3.26721600	C	-4.17165000	-1.48319600	1.13400000
H	4.34102900	-0.64392100	3.31055900	C	-4.27176700	-2.95875400	1.57485500
C	4.02440700	-0.65002000	0.66340600	H	-4.88933900	-1.26171000	0.33722700
C	3.33831700	-1.12102300	-0.62852700	H	-4.45405600	-0.81449500	1.95624800
O	4.37563200	0.48159300	0.91448600	C	-5.68118400	-3.31677100	2.06383100
C	4.33359400	-2.02673100	-1.38285100	H	-3.99875200	-3.61028800	0.73420900
O	4.04208900	-3.04079700	-1.97586100	H	-3.54297600	-3.15434400	2.37198900
O	5.57448000	-1.50892000	-1.34368500	C	-5.80507400	-4.77818000	2.50567100
C	6.58018600	-2.23978400	-2.07170700	H	-5.95239400	-2.65209000	2.89704300
H	6.31780600	-2.29437400	-3.13054300	H	-6.40406000	-3.10985800	1.26397400
H	7.50449300	-1.68047600	-1.93280100	H	-6.81941400	-5.00366700	2.84962900
H	6.67637300	-3.25292900	-1.67463800	H	-5.57328800	-5.46342300	1.68235000
C	-0.33298000	-1.74359500	0.17531100	H	-5.11708000	-5.00435500	3.32826000
C	-0.11423400	1.28073100	0.50708400	C	-2.29413900	2.90327800	-0.23127100
H	0.06508900	2.29645600	0.17863000	O	-2.36157000	4.02916800	-0.42731800
C	3.00508100	0.07943300	-1.53490300	C	-2.05810900	1.50667800	-3.23532800
H	2.70514700	-0.30588900	-2.51904000	C	-1.81106700	0.93742100	-4.62486200
H	3.89258200	0.68823200	-1.70041000	C	-3.09695300	-0.94228900	-4.11299700
S	1.96550800	2.64403900	-1.53735100	C	-3.36235600	-0.39774400	-2.71513300
O	0.61969800	3.03235000	-2.01428000	O	-2.89089100	0.11045200	-5.04421900
O	3.09383000	2.68066000	-2.48487000	O	-2.26284000	0.43067300	-2.29435100
C	2.37198500	3.76627500	-0.18511500	H	-2.21741600	-1.60816000	-4.09002200
C	1.57468900	4.90008000	-0.01790000	H	-3.95969500	-1.51678300	-4.46557400
C	3.52371000	3.55871500	0.57750200	H	-4.28784900	0.18968800	-2.68563800
C	1.93513500	5.84280000	0.94626000	H	-3.43383100	-1.20826600	-1.98655400
H	0.69366000	5.03130400	-0.63613100	H	-1.72551100	1.74682700	-5.35606700
C	3.86366200	4.50444700	1.54527400	H	-0.86953300	0.36373700	-4.62604000
H	4.12689200	2.66919100	0.43866300	H	-1.19182600	2.06961700	-2.88576800
C	3.07488100	5.64384400	1.72777100	H	-2.95005200	2.14904500	-3.24234500
H	1.32481700	6.73014200	1.08472600	H	-2.30364600	0.55918200	2.67861500
H	4.75006800	4.35195400	2.15369900	H	-2.25906800	2.33289900	2.44743200
H	3.35055600	6.37803000	2.47928000	TS3bb			
C	-0.29675400	1.33643000	2.07340300	C	-0.20000800	-1.35340700	0.47358600
C	-1.83636400	1.37884700	2.13031400	C	0.06230900	-2.76013100	0.13302200
C	0.27418200	0.15650500	2.87585300	Rh	-0.89748400	-0.46357000	-2.55557700
H	-0.19074800	-0.79534200	2.61729700	Cl	-0.18786900	-0.24860600	-4.87869200
H	1.35560100	0.06129800	2.72529200	C	1.24503700	-3.48762400	0.72455100

C	0.63820800	-0.69599900	1.31478600	C	-0.70853600	-4.70819800	-1.30674700
H	1.02471100	-4.54328600	0.89568500	H	-0.14521600	-5.36192000	-0.63809600
H	2.07730200	-3.46657000	0.01175100	H	-1.71895900	-5.12028200	-1.41230500
H	0.39202300	-4.67468700	5.39045200	H	-0.23861500	-4.76194900	-2.29692700
C	-0.05961400	-5.00195600	4.45109100	C	-1.77091300	-2.38887600	-1.46356200
O	0.72420200	-4.54788800	3.33288700	C	-1.59802000	-2.15014000	-2.86009000
H	-0.06320700	-6.08942600	4.38404000	C	-1.96125400	-2.93471800	-4.07608600
H	-1.07705000	-4.60856800	4.38982100	C	-3.27357300	-2.43512000	-4.73344500
C	0.87094200	-3.21152500	3.22751600	H	-2.06770000	-3.99907700	-3.82573500
C	1.76782900	-2.85720900	2.03065600	H	-1.15787200	-2.81924400	-4.81143300
O	0.36276400	-2.42653300	3.99768400	C	-3.62324100	-3.23618000	-5.99303000
C	3.17346700	-3.42124900	2.31885700	H	-4.10071500	-2.49998900	-4.01373600
O	3.86076900	-4.02153500	1.52447300	H	-3.14332900	-1.37777200	-4.98473200
O	3.55989800	-3.11718800	3.57157000	C	-4.90902400	-2.74619700	-6.66709100
C	4.88846100	-3.54063300	3.93404700	H	-2.78793900	-3.16707100	-6.70161600
H	5.62721600	-3.07111400	3.28078200	H	-3.72453800	-4.30010000	-5.73726100
H	5.02642900	-3.21753500	4.96513400	H	-5.13213700	-3.32683500	-7.56818800
H	4.97763700	-4.62637600	3.85242400	H	-5.76986600	-2.83337200	-5.99397300
C	-0.75482900	-3.28885200	-0.80621600	H	-4.82328300	-1.69437900	-6.96098700
C	-1.40916700	-0.77735700	-0.18206700	H	-3.43412000	-3.29227800	-0.37035700
H	-1.33795800	0.30280000	-0.21679900	H	-3.91211100	-2.00333800	-1.48945800
C	1.89259800	-1.32356600	1.88502200	C	2.35139600	-0.89502000	-2.46276900
H	2.72804600	-1.09522700	1.20838600	C	3.81761700	-0.56005800	-2.13606700
H	2.14315600	-0.88292800	2.84898500	C	3.28541100	1.41720000	-0.99178800
S	0.47889900	1.07209300	1.71181100	C	2.06589400	1.40255500	-1.93674600
O	0.04401300	1.82575000	0.51521800	O	3.88963400	0.12261200	-0.89527200
O	1.74713600	1.44545400	2.36466500	O	1.47224800	0.10007600	-1.90699900
C	-0.83946500	1.25913200	2.93070800	H	4.02208200	2.15521300	-1.34993400
C	-1.84104400	2.19728900	2.67172000	H	2.99164500	1.68414700	0.02524300
C	-0.79136400	0.55231000	4.13499100	H	1.30514300	2.09875200	-1.58531200
C	-2.82077500	2.42553000	3.63991400	H	2.33759800	1.65996200	-2.96911500
H	-1.83669900	2.73781500	1.73188200	H	4.40679300	-1.47676400	-2.03998300
C	-1.78312700	0.78447700	5.08838400	H	4.27300000	0.04505300	-2.93589100
H	-0.01929000	-0.18593500	4.31548800	H	2.18578900	-0.97238000	-3.54477300
C	-2.79296200	1.71922400	4.84400900	H	2.04991600	-1.83495500	-1.99196900
H	-3.60207700	3.15589800	3.45223100	C	-1.63069100	1.39444000	-2.63048000
H	-1.76315200	0.23466100	6.02445500	O	-2.32171900	2.27935100	-2.88195200
H	-3.55814200	1.89785000	5.59392500	INT-4bb			
C	-2.84793500	-1.23047200	0.27642700	C	-0.30520500	-1.64461400	0.94850800
C	-3.14023900	-2.31828500	-0.78147600	C	0.11041000	-3.00388600	0.59099100
C	-2.89948400	-1.76714900	1.71623100	Rh	-2.85855300	-2.46148200	-3.64858300
H	-2.24042400	-2.62879300	1.85374200	Cl	-2.90327200	-0.16784500	-4.36674000
H	-2.61177400	-1.00211400	2.44204500	C	1.34045700	-3.61646400	1.20147200
H	-3.92109700	-2.08673500	1.95220000	C	0.44585700	-0.88605300	1.77827400
C	-3.82348500	-0.05238500	0.13365700	H	1.23019600	-4.69462000	1.33672800
H	-4.85120200	-0.38099100	0.32573300	H	2.19832000	-3.47737100	0.53385600
H	-3.58259900	0.74079800	0.84887300	H	0.21704900	-4.94026600	5.76058100
H	-3.78822000	0.37349600	-0.87385300	C	-0.17955600	-5.24114000	4.78812200

O	0.64748500	-4.72529000	3.72874600	C	-1.61377700	-2.14762800	-2.25826300
H	-0.15244400	-6.32488400	4.67945400	C	-0.38155400	-1.35471800	-2.58246000
H	-1.20192300	-4.86890200	4.69027900	C	0.44156900	-1.86795400	-3.78519900
C	0.75911400	-3.38286000	3.67934000	H	0.26900200	-1.25463800	-1.70587200
C	1.71150300	-2.95586100	2.54946400	H	-0.75046300	-0.34844700	-2.83911500
O	0.18918000	-2.63984000	4.44781600	C	1.65267100	-0.97251800	-4.07520500
C	3.13478600	-3.40089000	2.93655000	H	0.78152200	-2.89343400	-3.58634800
O	3.94439600	-3.87704300	2.17340700	H	-0.20594500	-1.91559800	-4.66702300
O	3.38229900	-3.14640800	4.23459300	C	2.48993700	-1.47443600	-5.25563600
C	4.70869700	-3.47286300	4.69269400	H	1.30148100	0.04714200	-4.27844800
H	5.45438200	-2.90002400	4.13699200	H	2.28376900	-0.90656500	-3.17868200
H	4.72650200	-3.20519700	5.74843100	H	3.34511600	-0.81738400	-5.44359500
H	4.90560000	-4.53911300	4.55952800	H	2.87972900	-2.48175700	-5.06810800
C	-0.68090600	-3.52869300	-0.37594300	H	1.89365100	-1.51543000	-6.17413800
C	-1.59355900	-1.35763400	0.22200500	H	-3.33835700	-3.87794800	0.09078800
H	-1.63201300	-0.34797200	-0.18438700	H	-3.97558000	-2.58049600	-0.94724500
C	1.71584700	-1.41183400	2.42019300	C	-3.58182500	-2.72108100	-6.75495400
H	2.58438900	-1.11203100	1.82026000	C	-4.57880300	-2.90280900	-7.88772900
H	1.85966700	-0.96533200	3.40436700	C	-5.78643000	-1.30450300	-6.58708400
S	0.15892800	0.87790200	2.01394200	C	-5.57453200	-2.27716100	-5.43842200
O	-0.35300200	1.44618300	0.75190800	O	-5.62564700	-1.93451000	-7.85666100
O	1.40261400	1.40233800	2.60576700	O	-4.24286100	-2.86130200	-5.47659400
C	-1.15442800	1.07140500	3.23674000	H	-6.81154400	-0.92154000	-6.55250700
C	-2.16578100	1.99395900	2.96083000	H	-5.10058200	-0.45482700	-6.47461000
C	-1.10017400	0.38897300	4.45510400	H	-5.67498900	-1.76184100	-4.48061800
C	-3.14435100	2.23590500	3.92680100	H	-6.29939500	-3.09871800	-5.48886600
H	-2.17431000	2.50517700	2.00444200	H	-4.05832600	-2.80790200	-8.84856700
C	-2.09191500	0.63255300	5.40610900	H	-5.00757200	-3.91562500	-7.83694600
H	-0.32419200	-0.34258900	4.65049200	H	-2.81599700	-3.50063300	-6.78740800
C	-3.10803600	1.55603900	5.14585500	H	-3.09292900	-1.74199200	-6.80077500
H	-3.93379200	2.95363000	3.72458300	C	-3.21599200	-4.21385700	-3.11449000
H	-2.06752500	0.10018400	6.35218500	O	-3.53103500	-5.28578000	-2.81637200
H	-3.87305300	1.74415400	5.89364700	TS4bb			
C	-2.97940300	-1.79095900	0.88098000	C	1.79817000	0.28355500	-0.53476100
C	-3.18166200	-2.84851000	-0.24629400	C	1.20467500	-1.03419800	-0.31085400
C	-2.89885100	-2.40017400	2.28259600	C	2.02488000	-2.28188400	-0.42014800
H	-2.19497000	-3.23623900	2.32337400	C	3.09507900	0.39430900	-0.89560100
H	-2.59444300	-1.66295100	3.03080700	H	1.67747300	-3.05015600	0.27428800
H	-3.88535700	-2.78369300	2.56895200	H	1.90789900	-2.71168700	-1.42311500
C	-4.01264700	-0.66246300	0.83463400	H	4.76362200	-2.52266500	3.63697300
H	-5.00723100	-1.04730800	1.08974500	C	3.69372600	-2.64914500	3.45695600
H	-3.76438700	0.13123500	1.54619100	O	3.43584600	-2.77578100	2.04507200
H	-4.07166000	-0.21771800	-0.16441800	H	3.33305900	-3.57453300	3.90434500
C	-0.56003300	-4.88854800	-0.99148100	H	3.15875400	-1.78934400	3.86661800
H	0.18193000	-5.50260200	-0.47598500	C	3.83282700	-1.73644000	1.28486500
H	-1.51904500	-5.41767900	-0.96919700	C	3.52986800	-2.01032900	-0.20077400
H	-0.26665100	-4.82359900	-2.04672200	O	4.35274600	-0.73669100	1.72523700
C	-1.76648300	-2.54239600	-0.81405100	C	4.32383100	-3.25565700	-0.63409200

O	3.87506200	-4.17653600	-1.27738900	H	-4.62433400	6.29316400	-1.44069800
O	5.60605000	-3.16410200	-0.23633500	H	-5.45996500	4.90184300	-0.73578400
C	6.45646700	-4.26463400	-0.61516500	H	-4.26646700	5.78983700	0.21752300
H	6.48735100	-4.36481200	-1.70233700	H	-1.07939600	0.62797800	2.07794500
H	7.44234700	-4.01997600	-0.22188700	H	-1.70137000	2.20602100	1.62553300
H	6.08695800	-5.19638100	-0.18104400	Rh	-3.60755700	-0.00492900	0.17775700
C	-0.14611500	-0.95957400	-0.08403900	C	-3.53296500	-0.58841000	-1.55714500
C	0.69685100	1.29363300	-0.34319000	O	-3.47463900	-0.97598200	-2.65349200
H	0.69979300	2.05413600	-1.11974800	Cl	-3.83549900	0.64873000	2.53025100
C	3.99974000	-0.80831800	-1.05323800	C	-7.04461000	-2.65253500	1.62336200
H	4.02940000	-1.10047300	-2.11063300	C	-5.62731600	-2.14790200	1.40289100
H	5.02076700	-0.55317100	-0.76157700	C	-6.77507900	-0.15664400	0.63297800
S	3.82207300	1.94381800	-1.45158200	C	-7.43204800	-0.32593100	1.99261900
O	2.89133000	3.04611900	-1.14985800	O	-5.62658900	-1.03167000	0.48614200
O	4.27492700	1.69491100	-2.83186300	O	-7.89314700	-1.66245600	2.19984100
C	5.29564000	2.18436200	-0.44612400	H	-7.48326400	-0.39402800	-0.17111100
C	6.53906900	1.84264400	-0.98207300	H	-6.41491200	0.86583500	0.50517900
C	5.17872300	2.74814000	0.82630700	H	-6.72207700	-0.02725300	2.77441600
C	7.68648400	2.05803300	-0.21750800	H	-8.31065500	0.32476800	2.05661800
H	6.59574600	1.43959400	-1.98734700	H	-5.16219400	-1.83729400	2.34467100
C	6.33197600	2.95658500	1.58074800	H	-5.00940700	-2.92188900	0.93947300
H	4.20559900	3.03554500	1.20775200	H	-7.46476400	-2.99486500	0.66439900
C	7.58190200	2.60928300	1.06111700	H	-7.02289300	-3.51283900	2.30351100
H	8.66034500	1.80262200	-0.62397100	C	-1.03183500	-2.12858600	0.21595100
H	6.25588400	3.39564500	2.57067100	H	-0.48275200	-2.90673300	0.75511500
H	8.47734500	2.77674600	1.65240300	H	-1.42097800	-2.57230700	-0.70799100
C	0.48728200	1.92782400	1.09498400	H	-1.90511000	-1.81326200	0.79551100
C	-0.98077000	1.43274600	1.35472400	INT-5bb			
C	1.40690200	1.34347500	2.17570600	C	0.09284600	0.47829400	-0.43954500
H	1.34153700	0.25307400	2.22475300	C	-0.11757000	-0.65588500	-1.37909000
H	2.45328000	1.60859600	2.00436800	C	0.97736000	-1.12714200	-2.28617900
H	1.10965700	1.73395700	3.15523600	C	1.34212500	0.99533600	-0.34008400
C	0.60090000	3.45830000	1.10193000	H	0.82521900	-2.16423400	-2.58660200
H	0.35054200	3.84281600	2.09730400	H	0.98336400	-0.53531100	-3.21004000
H	1.61570300	3.77075200	0.84590100	H	3.40094400	-4.27332800	0.50458800
H	-0.07714300	3.92689500	0.38492200	C	2.34711600	-4.18013700	0.23084600
C	-0.57160700	0.43049600	-0.27021700	O	2.18193900	-3.19332700	-0.80440900
C	-1.86130200	1.02404600	-0.16174200	H	1.97669000	-5.11361100	-0.19328300
C	-2.09295700	2.32796700	-0.94848800	H	1.76826300	-3.89048400	1.11052100
C	-3.19050200	3.25829800	-0.41632300	C	2.59276600	-1.95226000	-0.47404100
H	-2.37633300	2.00114800	-1.95765800	C	2.36258400	-0.96856200	-1.63889200
H	-1.17297300	2.90968300	-1.07650200	O	3.11140300	-1.67186600	0.58028500
C	-3.39512400	4.49247300	-1.30565400	C	3.43753000	-1.24291300	-2.70709800
H	-4.12678400	2.69468900	-0.33475900	O	3.22512000	-1.34482900	-3.89504100
H	-2.95004500	3.58669000	0.60402000	O	4.66216200	-1.32190000	-2.15499700
C	-4.49723400	5.42253600	-0.78890500	C	5.74713100	-1.53562800	-3.07614200
H	-2.45233200	5.05204200	-1.38533100	H	5.81013300	-0.71032400	-3.78931800
H	-3.63994800	4.16688300	-2.32605700	H	6.64586300	-1.58287100	-2.46226600

H	5.60379500	-2.46933700	-3.62507300	H	-8.62028200	-1.50394000	0.65840100
C	-1.39159300	-1.14805700	-1.34805400	H	-8.77482200	0.16971000	0.10883500
C	-1.33976600	0.85745300	-0.01527700	H	-4.03976000	0.79607900	1.92301700
H	-1.61746400	1.47935400	-0.88753600	H	-4.18985500	1.69343900	0.42672200
C	2.53533500	0.47598500	-1.13092000	Rh	-2.53655100	-1.97375600	1.36700100
H	2.70014800	1.14596700	-1.98367400	C	-4.05521600	-2.87832500	0.86703400
H	3.43694200	0.51860300	-0.51658400	O	-4.90234800	-3.62424900	0.60327600
S	1.84702400	2.44503800	0.59787700	Cl	-0.21000200	-1.68855900	2.04176200
O	0.71296300	3.01381400	1.34291400	C	-1.81627800	-5.70577200	3.86817400
O	2.59487200	3.30355100	-0.34098000	C	-1.71464100	-4.74013900	2.69864100
C	3.02140400	1.80527600	1.80493500	C	-2.38102500	-3.07481000	4.34879100
C	4.28247400	2.39849200	1.87671700	C	-1.21411500	-3.73041700	5.06912900
C	2.63327500	0.78785900	2.67946000	O	-2.48998300	-3.54991600	2.97439600
C	5.17370800	1.96785800	2.86049400	O	-1.32129200	-5.15135100	5.08555700
H	4.54651800	3.17936100	1.17177400	H	-3.32963300	-3.30888400	4.84527000
C	3.53835400	0.36316500	3.65129600	H	-2.24375800	-1.99292300	4.30941700
H	1.65882900	0.31709200	2.59234200	H	-0.27262900	-3.40737200	4.60603200
C	4.80127300	0.95341800	3.74498600	H	-1.20884700	-3.40227100	6.11352300
H	6.15753600	2.42211500	2.93260700	H	-0.67977800	-4.45074200	2.49121200
H	3.25660300	-0.43566100	4.33024500	H	-2.14766900	-5.17926900	1.79657800
H	5.49973400	0.61721100	4.50614000	H	-2.86615100	-6.00825200	3.99999000
C	-2.11142300	1.59526200	1.15238900	H	-1.23421800	-6.60798200	3.64246700
C	-3.54780400	0.97841400	0.96193200	P2^B			
C	-1.62479800	1.37690400	2.59253700	C	0.28356400	0.78929200	-0.96848500
H	-1.62575900	0.32463400	2.87611600	C	-0.15416500	-0.26580100	-1.89679800
H	-0.61798400	1.77043100	2.72894200	C	0.84718900	-1.13361800	-2.60193500
H	-2.29423300	1.91771800	3.27279300	C	1.61185500	0.98674300	-0.76617100
C	-2.23024900	3.11218300	0.88514600	H	0.43018700	-2.10955800	-2.85796400
H	-2.95024100	3.55151600	1.58549200	H	1.15872300	-0.67210700	-3.54682800
H	-1.27659800	3.62067900	1.00727600	H	1.93752400	-4.51134700	0.76031100
H	-2.60220800	3.30569500	-0.12894100	C	1.01957200	-4.26464900	0.22153800
C	-1.94740000	-2.25994500	-2.18862600	O	1.30106000	-3.36079900	-0.86186400
H	-2.46245500	-2.99833500	-1.56640900	H	0.59474100	-5.15453900	-0.24199000
H	-2.67604500	-1.87888800	-2.91474800	H	0.30828000	-3.81548200	0.91852900
H	-1.16626700	-2.77698500	-2.74920300	C	1.83583300	-2.17535400	-0.50685100
C	-2.13423000	-0.40719900	-0.33952800	C	2.11967400	-1.31621900	-1.74914400
C	-3.46058300	-0.27926900	0.10180600	O	2.05971800	-1.86755200	0.64360900
C	-4.69097000	-0.61529200	-0.73373500	C	3.19031200	-2.03309000	-2.58911000
C	-6.04563500	-0.55841300	-0.00921000	O	3.15271900	-2.17867700	-3.78967000
H	-4.57521600	-1.57450500	-1.24518600	O	4.21089600	-2.44564600	-1.81202800
H	-4.71059600	0.14456500	-1.53250700	C	5.30050300	-3.08470200	-2.50331900
C	-7.21459100	-0.95918600	-0.91835000	H	5.74784100	-2.39786700	-3.22542900
H	-6.03458900	-1.20965900	0.87240000	H	6.02040100	-3.35176300	-1.73048200
H	-6.21455900	0.45815300	0.36767700	H	4.94858000	-3.97523600	-3.02932200
C	-8.57589600	-0.85543200	-0.22386900	C	-1.51108800	-0.25811200	-2.07563600
H	-7.21197600	-0.32575300	-1.81623500	C	-0.97275000	1.55535600	-0.55157400
H	-7.06007900	-1.98821800	-1.26937800	H	-0.91982400	2.53992900	-1.03701500
H	-9.38924600	-1.15079700	-0.89440000	C	2.67753500	0.06521300	-1.33739600

H	3.13839300	0.53654500	-2.21329800	C	-0.08068700	-1.86046400	0.96528600
H	3.48439000	-0.07621300	-0.61507200	C	0.11164300	-3.29287900	0.72469800
S	2.30328900	2.50007600	-0.09270500	Rh	-2.43153900	-2.93905600	-3.87457400
O	1.32429600	3.59374100	-0.23454200	Cl	-3.27773700	-0.61663400	-3.75300900
O	3.62666800	2.64487400	-0.72970600	C	1.13974000	-4.07165400	1.49863000
C	2.58926300	2.26167200	1.67563900	C	0.74558600	-1.18026100	1.79202600
C	2.75224900	3.41906800	2.44387400	H	0.79833800	-5.08826000	1.70833900
C	2.71328500	0.99126100	2.24027900	H	2.05981700	-4.17436500	0.91240500
C	3.04829500	3.29791400	3.80049900	H	-0.58655500	-4.71094800	6.01437100
H	2.63271500	4.39416600	1.98344500	C	-0.96235000	-5.01403300	5.03430500
C	3.00460700	0.88640700	3.60336400	O	0.03098300	-4.77335600	4.02090300
H	2.57043200	0.09434800	1.64625800	H	-1.15210700	-6.08667600	5.00938100
C	3.17545200	2.03263400	4.38051300	H	-1.87518700	-4.45573800	4.81429300
H	3.17437700	4.19109400	4.40528000	C	0.42522300	-3.49134200	3.88597000
H	3.09578700	-0.09759500	4.05367300	C	1.52804200	-3.36736300	2.82058000
H	3.40284700	1.94217800	5.43880600	O	-0.03208100	-2.58313800	4.54457500
C	-1.52726100	1.78097800	0.90601400	C	2.80221100	-4.03214100	3.37488000
C	-3.05886600	1.87746700	0.58611200	O	3.57619300	-4.69833700	2.72523200
C	-1.25870200	0.55208600	1.79243900	O	2.97639700	-3.73285200	4.67571200
H	-1.64528800	-0.36535600	1.33688300	C	4.17468000	-4.25462800	5.28091300
H	-0.18730700	0.41816300	1.96673100	H	5.05863200	-3.86258800	4.77288000
H	-1.74276900	0.67355500	2.76816700	H	4.14713900	-3.92054800	6.31738700
C	-1.06390200	3.05423000	1.62230900	H	4.18574300	-5.34559700	5.22529300
H	-1.69203900	3.22047500	2.50649200	C	-0.66450500	-3.72850200	-0.29863600
H	-0.02957200	2.98866200	1.95961000	C	-1.24480400	-1.42085000	0.12046500
H	-1.14370700	3.93201000	0.97507700	H	-1.10782500	-0.42856300	-0.30868800
C	-2.29281800	-1.15530700	-2.98764300	C	1.84730200	-1.87093400	2.57198900
H	-3.02668500	-1.74464600	-2.42557100	H	2.79580000	-1.80242200	2.02393900
H	-2.85459500	-0.56779600	-3.72320800	H	2.00952100	-1.36867000	3.52610600
H	-1.65008200	-1.84883400	-3.53406800	S	0.78279200	0.61593800	1.85384000
C	-2.08614100	0.72901100	-1.18047400	O	0.56451900	1.13732400	0.48753200
C	-3.27851000	0.93908300	-0.58608800	O	2.01893200	0.96654900	2.57672300
C	-4.62283100	0.33844500	-0.88837500	C	-0.61454400	1.16939300	2.85107400
C	-5.03217000	-0.79263600	0.08013700	C	-1.37298200	2.24039100	2.37510800
H	-4.65122000	-0.04158400	-1.91515700	C	-0.85996000	0.59767200	4.10259400
H	-5.38384900	1.13101300	-0.83580800	C	-2.40048100	2.74980500	3.17137300
C	-6.44030100	-1.33710500	-0.19154500	H	-1.15505500	2.65488500	1.39700300
H	-4.30096800	-1.60916700	0.00627100	C	-1.89779100	1.11010700	4.88199800
H	-4.97653200	-0.42906900	1.11461800	H	-0.27732200	-0.24747200	4.45324900
C	-6.84215500	-2.46895500	0.75940800	C	-2.66263800	2.18535200	4.42135800
H	-7.16582000	-0.51617800	-0.11224500	H	-2.99599100	3.58394600	2.81250400
H	-6.49772400	-1.69222100	-1.22967200	H	-2.10623100	0.66840000	5.85184600
H	-7.85075200	-2.83505400	0.54157200	H	-3.46545800	2.58139600	5.03654800
H	-6.15519200	-3.31905700	0.67730100	C	-2.73525100	-1.62035100	0.65889300
H	-6.82827300	-2.13389000	1.80280200	C	-2.99322700	-2.64264700	-0.49258600
H	-3.67029300	1.61416800	1.45929700	C	-2.87217900	-2.21660000	2.06149500
H	-3.33029800	2.91206600	0.32138900	H	-2.32423600	-3.15792600	2.16089000
				H	-2.50903000	-1.52743200	2.83016300

TS4dd

H	-3.92883300	-2.42536700	2.26755700	C	0.68467300	-1.04135300	1.71371900
C	-3.57396800	-0.34621800	0.52927300	H	0.70653700	-4.94137700	1.43849300
H	-4.63176300	-0.56992100	0.71339400	H	1.91297900	-3.99705100	0.59609700
H	-3.25911100	0.41283600	1.25251800	H	-0.33043500	-4.78129900	5.85192700
H	-3.49708900	0.08070400	-0.47597100	C	-0.77851600	-5.04386700	4.89075000
C	-0.73813400	-5.13074100	-0.81570800	O	0.13231500	-4.74916100	3.81619600
H	-0.33118500	-5.84899400	-0.09878300	H	-0.96341200	-6.11607900	4.83216100
H	-1.77360200	-5.40950300	-1.03853200	H	-1.70894700	-4.48484300	4.76725900
H	-0.18022700	-5.24664900	-1.75166400	C	0.51127000	-3.45916200	3.71221200
C	-1.49035900	-2.59422700	-0.89531900	C	1.53055600	-3.27898000	2.57472200
C	-1.15033900	-2.34045700	-2.37360800	O	0.10148600	-2.58680800	4.44606200
C	0.03077000	-1.65036600	-2.62462400	C	2.83991000	-3.97138200	2.99803200
C	0.58018200	-1.28436200	-3.96365600	O	3.55168100	-4.61928100	2.26425100
H	0.61074000	-1.28090200	-1.77115800	O	3.12260800	-3.72009800	4.28999500
H	-1.46992900	-1.20684800	-2.71961600	C	4.36176400	-4.27083800	4.77549100
C	0.93124500	0.21022500	-4.09843500	H	5.20447700	-3.86749100	4.20955600
H	1.49851900	-1.88409200	-4.07859500	H	4.42334700	-3.97290800	5.82147300
H	-0.11255800	-1.61189500	-4.74620500	H	4.35756100	-5.35927000	4.68190600
C	1.62535500	0.52409800	-5.42654500	C	-0.89280200	-3.49238900	-0.38111700
H	0.00767600	0.79478900	-4.01419400	C	-1.41162400	-1.19518700	0.17180100
H	1.57102100	0.51457200	-3.26042500	H	-1.28170400	-0.19557300	-0.24151500
H	1.85241600	1.59142600	-5.50623600	C	1.83588400	-1.77179500	2.37789900
H	2.56816100	-0.02642100	-5.52292800	H	2.74216100	-1.67571300	1.76632300
H	0.99196400	0.25367800	-6.27853300	H	2.06929700	-1.31863100	3.34167600
H	-3.36299300	-3.62679700	-0.18671700	S	0.72683700	0.74984100	1.88075400
H	-3.64640400	-2.24958400	-1.27472700	O	0.39163900	1.35687600	0.57626900
C	-3.78855900	-2.67728700	-6.69471400	O	2.01904000	1.05901100	2.51956900
C	-4.95383200	-2.95472300	-7.63009300	C	-0.58115300	1.23743100	3.02506400
C	-6.19947700	-2.38848500	-5.67315200	C	-1.37214900	2.33510300	2.68033800
C	-5.35151700	-3.45855100	-5.00560900	C	-0.72275800	0.59293300	4.25699900
O	-6.20091400	-2.51733800	-7.09376000	C	-2.32702200	2.79486500	3.58935400
O	-3.96849000	-3.38819500	-5.44677400	H	-1.23411500	2.80941200	1.71493500
H	-7.23873300	-2.49147700	-5.34383300	C	-1.68932000	1.05653000	5.15057700
H	-5.84221300	-1.39585200	-5.36768600	H	-0.11593800	-0.27059000	4.50646800
H	-5.34810700	-3.32842100	-3.92152200	C	-2.48605500	2.15625900	4.82090000
H	-5.72855700	-4.45957600	-5.24786800	H	-2.94635500	3.64930700	3.33304900
H	-4.79285100	-2.42694700	-8.57756700	H	-1.81658500	0.55749400	6.10660000
H	-4.99725300	-4.03273900	-7.84991400	H	-3.23252700	2.51428900	5.52410600
H	-2.85131700	-3.04499200	-7.11970200	C	-2.86446100	-1.38809700	0.80467400
H	-3.68777800	-1.60706800	-6.48513900	C	-3.21927500	-2.36289800	-0.36078500
C	-1.63585500	-4.57939100	-4.05224800	C	-2.91512800	-2.03835900	2.18931200
O	-1.11406800	-5.60382900	-4.22007000	H	-2.37880500	-2.99119800	2.21370100
INT-5dd				H	-2.48574600	-1.38648400	2.95605900
C	-0.19478400	-1.67764000	0.90777100	H	-3.95845000	-2.23878500	2.46169500
C	-0.03249700	-3.09790100	0.59110800	C	-3.68569600	-0.09658400	0.78936500
Rh	-2.40622500	-2.77959900	-4.07481500	H	-4.73479400	-0.31027500	1.02718300
Cl	-3.53369000	-0.67575700	-4.45517800	H	-3.31195300	0.62051400	1.52697100
C	1.03980400	-3.91692600	1.25346600	H	-3.65934000	0.38315700	-0.19477300

C	-1.04069600	-4.90238800	-0.86920800	H	-1.85745900	-4.75002100	4.51211200
H	-0.78555800	-5.62208700	-0.08487300	C	0.40965000	-3.55724600	3.78545900
H	-2.06548200	-5.10303800	-1.19545300	C	1.51971400	-3.23129800	2.77252000
H	-0.38466200	-5.11883700	-1.71920500	O	-0.09874300	-2.77910500	4.56239400
C	-1.74455200	-2.33161600	-0.87334400	C	2.80811800	-3.92984000	3.24618700
C	-1.55138300	-1.80680200	-2.28032300	O	3.59745400	-4.49720500	2.52528900
C	-0.50592800	-2.05926100	-3.17744800	O	2.97347900	-3.78656900	4.57514600
C	0.10754200	-0.99953900	-4.06525700	C	4.18182100	-4.35204100	5.11694100
H	0.15553600	-2.89583800	-2.95057000	H	5.05780500	-3.88779300	4.65835000
H	-2.04069700	-0.84286500	-2.40307800	H	4.14967100	-4.14062700	6.18513600
C	1.31321000	-0.32938000	-3.36846700	H	4.21337600	-5.42902400	4.93600800
H	0.44461300	-1.45105500	-5.00700000	C	-0.68306800	-3.23425900	-0.34978900
H	-0.64393500	-0.24606000	-4.31933000	C	-1.23927700	-0.96696100	0.28599600
C	1.96937200	0.74061300	-4.24687500	H	-1.05933700	0.04636000	-0.07032800
H	0.98460700	0.11946500	-2.42295400	C	1.78926400	-1.70463400	2.75486100
H	2.05492700	-1.09572600	-3.10560100	H	2.75183900	-1.52491300	2.25975000
H	2.81838800	1.20347500	-3.73419500	H	1.90502400	-1.34670400	3.77826200
H	2.33676400	0.31413800	-5.18747700	S	0.68197600	0.83307900	2.37527600
H	1.25798800	1.53508200	-4.49728100	O	0.36033600	1.56188600	1.13266000
H	-3.58462200	-3.35089000	-0.06209400	O	1.94860700	1.10984300	3.07810000
H	-3.92146300	-1.93712300	-1.08309900	C	-0.66458100	1.18130900	3.52923600
C	-3.64111100	-3.13938300	-6.94807600	C	-1.45715200	2.30326100	3.27748700
C	-4.67964200	-3.75482300	-7.87142500	C	-0.83936600	0.41006600	4.68131500
C	-6.13250700	-2.87529400	-6.19181800	C	-2.44358700	2.65930400	4.19904200
C	-5.26387600	-3.62219400	-5.19315600	H	-1.29405000	2.87773800	2.37221200
O	-6.01553700	-3.40949300	-7.50659900	C	-1.83679500	0.77152200	5.58835100
O	-3.85917900	-3.59362500	-5.58864800	H	-0.23870000	-0.47538600	4.85636900
H	-7.18270700	-2.98063900	-5.90165500	C	-2.63332900	1.89493100	5.35204300
H	-5.87896400	-1.80750300	-6.16772100	H	-3.06320500	3.53185100	4.01398400
H	-5.33591800	-3.15935300	-4.20735100	H	-1.98904000	0.17255700	6.48126600
H	-5.55731700	-4.67631400	-5.13112800	H	-3.40396400	2.17244900	6.06554100
H	-4.50123300	-3.40526100	-8.89609400	C	-2.73210500	-1.16600400	0.81250600
H	-4.57042600	-4.84968100	-7.86567800	C	-3.00812900	-2.11204500	-0.39637200
H	-2.63704200	-3.47527300	-7.21830400	C	-2.88934100	-1.85290400	2.17093000
H	-3.66712600	-2.04555800	-6.97004600	H	-2.35153300	-2.80444800	2.20953900
C	-1.69263000	-4.48218100	-4.00692500	H	-2.52510400	-1.22463000	2.98868400
O	-1.28420600	-5.56004400	-4.10748100	H	-3.94997400	-2.06418600	2.35451700
P1^B				C	-3.54286900	0.13150600	0.77069400
C	-0.08935500	-1.50614300	1.09586900	H	-4.60905500	-0.07673600	0.92282800
C	0.11687200	-2.90213700	0.69291500	H	-3.21965600	0.82566000	1.55303100
C	1.17417600	-3.74222200	1.35458700	H	-3.43585000	0.63884100	-0.19432300
C	0.69378400	-0.93469300	2.03958400	C	-0.79667600	-4.57214000	-1.01188000
H	0.88649700	-4.79474300	1.40045900	H	-0.18616300	-5.33408500	-0.52176100
H	2.10148200	-3.70283000	0.77206400	H	-1.83999500	-4.91370100	-1.00542600
H	-0.57728900	-5.11453200	5.69188100	H	-0.49959600	-4.51585600	-2.06486600
C	-0.92160800	-5.29113400	4.67015500	C	-1.50593700	-2.04948500	-0.82332000
O	0.07391200	-4.86211200	3.72417900	C	-1.24357600	-1.62808800	-2.24862400
H	-1.05840100	-6.35682100	4.48866600	C	-0.11940100	-1.82831300	-2.94466100

C	0.13584100	-1.31539700	-4.33525500	O	-3.43270900	-6.20112100	-6.86939300
H	0.70266700	-2.37652900	-2.48141600	O	-1.90445600	-6.97925300	-5.40486000
H	-2.04948200	-1.06005600	-2.71677900	C	-0.47904300	-4.58039700	-6.48671500
C	1.32394700	-0.33603100	-4.40566000	O	0.45939200	-3.93429800	-6.06732000
H	0.34327100	-2.16161400	-5.00811200	O	-0.45189900	-5.28007500	-7.63105600
H	-0.76751700	-0.82588200	-4.72162400	C	-2.48215300	-8.29556300	-5.54232900
C	1.60854100	0.15372600	-5.82863800	H	-2.45263700	-8.61398100	-6.58679400
H	1.12034000	0.51850100	-3.74895800	H	-1.86689600	-8.94709000	-4.92241900
H	2.21878000	-0.82558300	-3.99882000	H	-3.51409900	-8.27795100	-5.18653100
H	2.45737600	0.84476000	-5.84937900	C	0.77899000	-5.21624100	-8.37779300
H	1.84305800	-0.68266000	-6.49735000	H	0.61453800	-5.83163400	-9.26123400
H	0.74268900	0.67872000	-6.24823500	H	0.99741500	-4.18419700	-8.66121200
H	-3.38487600	-3.10841700	-0.14215200	H	1.60623000	-5.60756000	-7.78149400
H	-3.67877900	-1.67507400	-1.14368500	S	-2.86700900	-0.69735100	-6.13001800
TS1b^H				O	-2.33730100	-0.79212000	-7.50229900
C	-1.86394600	-4.63643400	-5.82240700	O	-4.08446600	0.08951000	-5.85088000
C	-2.73611500	-3.51612300	-6.49732200	C	-1.56026400	-0.05459600	-5.06907100
H	-2.21631100	-3.08451500	-7.35411300	C	-0.27995500	-0.61225000	-5.13871200
H	-3.63302800	-4.00228900	-6.88677000	C	-1.84901300	1.01390700	-4.21959300
C	-1.65663600	-4.41652800	-4.30297400	C	0.72306500	-0.09237100	-4.32095600
H	-1.08526200	-5.25550400	-3.89779500	H	-0.06487300	-1.43945800	-5.80718200
H	-1.05056700	-3.51354100	-4.18361300	C	-0.83194700	1.52997200	-3.41385500
C	-3.16138700	-2.40344600	-5.57749300	H	-2.84976200	1.43152000	-4.20811400
C	-3.80904300	-2.55571200	-4.42214400	C	0.44851700	0.97560300	-3.46173800
C	-4.64176000	-1.94300100	-3.48068800	H	1.71982000	-0.52083400	-4.35981600
H	-5.44530600	-1.35524700	-3.92309400	H	-1.04155100	2.36473400	-2.75184200
C	-4.19189800	-1.45101100	-2.11951400	H	1.23586300	1.37742800	-2.83069800
C	-5.34691000	-1.28488900	-1.11035600	Rh	-5.10104200	-4.09714300	-3.74963500
H	-6.12965900	-0.65346800	-1.55378100	Cl	-5.48238400	-6.54218900	-3.79020700
H	-5.81232100	-2.26170500	-0.92818900	C	-6.88166900	-3.95946400	-2.90631600
C	-4.90809300	-0.70466500	0.15940700	O	-7.87633500	-3.86880600	-2.34507100
C	-4.52804300	-0.23235200	1.20709500	C	-3.57723200	-5.05290100	-1.07633800
C	-4.08938700	0.36859100	2.46813300	H	-4.17745000	-5.96690900	-1.03538000
C	-4.22955200	1.90525900	2.49664300	H	-2.55842400	-5.27536600	-0.73824000
H	-3.04168400	0.09629700	2.65796800	H	-4.01786400	-4.32639200	-0.38434400
H	-4.66649000	-0.06357200	3.29753000	C	-6.62146500	-4.89866500	-8.18175500
C	-3.76876300	2.51769500	3.82422200	C	-6.68235800	-5.02869500	-6.66793900
H	-3.64959200	2.33157800	1.66844900	C	-6.72662500	-2.65701300	-6.50191900
H	-5.27710100	2.17086100	2.30746000	C	-6.67158600	-2.56875600	-8.02318700
C	-3.90318000	4.04328300	3.85862100	O	-6.08608600	-3.86406900	-6.05322100
H	-4.35050800	2.07959100	4.64674000	O	-7.26945400	-3.70821000	-8.62272500
H	-2.72265100	2.23741900	4.00949900	H	-6.18719700	-1.81930500	-6.05428400
H	-3.56729100	4.45224600	4.81697800	H	-7.77223600	-2.65142300	-6.15949600
H	-3.30495800	4.51184800	3.06890900	H	-7.22586500	-1.69140100	-8.37057000
H	-4.94401900	4.35288100	3.71131900	H	-5.62270300	-2.46743300	-8.34601800
C	-2.92343500	-4.28376500	-3.54000400	H	-7.72549500	-5.11274200	-6.33144700
C	-3.56173100	-4.53745000	-2.45791400	H	-6.11496100	-5.88704600	-6.30952900
C	-2.51165200	-6.01112400	-6.10658200	H	-5.57071900	-4.91043600	-8.51005000

H	-7.14287400	-5.73756000	-8.65275200	H	2.47671800	-4.78843300	-7.36322200
H	-3.42278800	-2.10564500	-1.70520000	H	1.92909100	-6.47998700	-7.41855800
H	-3.71611400	-0.47179200	-2.26658000	S	-2.78806400	-0.77550000	-5.76861500
INT-2b^H				O	-2.40537900	-0.76163600	-7.19090600
C	-1.14303100	-4.59311700	-5.51922600	O	-4.13460300	-0.32414200	-5.36045200
C	-1.29568000	-3.09404400	-5.86038100	C	-1.59836800	0.25816000	-4.89279700
H	-0.36655200	-2.57562100	-5.58558100	C	-0.32074500	0.42855600	-5.43206400
H	-1.42004100	-2.97737400	-6.93887200	C	-1.97575300	0.88597600	-3.70334400
C	-1.35273300	-4.80613800	-3.99858300	C	0.60124200	1.22372700	-4.74997900
H	-1.17595700	-5.84935100	-3.73943400	H	-0.07086400	-0.03169500	-6.38187900
H	-0.60972000	-4.19989600	-3.46739300	C	-1.04636100	1.68086600	-3.03271100
C	-2.47107500	-2.44170900	-5.15723100	H	-2.98746100	0.77239100	-3.33042400
C	-3.19227400	-3.04431100	-4.17283400	C	0.24107400	1.84340900	-3.55115500
C	-4.46232400	-2.58128200	-3.50766500	H	1.59622800	1.36705100	-5.16042000
H	-5.01857500	-1.87138400	-4.11373800	H	-1.33064200	2.17845200	-2.11052900
C	-4.25141200	-1.99973300	-2.10509700	H	0.96123100	2.46349800	-3.02551200
C	-5.47678400	-1.21889900	-1.58453900	Rh	-5.42407300	-4.45441000	-3.76426300
H	-5.73357200	-0.44176000	-2.31731400	Cl	-6.16964100	-6.71750100	-4.48020000
H	-6.35287900	-1.87654900	-1.52734500	C	-6.29713600	-4.43439600	-2.17340400
C	-5.24407300	-0.60422100	-0.27682300	O	-6.84525200	-4.50389000	-1.16316600
C	-5.03741600	-0.10333200	0.80563500	C	-3.54048800	-6.37752100	-2.25831200
C	-4.79302700	0.53587500	2.10003400	H	-4.12215000	-7.19259900	-2.69839500
C	-4.21987500	1.96347500	1.97821700	H	-2.48859800	-6.67077300	-2.17464800
H	-4.10328900	-0.08294100	2.69086800	H	-3.92139500	-6.22003000	-1.24135400
H	-5.73081600	0.56911500	2.67209000	C	-8.01524900	-4.89093000	-7.11250600
C	-3.97818700	2.62625800	3.33918600	C	-8.16813900	-4.28989100	-5.72164000
H	-3.28029800	1.92203700	1.41244000	C	-6.64830400	-2.56979900	-6.33512200
H	-4.91041600	2.57476500	1.38389000	C	-6.50276900	-3.21046500	-7.70760700
C	-3.40588400	4.04233500	3.22181000	O	-6.96300200	-3.58102800	-5.34621500
H	-4.92247600	2.65822100	3.89966400	O	-7.70032600	-3.88748000	-8.07215500
H	-3.29485900	2.00198600	3.93111800	H	-5.72970500	-2.07239200	-6.02534800
H	-3.24504200	4.49134000	4.20720700	H	-7.46434000	-1.83450700	-6.34203600
H	-2.44365500	4.03869100	2.69699900	H	-6.32626600	-2.43837900	-8.46257300
H	-4.08344300	4.69835600	2.66367700	H	-5.64664500	-3.90273500	-7.70660800
C	-2.75430800	-4.36442700	-3.66404500	H	-8.99973100	-3.57187600	-5.70007600
C	-3.69677800	-5.13226700	-3.05853900	H	-8.32022900	-5.06959800	-4.97567100
C	-2.19193600	-5.41425600	-6.29637000	H	-7.23538100	-5.66477500	-7.08537000
O	-3.07148600	-4.94483900	-6.98441200	H	-8.95837800	-5.34908100	-7.42692800
O	-2.02126000	-6.72644300	-6.07267600	H	-3.95560400	-2.77001600	-1.38554200
C	0.26457400	-5.05461100	-5.91286000	H	-3.40910800	-1.29607000	-2.14858100
O	1.14585200	-5.34185500	-5.13417300	Z-TS2bb^{III}			
O	0.40767200	-5.05914900	-7.25175400	C	4.26267300	-2.04197500	-2.13163200
C	-3.00037200	-7.60070600	-6.68170100	C	4.35448400	-0.58401100	-2.61907800
H	-3.05198300	-7.41607100	-7.75658100	H	5.38395800	-0.22103500	-2.50047500
H	-2.64755100	-8.61144000	-6.47926600	H	4.09842900	-0.53225400	-3.68122700
H	-3.98042100	-7.43450500	-6.22795100	C	4.22103000	-2.03588800	-0.59091400
C	1.70166600	-5.46059800	-7.73891200	H	4.31878100	-3.05442500	-0.23093300
H	1.63565100	-5.40360000	-8.82475800	H	5.11308100	-1.49966800	-0.24209800

C	3.39184100	0.27078800	-1.84043500	H	4.75858800	2.61623500	-0.35521300
C	2.67834200	-0.08174200	-0.72877400	C	6.81042400	4.36241100	-2.43732400
C	1.55293400	0.80347500	-0.31790400	H	6.55119700	4.55139500	-4.57003700
H	0.63303500	0.64180800	-0.87460700	H	6.81775100	4.00241800	-0.30885600
C	1.39956100	1.35111600	0.97328500	H	7.71211900	4.96714000	-2.41494800
C	2.62388600	1.81415800	1.76632700	Rh	0.52779000	-1.40640000	1.85235900
H	3.39422100	1.03372700	1.72866400	Cl	-0.71003800	-1.77147700	-0.20522300
H	3.03836900	2.69586100	1.25828500	C	1.42813600	-1.34841300	3.48061400
C	2.33432000	2.16071600	3.15890300	O	1.97114600	-1.36358900	4.50259200
C	2.13701200	2.47916000	4.31015000	C	2.63726400	-3.36498700	1.41204900
C	1.93636100	2.84923000	5.71297000	H	1.88866900	-3.80190600	2.07385600
C	1.24802700	1.75554000	6.55647400	H	2.76984200	-4.05261100	0.56957000
H	1.35035100	3.77710200	5.76944500	H	3.58492000	-3.32859400	1.96701300
H	2.91309900	3.08421200	6.15868000	C	-3.94490300	-0.97268700	2.71176200
C	1.12563300	2.14111600	8.03512700	C	-2.63620800	-1.74662700	2.67303000
H	0.24993400	1.56135600	6.14286000	C	-1.62736600	-0.03554800	3.98564800
H	1.80924800	0.81925200	6.45629200	C	-2.95700700	0.70889600	4.00014200
C	0.43246100	1.06613900	8.87809000	O	-1.52969100	-0.82760200	2.79166200
H	2.12754700	2.33543300	8.44162300	O	-4.04634900	-0.19680600	3.90341600
H	0.57434900	3.08768700	8.12059900	H	-0.78194500	0.65640700	3.97060200
H	0.36386600	1.36556300	9.92882400	H	-1.54751100	-0.68879900	4.86710800
H	-0.58584600	0.87624900	8.51997000	H	-3.07665100	1.25659900	4.94041200
H	0.97902900	0.11743800	8.83642000	H	-2.98185900	1.43013600	3.16681000
C	2.95780100	-1.36651600	-0.05016500	H	-2.59091600	-2.46745500	3.50230500
C	2.21994700	-1.98239900	0.92881200	H	-2.49760000	-2.25699200	1.71882500
C	2.98885500	-2.69002800	-2.71352400	H	-4.01306400	-0.32260000	1.82553100
O	2.28208600	-2.19198600	-3.55755200	H	-4.79477100	-1.66172600	2.70814800
O	2.76589900	-3.89199100	-2.14989900	H	0.99995600	0.28517300	1.49502700
C	5.49140600	-2.82082300	-2.61624500	H	0.53160500	2.00343300	1.07400200
O	6.39172900	-3.21380500	-1.90831300	E-TS2bb^{BH}			
O	5.46047900	-2.98533800	-3.95358700	C	4.21325200	-2.03837900	-2.33802200
C	1.52910100	-4.53027300	-2.53883600	C	4.34852500	-0.55568200	-2.73216700
H	1.47666600	-4.62631400	-3.62519000	H	5.38373800	-0.22709300	-2.56931400
H	1.54693800	-5.51048000	-2.06311000	H	4.11629800	-0.43240200	-3.79361600
H	0.68267100	-3.94043200	-2.17855400	C	4.16198200	-2.13053300	-0.80117900
C	6.57784700	-3.69401000	-4.51930300	H	4.21674400	-3.17423900	-0.50987000
H	6.38467800	-3.73675400	-5.59064200	H	5.07293200	-1.65536600	-0.41487100
H	7.51093900	-3.16295100	-4.31603400	C	3.38628800	0.26823700	-1.92129300
H	6.64381000	-4.70010500	-4.09851200	C	2.66700000	-0.13268100	-0.83017500
S	3.00043100	1.84065500	-2.55310100	C	1.55619700	0.74859100	-0.38153300
O	2.60958600	1.73475100	-3.96563700	H	0.61738400	0.60575700	-0.91197200
O	2.03970400	2.43525100	-1.55727400	C	1.47675500	1.27684800	0.92415200
C	4.51116200	2.81678300	-2.49286800	C	0.39239200	2.32273700	1.21246000
C	5.00214300	3.34910900	-3.68570500	H	0.58307200	3.20015000	0.58108900
C	5.15138700	3.04408900	-1.27098700	H	-0.58100000	1.92209800	0.90289900
C	6.15951200	4.12897000	-3.64986400	C	0.35252500	2.73391300	2.61714500
H	4.47739900	3.15136000	-4.61374700	C	0.34268400	3.10013800	3.77152700
C	6.30881600	3.81983500	-1.25023900	C	0.35341600	3.57450900	5.15760300

C	1.61000800	4.39749600	5.51220400	H	2.66922200	-4.14679300	0.31064200
H	0.27838300	2.71806000	5.84225200	H	3.55139800	-3.51123100	1.71065800
H	-0.54259800	4.18441300	5.33847300	C	-3.78130400	-1.24550600	3.13906700
C	1.60425700	4.89079600	6.96366100	C	-2.45396500	-1.93977700	2.87513700
H	2.50057700	3.78270300	5.33130800	C	-1.37295100	-0.31479500	4.23930100
H	1.67984600	5.25245300	4.82817800	C	-2.72345500	0.34737900	4.48120200
C	2.84872000	5.70944500	7.32127200	O	-1.38007700	-0.97925300	2.96414100
H	0.70439400	5.49657600	7.13727500	O	-3.77911300	-0.60062300	4.40942400
H	1.52566900	4.02851700	7.63973800	H	-0.57628200	0.43040800	4.19455200
H	2.81716500	6.04955300	8.36129200	H	-1.15735600	-1.04738500	5.03093900
H	3.76235000	5.11823200	7.19214000	H	-2.75590100	0.78812700	5.48273200
H	2.93592600	6.59632700	6.68351400	H	-2.87328600	1.14857300	3.73965600
C	2.92703300	-1.44844700	-0.21218800	H	-2.28315900	-2.73504400	3.61533700
C	2.20644600	-2.07393500	0.77359100	H	-2.40541400	-2.34766700	1.86439100
C	2.92597700	-2.61431300	-2.96236300	H	-3.97836400	-0.51419900	2.33936300
O	2.22437200	-2.04107600	-3.76200300	H	-4.59558500	-1.97627600	3.15427700
O	2.68044900	-3.85064800	-2.48829200	H	2.43245700	1.46742700	1.41657600
C	5.42351600	-2.81874700	-2.86513400	H	1.11252700	0.21074500	1.45504600
O	6.31344300	-3.27157600	-2.18041600	E-INT-2b^{PH}			
O	5.39029800	-2.90829400	-4.20973600	C	2.92117700	-2.03551100	-1.87574100
C	1.43513000	-4.43741600	-2.92409600	C	2.73317100	-0.54003500	-2.22182600
H	1.38634600	-4.46057100	-4.01467900	H	3.63662300	0.01031900	-1.92983100
H	1.43052900	-5.44689700	-2.51393100	H	2.62115100	-0.44143800	-3.30513500
H	0.59661100	-3.85732800	-2.53129600	C	2.67842500	-2.26350700	-0.36707100
C	6.49053200	-3.61283100	-4.81313100	H	2.87018200	-3.30630000	-0.12285200
H	6.29512600	-3.59731400	-5.88480000	H	3.41600400	-1.66473700	0.18074000
H	7.43574700	-3.11390800	-4.58574300	C	1.51622600	0.05616900	-1.54467900
H	6.53430900	-4.63991700	-4.44332100	C	0.79348400	-0.57854800	-0.58695400
S	3.03121100	1.88245700	-2.54725400	C	-0.49595100	-0.12767900	0.00867700
O	2.79223600	1.87028600	-3.99629900	H	-1.15070900	0.44545100	-0.63733100
O	1.97099000	2.39265700	-1.60595800	C	-0.45820000	0.32529100	1.43168600
C	4.49685800	2.88064900	-2.25338500	C	-1.26123300	1.60247800	1.74088700
C	5.34829500	3.15174500	-3.32629100	H	-0.72079800	2.43953800	1.28310200
C	4.76211600	3.35738800	-0.96675300	H	-2.22236400	1.54050400	1.21996900
C	6.49650000	3.91194900	-3.09835700	C	-1.47509300	1.83099000	3.17013700
H	5.09755900	2.78629300	-4.31599300	C	-1.65982800	1.99100500	4.35674600
C	5.91170400	4.11569400	-0.75390800	C	-1.85669000	2.23080400	5.78812300
H	4.07192400	3.15154500	-0.15575800	C	-0.90407100	3.29819100	6.36748800
C	6.77800600	4.38931400	-1.81680300	H	-1.72310800	1.28903400	6.33823700
H	7.16641200	4.13457700	-3.92312900	H	-2.89656000	2.53827400	5.96655100
H	6.12874400	4.49777900	0.23881300	C	-1.12791400	3.53689300	7.86520000
H	7.67198600	4.98140600	-1.64508100	H	0.13222300	2.98454100	6.19038400
Rh	0.59880100	-1.48235000	1.83054200	H	-1.04164300	4.23596400	5.81518100
Cl	-0.78931300	-1.68636200	-0.15241000	C	-0.18478700	4.59289200	8.44996000
C	1.63885800	-1.43394800	3.37210700	H	-2.16975900	3.84303300	8.03183700
O	2.28205900	-1.40170000	4.33425200	H	-0.99928200	2.58967200	8.40668700
C	2.58725000	-3.49013600	1.18394200	H	-0.36747700	4.74261300	9.51884400
H	1.84314400	-3.92693200	1.85136100	H	0.86369400	4.29783400	8.32953200

H	-0.31507200	5.55991600	7.95132100	H	-4.77102000	1.65719200	1.89024400
C	1.26813400	-1.84533400	-0.01799000	H	-4.98626600	-1.69694700	-0.15068400
C	0.40312000	-2.54237300	0.75687800	H	-3.80298900	-0.82104800	-1.14538000
C	1.95118800	-2.87977700	-2.73102400	H	-4.87054900	1.35133900	-0.54002800
O	1.30825400	-2.46638100	-3.66585900	H	-6.13396400	0.25679100	-1.15946500
O	1.93318900	-4.15767200	-2.30425500	H	0.55255300	0.34970100	1.84936900
C	4.35933200	-2.44750400	-2.22120700	H	-0.92194200	-0.50365900	2.15216600
O	5.21792700	-2.72430600	-1.41303400	Z-INT-2b^{PH}			
O	4.56160700	-2.43186900	-3.55340000	C	3.81040700	-1.61879400	-1.08259300
C	0.99986000	-5.01735300	-2.98951500	C	3.82163700	-0.09040100	-1.30554900
H	1.19607700	-5.01388700	-4.06399400	H	4.66081600	0.35876100	-0.76166700
H	1.15824700	-6.01110500	-2.57073300	H	3.98911700	0.11236200	-2.36660800
H	-0.02081300	-4.67618200	-2.80228700	C	3.25468500	-1.93926400	0.32327400
C	5.88752000	-2.78586000	-3.98452300	H	3.30409900	-3.01264600	0.49602500
H	5.86635600	-2.72819500	-5.07228300	H	3.92089300	-1.46698000	1.05520700
H	6.62254500	-2.08844800	-3.57524300	C	2.52887800	0.55519100	-0.85631100
H	6.13857600	-3.79737500	-3.65644900	C	1.59617200	-0.05660500	-0.08272300
S	1.08169500	1.68870200	-2.16128900	C	0.26746400	0.49368100	0.31532900
O	0.82264200	1.60811200	-3.60844600	H	-0.21354800	1.14631200	-0.40263200
O	0.08924100	2.31361000	-1.26098300	C	0.05582500	0.89057900	1.74199400
C	2.61574300	2.62188600	-1.95594200	C	1.28500000	1.18799800	2.62566400
C	3.40399700	2.88955900	-3.07575800	H	2.00208800	0.36418800	2.54939600
C	2.97084400	3.08843300	-0.68771400	H	1.77035100	2.07245000	2.19404400
C	4.57664900	3.63091500	-2.91746000	C	0.93321600	1.42019700	4.02558300
H	3.08525300	2.53165100	-4.04882500	C	0.62723600	1.60538400	5.18227900
C	4.14634700	3.82330100	-0.54010100	C	0.28144000	1.80984000	6.59004800
H	2.32696100	2.89006200	0.16254500	C	-0.02841700	0.49909400	7.34352900
C	4.94854400	4.09215900	-1.65316800	H	-0.58294800	2.48460900	6.66190700
H	5.19615200	3.85023300	-3.78193700	H	1.10957100	2.32955900	7.09158500
H	4.43287800	4.19286400	0.43998700	C	-0.37718500	0.73143000	8.81812400
H	5.86194300	4.66765900	-1.53404200	H	-0.85861500	-0.01396300	6.84123300
Rh	-1.45261000	-1.75442600	0.89941100	H	0.83832600	-0.16900100	7.26595200
Cl	-1.98811200	-2.96657100	-1.09767600	C	-0.69051400	-0.56559600	9.57051400
C	-2.23927800	-3.19263900	2.06154700	H	0.45744900	1.24879800	9.31047200
O	-2.69048000	-4.02542600	2.70470100	H	-1.23769600	1.41129400	8.88522900
C	0.67377200	-3.85983800	1.41638900	H	-0.93447000	-0.36933800	10.61947300
H	0.01939500	-4.63246800	0.99648000	H	-1.54368400	-1.08748300	9.12244400
H	1.70997400	-4.18435700	1.28052200	H	0.16365100	-1.25174600	9.55017700
H	0.47975100	-3.81558400	2.49454900	C	1.84500700	-1.40478400	0.44588000
C	-5.41959800	0.41560900	-0.34640600	C	0.79086700	-2.06685000	0.97806300
C	-4.44525800	-0.74921100	-0.26746100	C	2.95152900	-2.28612800	-2.17576300
C	-4.32586800	-0.44520900	2.08932100	O	2.48313000	-1.72254600	-3.13780800
C	-5.31964000	0.70457400	1.97175700	O	2.79339600	-3.59906000	-1.92063100
O	-3.56829300	-0.56743700	0.86969800	C	5.24626500	-2.15053000	-1.19174900
O	-6.17695200	0.52699600	0.85502600	O	5.90338400	-2.57708900	-0.26869300
H	-3.60585600	-0.25734400	2.88975800	O	5.70226100	-2.05088700	-2.45593100
H	-4.85482600	-1.38968500	2.28158600	C	1.94187400	-4.30578800	-2.84456200
H	-5.95488800	0.74656700	2.86197900	H	2.31482200	-4.19875700	-3.86561000

H	1.97270600	-5.34873100	-2.52973500	H	3.89365800	0.22871000	-2.50157100
H	0.92402000	-3.91316900	-2.78501800	C	3.36342200	-1.60869500	0.38441600
C	7.05671500	-2.49015500	-2.66403400	H	3.43704400	-2.66351700	0.64010200
H	7.25354600	-2.33847200	-3.72479600	H	4.07123600	-1.07364000	1.02913800
H	7.74686200	-1.90084800	-2.05567900	C	2.52980400	0.77521400	-0.95219400
H	7.16120100	-3.54483800	-2.39851800	C	1.66193800	0.22207300	-0.06563700
S	2.37348300	2.25959200	-1.39527800	C	0.36394500	0.81644000	0.35978700
O	1.28564300	2.91915700	-0.64313500	H	-0.22726000	1.31025300	-0.40019700
O	3.72517000	2.84907000	-1.35458300	C	0.13015200	1.17950600	1.71584300
C	1.88955600	2.15434300	-3.13009900	C	1.23497800	1.33199900	2.76023100
C	0.91887000	1.24189500	-3.55016200	H	1.96011000	0.51999700	2.65692400
C	2.48197800	3.05324800	-4.01931100	H	1.77102600	2.25845300	2.50767300
C	0.53171600	1.24307700	-4.89040100	C	0.73791000	1.40106400	4.13381300
H	0.49111900	0.51958100	-2.86224000	C	0.32059800	1.45852800	5.26885600
C	2.07804900	3.04924100	-5.35447900	C	-0.16078500	1.49907800	6.65087100
H	3.24975100	3.73097700	-3.66208600	C	-0.29723700	0.10265600	7.29445400
C	1.10394000	2.14713700	-5.78832500	H	-1.13152100	2.01268000	6.68651200
H	-0.21084300	0.52841100	-5.23150500	H	0.52469500	2.11136500	7.25305300
H	2.52995800	3.74457100	-6.05567100	C	-0.79932100	0.16574100	8.74147900
H	0.79754500	2.14135100	-6.83045800	H	-0.98199800	-0.50397300	6.68829600
Rh	-0.96673600	-1.08154600	0.89598800	H	0.67582700	-0.40240200	7.25872100
Cl	-1.24667900	-1.94624700	-1.32654200	C	-0.93754900	-1.21666700	9.38702600
C	-2.08740700	-2.51640300	1.74398200	H	-0.11188700	0.78175200	9.33712400
O	-2.74228500	-3.33996800	2.19587400	H	-1.76902100	0.68161300	8.76689500
C	0.80625900	-3.45944600	1.53000800	H	-1.29816000	-1.14095400	10.41778500
H	0.16384800	-4.11167600	0.92703300	H	-1.64416300	-1.84430100	8.83240900
H	1.81194700	-3.89089300	1.53775400	H	0.02392200	-1.74173100	9.40859400
H	0.42735600	-3.48531700	2.55825800	C	1.95808100	-1.07670100	0.56061700
C	-4.39240700	1.69978200	-0.64007000	C	0.95822300	-1.72077300	1.20987900
C	-3.68258300	0.36308200	-0.49120200	C	2.90255300	-2.15318800	-2.06628400
C	-3.70399100	0.64923200	1.86651900	O	2.45230800	-1.68385000	-3.08373200
C	-4.42096400	1.98183900	1.68151200	O	2.68257800	-3.41498800	-1.64990400
O	-2.88657800	0.37312900	0.71560200	C	5.25476200	-1.92576300	-1.23136100
O	-5.20435800	1.97303800	0.49841800	O	5.99560200	-2.20270300	-0.31338300
H	-3.03548700	0.67485400	2.73121900	O	5.60613300	-2.00418300	-2.52835800
H	-4.43469500	-0.16209300	1.99731300	C	1.76048600	-4.17192500	-2.46226700
H	-5.10209000	2.16720700	2.51780800	H	2.09880800	-4.19572200	-3.50039900
H	-3.67770800	2.79538300	1.64595700	H	1.75266700	-5.17471200	-2.03499200
H	-4.41205700	-0.45571500	-0.42769700	H	0.76817100	-3.71810200	-2.40777600
H	-2.99466700	0.15689100	-1.31151800	C	6.94763300	-2.45567400	-2.78519900
H	-3.65106700	2.50246800	-0.78179500	H	7.04921500	-2.46640600	-3.86980000
H	-5.05821800	1.68151500	-1.50785200	H	7.67371400	-1.77309200	-2.33684200
H	-0.48087600	0.01057900	2.33408900	H	7.09971900	-3.45587400	-2.37259100
H	-0.68506100	1.68816600	1.81380600	S	2.28024400	2.40726300	-1.69076800
Z-TS2bb^{BH}				O	3.07008400	2.44239400	-2.93171200
C	3.81966500	-1.40260300	-1.07561000	O	0.84882100	2.76189400	-1.69849900
C	3.80170900	0.10256900	-1.42184200	C	3.08759600	3.53406100	-0.53153800
H	4.67324600	0.58664200	-0.95881500	C	4.46924100	3.72324800	-0.61310900

C	2.31715400	4.21662100	0.41274700	H	-2.30924000	1.46346600	1.18055700
C	5.09022000	4.58936800	0.28776600	C	-1.53518600	1.66658100	3.13860300
H	5.03749600	3.21997200	-1.38800100	C	-1.68538800	1.73945200	4.33821800
C	2.94819400	5.08376200	1.30631600	C	-1.84401500	1.86796900	5.78843900
H	1.24027800	4.08710000	0.41632600	C	-1.02980100	3.03213100	6.39218000
C	4.33283100	5.26329800	1.24880800	H	-1.54635300	0.92700100	6.27115400
H	6.16327100	4.74606500	0.23180300	H	-2.90744900	2.00626500	6.02796000
H	2.35836100	5.62774700	2.03824600	C	-1.20557400	3.14844000	7.91063400
H	4.81996500	5.93974200	1.94493900	H	0.03047600	2.88939200	6.14917600
Rh	-0.84766300	-0.81904500	1.12977100	H	-1.33438600	3.96846000	5.90841500
Cl	-1.19528400	-1.85393300	-1.08417300	C	-0.40483000	4.30415600	8.51860200
C	-1.84894800	-2.28108300	1.94968400	H	-2.27137000	3.27814500	8.14340300
O	-2.46077700	-3.12371400	2.42483300	H	-0.90388100	2.20401300	8.38384500
C	1.06490400	-3.05357000	1.88601500	H	-0.55032300	4.36281100	9.60192100
H	0.44664700	-3.79234100	1.36258600	H	0.66842900	4.18373000	8.33314500
H	2.09144400	-3.43061700	1.90643400	H	-0.70846600	5.26557500	8.08943800
H	0.71033800	-3.00123300	2.92167400	C	1.32021800	-1.74113400	-0.02013800
C	-4.38713700	1.73383300	-0.51659400	C	0.49984400	-2.38190400	0.84636300
C	-3.61219800	0.43943000	-0.33003300	C	1.90910400	-3.03709400	-2.65096800
C	-3.66931500	0.78266600	2.02139500	O	1.26299200	-2.72815600	-3.62299000
C	-4.45319300	2.07096200	1.79754400	O	1.88054600	-4.25408700	-2.07519300
O	-2.82716800	0.52346400	0.88449500	C	4.33059900	-2.55036300	-2.26969000
O	-5.22255000	1.99595800	0.60901200	O	5.21640100	-2.74879400	-1.46751300
H	-3.01079300	0.86041900	2.89067700	O	4.48839000	-2.66222300	-3.60273500
H	-4.35903100	-0.06192200	2.16360400	C	0.92498200	-5.17473600	-2.64332100
H	-5.15091900	2.24033700	2.62371500	H	1.10645000	-5.29895200	-3.71319900
H	-3.75231500	2.92152400	1.75037500	H	1.07812800	-6.11511900	-2.11375300
H	-4.29735600	-0.41444800	-0.24786100	H	-0.08752500	-4.79762500	-2.48219600
H	-2.90835600	0.24467500	-1.13949800	C	5.80003000	-3.05650300	-4.04238400
H	-3.68673900	2.56968600	-0.67398800	H	5.74141800	-3.10541600	-5.12917600
H	-5.04340300	1.66019500	-1.38841900	H	6.54617000	-2.32232800	-3.72860600
H	-0.58491700	-0.05128100	2.51884200	H	6.06553800	-4.03103300	-3.62575200
H	-0.71259700	1.85047000	1.86913100	S	1.06001000	1.57455300	-2.49149900
E-TS2bb^{pH}				O	0.97281200	1.39136400	-3.94922100
C	2.90280000	-2.10915300	-1.91567700	O	-0.05259900	2.19826200	-1.74557500
C	2.69114400	-0.65784000	-2.40339200	C	2.52082200	2.59289600	-2.18058800
H	3.60076800	-0.07516900	-2.20720400	C	3.45677900	2.77001200	-3.20073500
H	2.53127900	-0.66897200	-3.48455000	C	2.67804100	3.20624600	-0.93527700
C	2.71926400	-2.18419100	-0.38472500	C	4.57737000	3.56795100	-2.96142200
H	2.92881400	-3.19620800	-0.04629000	H	3.28884700	2.30222200	-4.16480800
H	3.47148300	-1.52936600	0.07147100	C	3.80140400	3.99943300	-0.70635300
C	1.49954800	0.00060700	-1.73978600	H	1.92057800	3.07643900	-0.16972800
C	0.82049700	-0.53483900	-0.69299100	C	4.75088900	4.17702100	-1.71703900
C	-0.43457200	0.00823500	-0.10352100	H	5.31031300	3.71752300	-3.74858100
H	-1.16266900	0.45004900	-0.77128400	H	3.93326200	4.48466300	0.25618000
C	-0.42785400	0.43743800	1.24776500	H	5.62379700	4.79720700	-1.53519500
C	-1.34710500	1.56687000	1.69116200	Rh	-1.37726200	-1.64517300	0.96192000
H	-0.89434500	2.49190100	1.30505000	Cl	-1.94019800	-2.90101200	-1.09089900

C	-2.10919600	-3.11348100	2.02227100	H	0.31292600	-0.70210700	8.45429500
O	-2.56040800	-3.96682600	2.63716000	H	-1.40670900	-0.67249900	8.10363400
C	0.84279700	-3.60775300	1.63717600	H	-0.84273700	-2.61861500	9.57607000
H	0.23641000	-4.45867100	1.30481300	H	-1.43891500	-3.19970000	8.01583200
H	1.89541300	-3.88695700	1.53427600	H	0.29362300	-3.22922500	8.36606900
H	0.64221600	-3.45860700	2.70434700	C	1.62128400	-2.27978800	-0.48276600
C	-5.48494400	0.28919900	-0.27995600	C	0.90719200	-3.01859300	0.40479900
C	-4.45477100	-0.82697000	-0.20937300	C	2.09491300	-3.22713400	-3.28688800
C	-4.32422500	-0.51227300	2.14420700	O	1.40236200	-2.79639100	-4.17717100
C	-5.37379500	0.58755900	2.03714200	O	2.07855500	-4.50572700	-2.86351200
O	-3.57323700	-0.59462200	0.91638300	C	4.53832900	-2.78087500	-2.95145600
O	-6.23358900	0.37022700	0.92954700	O	5.46752800	-3.02930100	-2.21469000
H	-3.60535300	-0.29337000	2.93693500	O	4.62784000	-2.77092600	-4.29449700
H	-4.80664800	-1.48131500	2.33642100	C	1.07430000	-5.33796900	-3.48216500
H	-6.00117600	0.59934000	2.93394500	H	1.19731200	-5.34047300	-4.56735400
H	-4.87272300	1.56601300	1.95075800	H	1.23197200	-6.33582700	-3.07297800
H	-4.94685400	-1.79903400	-0.07982700	H	0.07958000	-4.96526100	-3.22621300
H	-3.82089300	-0.87722000	-1.09453700	C	5.92181800	-3.09199000	-4.83521900
H	-4.98437800	1.24990000	-0.48383300	H	5.80693100	-3.04027300	-5.91729000
H	-6.20012300	0.09285300	-1.08401000	H	6.66935400	-2.37286300	-4.49157300
H	0.51545300	0.37208300	1.78687500	H	6.22658400	-4.09475300	-4.52636000
H	-0.97460900	-0.76505000	2.24597300	S	1.07829300	1.19824100	-2.68806300
Z-INT-3bb^{PH}				O	1.44239600	1.26106100	-4.11193000
C	3.12537800	-2.39897000	-2.48747000	O	-0.30883600	1.43179300	-2.24553900
C	2.89103900	-0.90151800	-2.77516200	C	2.10582300	2.41535500	-1.83519200
H	3.78160100	-0.33380700	-2.47124500	C	3.37877700	2.70712900	-2.33139800
H	2.75265900	-0.75247900	-3.84751400	C	1.60067100	3.06682800	-0.70752400
C	3.00512200	-2.65971000	-0.97271900	C	4.16864400	3.64466900	-1.66445200
H	3.23166000	-3.70448300	-0.77432000	H	3.72713200	2.22686000	-3.23937000
H	3.77740100	-2.06286700	-0.47237800	C	2.39716000	4.00643100	-0.05156100
C	1.66856000	-0.38454700	-2.05083300	H	0.58841100	2.85624600	-0.37940700
C	1.05084700	-1.04351600	-1.03599400	C	3.68172300	4.28790400	-0.52410100
C	-0.23044700	-0.60350500	-0.40995500	H	5.15896100	3.88077700	-2.04215400
H	-1.07963800	-0.47943600	-1.06930200	H	2.01160900	4.52636500	0.82048300
C	-0.32533100	-0.15837900	0.89067400	H	4.29866500	5.01971400	-0.01093100
C	0.84666200	0.18768100	1.79361500	Rh	-0.97482000	-2.41830500	0.80570200
H	1.68948100	-0.48006300	1.59234700	Cl	-1.86852000	-3.21405500	-1.42942000
H	1.18375100	1.19501300	1.50427100	C	-1.55040600	-4.11973600	1.45075700
C	0.52101500	0.18187900	3.22063000	O	-1.93470300	-5.12443500	1.84001300
C	0.26170700	0.19606700	4.40347700	C	1.40964900	-4.26924600	1.06988500
C	-0.03035600	0.18120100	5.83844400	H	0.88486000	-5.15094300	0.68113500
C	-0.17589400	-1.24111700	6.42008300	H	2.48012700	-4.42778300	0.91602500
H	-0.95025600	0.75025300	6.03243900	H	1.23230000	-4.23373300	2.14958300
H	0.76850200	0.71228600	6.37427800	C	-5.34184700	-0.73001900	0.67425500
C	-0.48350200	-1.23975600	7.92201400	C	-4.32218300	-1.85373100	0.58403200
H	-0.97063700	-1.76937400	5.87786900	C	-3.44198000	-1.17913100	2.69012300
H	0.74906000	-1.79916700	6.22932200	C	-4.48791900	-0.07186800	2.74939800
C	-0.62612100	-2.64974200	8.50358100	O	-3.13059900	-1.47965000	1.31642100

O	-5.65713000	-0.43427100	2.03262800	O	5.37681300	-2.63117500	-1.34539400
H	-2.50614700	-0.87388700	3.16460300	O	4.70290700	-2.65422400	-3.49982000
H	-3.82064200	-2.08708500	3.18163300	C	1.22337700	-5.34777900	-2.47314600
H	-4.78902100	0.10979600	3.78597600	H	1.45961100	-5.53420000	-3.52300900
H	-4.05985800	0.85929300	2.34156100	H	1.38702500	-6.24443800	-1.87518000
H	-4.72997800	-2.77563700	1.02216100	H	0.19089700	-5.00156900	-2.38385900
H	-4.00172000	-2.05499800	-0.43926200	C	6.04870100	-2.97403500	-3.89456700
H	-4.95158700	0.16790100	0.16886700	H	6.02156500	-3.06101300	-4.98019700
H	-6.27594100	-1.02570000	0.18798500	H	6.73640400	-2.18213200	-3.58770200
H	-0.48134500	-2.08702400	2.24851700	H	6.36687000	-3.91502400	-3.43953000
H	-1.28452800	0.25118500	1.19524100	S	0.93998500	1.34282900	-2.65320400
E-INT-3bb^{BH}				O	0.92090800	1.09695800	-4.10374600
C	3.04010500	-2.15585000	-1.87041000	O	-0.24852300	1.88798000	-1.96541000
C	2.73956500	-0.74674300	-2.42683500	C	2.29548000	2.49562300	-2.33775900
H	3.59767100	-0.09004000	-2.23253100	C	3.25882600	2.69948500	-3.32714400
H	2.61048900	-0.81405600	-3.51007700	C	2.34392200	3.18333200	-1.12254500
C	2.82959700	-2.17054200	-0.34179900	C	4.29736800	3.60103800	-3.08609800
H	3.10797500	-3.14642300	0.04829800	H	3.17372100	2.17175700	-4.27089000
H	3.52077700	-1.43892400	0.09421300	C	3.38612500	4.08034200	-0.89204100
C	1.48395100	-0.15645600	-1.82211200	H	1.56566300	3.02925900	-0.38280800
C	0.81818100	-0.69588800	-0.76842400	C	4.36293100	4.28556100	-1.87084300
C	-0.48969000	-0.19205800	-0.25986600	H	5.05026400	3.77235300	-3.84963700
H	-1.26723900	0.02248300	-0.98135600	H	3.43289800	4.62423600	0.04670400
C	-0.60120200	0.29439800	1.02637300	H	5.17220000	4.98644200	-1.68774900
C	-1.70345300	1.24855700	1.44067700	Rh	-1.31670800	-1.95412800	0.95077900
H	-1.41658300	2.23327800	1.03961100	Cl	-1.77165900	-2.96517300	-1.32269500
H	-2.63634000	0.97811400	0.93664700	C	-1.91212900	-3.63841000	1.63746000
C	-1.90627000	1.35673900	2.88650600	O	-2.29845100	-4.63836000	2.03636900
C	-2.06293000	1.46361900	4.08262300	C	1.10596900	-3.59320500	1.77170500
C	-2.22513500	1.62375100	5.52947900	H	0.67985200	-4.55428400	1.45756900
C	-1.17014000	2.55557500	6.16303700	H	2.19457800	-3.69547600	1.76192000
H	-2.17759000	0.63906400	6.01470800	H	0.79614600	-3.42336800	2.80797000
H	-3.22941000	2.01630700	5.74119600	C	-5.71192200	-0.56486800	-0.05922100
C	-1.35758600	2.71853600	7.67568500	C	-4.57655000	-1.57590800	-0.04463400
H	-0.17017400	2.15639300	5.95220400	C	-4.31897400	-1.20540100	2.28897300
H	-1.22124800	3.53588800	5.67318300	C	-5.47277200	-0.21159300	2.24130200
C	-0.31233800	3.64061800	8.31125700	O	-3.64742000	-1.23698600	1.01316500
H	-2.36378800	3.11122600	7.87630500	O	-6.38166700	-0.52825600	1.19742600
H	-1.31526600	1.73107000	8.15538900	H	-3.57228100	-0.90665600	3.02653800
H	-0.47006700	3.73787500	9.39009900	H	-4.69463000	-2.21247700	2.52176800
H	0.70192600	3.25564700	8.15659200	H	-6.03719400	-0.24348200	3.17855300
H	-0.35387300	4.64581700	7.87689300	H	-5.07241100	0.80705700	2.11116700
C	1.39301100	-1.81959400	-0.01871900	H	-4.96648600	-2.58638200	0.13708300
C	0.62842600	-2.48110600	0.88367500	H	-3.99955100	-1.58763800	-0.96941400
C	2.12900600	-3.17971000	-2.58673800	H	-5.32027800	0.43413500	-0.31205500
O	1.53065200	-2.96982300	-3.61400000	H	-6.45762900	-0.84479200	-0.80906500
O	2.11462300	-4.35284900	-1.92567500	H	0.27438800	0.27649700	1.66886900
C	4.50256500	-2.51343700	-2.17578100	H	-1.08514800	-1.47678400	2.42357000

Z-TS3bb^{BH}				O	3.08850900	1.04979900	-4.40651300
C	3.37824900	-2.39040700	-1.87155800	O	0.73396400	1.55173400	-3.52686900
C	3.55016800	-0.97052800	-2.44835600	C	2.80975500	2.72324100	-2.38661900
H	4.46108900	-0.52590300	-2.02325200	C	4.19200800	2.87606600	-2.24709000
H	3.69107200	-1.02118300	-3.52869400	C	1.91820100	3.67133700	-1.88131700
C	2.91317300	-2.30688600	-0.40501800	C	4.68497300	3.98479300	-1.55987400
H	2.79723100	-3.31443300	-0.00964600	H	4.86651800	2.15174700	-2.69158800
H	3.72154000	-1.83725400	0.16974800	C	2.42407500	4.78196000	-1.20172500
C	2.35564200	-0.09719100	-2.14615500	H	0.85394500	3.54313200	-2.04624200
C	1.46109300	-0.35050300	-1.15608300	C	3.80269600	4.93306200	-1.03418500
C	0.20302600	0.43293000	-0.95990400	H	5.75682600	4.11532700	-1.44524800
H	-0.49536000	0.45345100	-1.79142100	H	1.74204300	5.53263300	-0.81361700
C	-0.02355300	1.28502400	0.09552200	H	4.19152900	5.79795400	-0.50487100
C	1.00954800	1.69545000	1.12631300	Rh	-1.09103400	-0.78960600	0.49374500
H	1.84094200	0.98275400	1.13562000	Cl	-3.09253900	0.05918800	-0.54282600
H	1.43407200	2.64728400	0.77105600	C	-2.19649100	-2.05289500	1.41334400
C	0.47850600	1.87835400	2.47807600	O	-2.85866900	-2.80557800	1.96065700
C	0.06747700	2.04948700	3.60366000	C	0.81755800	-3.06043400	1.53239400
C	-0.42309800	2.25386700	4.96742000	H	0.75706600	-3.98628700	0.94652500
C	-1.60673600	1.34077600	5.35103700	H	1.78556600	-3.06370300	2.04682700
H	-0.72080700	3.30415700	5.09176100	H	0.04362000	-3.10514600	2.29843500
H	0.40366600	2.08983700	5.67279800	C	-6.13952400	0.80450800	1.76869900
C	-2.05229400	1.54438800	6.80422700	C	-6.19213800	-0.69930600	1.52866600
H	-2.44555500	1.53761700	4.67166400	C	-6.31915800	-1.06312100	3.84182200
H	-1.31758900	0.29410300	5.19363400	C	-6.26195500	0.44271000	4.08178400
C	-3.22198700	0.64098000	7.20602400	O	-5.63649800	-1.40286400	2.64153900
H	-1.20029800	1.35911700	7.47282100	O	-6.81404700	1.14849400	2.98016500
H	-2.33302500	2.59587600	6.95372100	H	-5.82920600	-1.61007800	4.65444600
H	-3.51065300	0.80324200	8.24947100	H	-7.37293300	-1.38430200	3.78525000
H	-4.10276700	0.83409700	6.58351900	H	-6.84556500	0.72288900	4.96564200
H	-2.96227200	-0.41768000	7.09290600	H	-5.21139300	0.74231700	4.24324300
C	1.63570400	-1.50381600	-0.26379900	H	-7.23716600	-1.01493200	1.37305500
C	0.66656300	-1.85404000	0.63108900	H	-5.59631100	-0.96799300	0.65313900
C	2.36487300	-3.17707600	-2.72308600	H	-5.08876600	1.13059900	1.80885800
O	1.81530300	-2.77015000	-3.71852400	H	-6.64214300	1.34787700	0.96288300
O	2.16551100	-4.40709100	-2.20086300	H	-0.93633900	1.87519100	0.07469600
C	4.73526800	-3.10903600	-1.92609700	H	-0.05813600	-0.74656700	1.65192400
O	5.45500100	-3.30596600	-0.97237500	E-TS3bb^{BH}			
O	5.04542000	-3.45356000	-3.18901000	C	3.04452000	-2.02161800	-1.54831700
C	1.24788600	-5.24196900	-2.93290500	C	3.21474100	-0.69049100	-2.30879800
H	1.60836800	-5.40088500	-3.95181400	H	4.09793700	-0.16676500	-1.91813500
H	1.20889300	-6.18404600	-2.38670100	H	3.39929200	-0.89471200	-3.36605200
H	0.25980100	-4.77789100	-2.97475100	C	2.38150100	-1.75357200	-0.18236800
C	6.31838400	-4.10345700	-3.36526900	H	2.30970900	-2.68336200	0.37800100
H	6.39697100	-4.30626800	-4.43257200	H	3.04928300	-1.09304400	0.38482800
H	7.12898900	-3.44926100	-3.03613200	C	1.99948500	0.20236600	-2.20069900
H	6.35420500	-5.03187800	-2.79071400	C	0.95981900	-0.00486900	-1.34977800
S	2.16496700	1.29923200	-3.28818400	C	-0.31483400	0.77385300	-1.40126200

H	-0.76887100	0.92428800	-2.37348000	H	3.51691300	5.05684100	-0.13317800
C	-0.79648400	1.48973600	-0.33211500	H	5.89607500	4.95822400	-0.83186600
C	-1.90108100	2.52737400	-0.42833800	Rh	-1.82419800	-0.65513200	-0.35840800
H	-2.34800900	2.49925400	-1.42622200	Cl	-3.52316200	-0.08735600	-1.96510700
H	-2.70621100	2.27145600	0.27263400	C	-3.00175400	-2.05562300	0.18396300
C	-1.40151200	3.86888900	-0.10837100	O	-3.71319900	-2.90583500	0.46505000
C	-1.04613700	4.99033500	0.17821800	C	-0.03684400	-2.67667800	1.28115000
C	-0.65465100	6.36050400	0.51411600	H	0.25580400	-3.60246000	0.77198400
C	0.86969200	6.59622100	0.52379700	H	0.69315600	-2.49855600	2.08014300
H	-1.06637200	6.62475900	1.49813900	H	-1.00208400	-2.84669700	1.75807100
H	-1.12027200	7.05023400	-0.20318400	C	-5.47402300	1.02935300	3.79163800
C	1.23919100	8.03978400	0.88555500	C	-4.78791300	0.49332700	2.54010700
H	1.33266900	5.90402700	1.23946600	C	-5.10928400	-1.70135000	3.30799800
H	1.27493200	6.34552100	-0.46423400	C	-5.79541700	-1.16112000	4.55828800
C	2.75105300	8.28609200	0.90124600	O	-4.15710500	-0.75776500	2.81793000
H	0.76421200	8.72398000	0.16970000	O	-6.42033300	0.08767200	4.28604600
H	0.81669200	8.28656300	1.86897600	H	-4.56021000	-2.62278100	3.52517100
H	2.98387800	9.32526400	1.15463400	H	-5.86299800	-1.91313200	2.53338500
H	3.24961500	7.64636800	1.63892100	H	-6.58189500	-1.84178800	4.89935600
H	3.19652300	8.07543600	-0.07766400	H	-5.05200900	-1.04794600	5.36495900
C	1.03045900	-1.09676100	-0.36565000	H	-5.52548400	0.37229800	1.73177700
C	-0.07839300	-1.52472200	0.30121400	H	-4.00162700	1.17256300	2.19779400
C	2.18935600	-2.99530100	-2.38006700	H	-4.71597200	1.24717600	4.56236500
O	1.73993500	-2.77704200	-3.47921200	H	-6.02630000	1.94855100	3.57277500
O	2.00238800	-4.15243500	-1.70584500	H	-0.22533800	1.50134100	0.59405000
C	4.42917300	-2.64650200	-1.32723100	H	-1.15858000	-0.54169200	1.04371200
O	5.00990300	-2.69265400	-0.26594400	Z-INT-4bb^{PH}			
O	4.93801200	-3.10438600	-2.48653300	C	1.95963300	0.02130000	-2.77028300
C	1.23370700	-5.15008600	-2.40542200	C	0.89762600	1.13903200	-2.64773200
H	1.71082100	-5.40080400	-3.35544600	H	1.35793500	2.10118800	-2.90982200
H	1.20869100	-6.01691800	-1.74555100	H	0.10468700	0.97880400	-3.38073800
H	0.22310500	-4.78454400	-2.60224500	C	2.65083800	-0.25831800	-1.41518600
C	6.25267500	-3.68575400	-2.40487900	H	3.30317600	-1.12310300	-1.51819000
H	6.49706600	-3.99853600	-3.41931100	H	3.29790600	0.60415700	-1.20579900
H	6.97395900	-2.94881400	-2.04393400	C	0.27866900	1.28812700	-1.28373600
H	6.24904600	-4.54185900	-1.72618900	C	0.61341000	0.61122900	-0.15835500
S	2.08325100	1.60419800	-3.33807000	C	-0.04307200	0.88026900	1.15909900
O	2.69582900	1.12405400	-4.58735600	H	-1.09687700	0.64019800	1.22792500
O	0.79594700	2.31954000	-3.35083000	C	0.54083900	1.42538100	2.23450800
C	3.29099300	2.68149700	-2.54003300	C	1.96725200	1.92632400	2.34859000
C	4.62354800	2.62400400	-2.95368900	H	2.56479800	1.20580500	2.92840200
C	2.87528400	3.55488800	-1.53122700	H	2.43411400	1.98056100	1.35769600
C	5.56209900	3.45006800	-2.33300700	C	2.03769600	3.23337800	3.01221700
H	4.90280600	1.95723200	-3.76229000	C	2.07518400	4.29670200	3.59005400
C	3.82427000	4.37187500	-0.91696900	C	2.10722700	5.57803200	4.29885100
H	1.82806700	3.60634100	-1.24990100	C	0.72618200	6.26047500	4.40102900
C	5.16362500	4.31721800	-1.31389800	H	2.81213400	6.25650900	3.79805600
H	6.60036300	3.41974600	-2.64957900	H	2.50931200	5.42250300	5.30953900

C	0.78243400	7.59581300	5.15164500	C	-0.17217300	-5.55504800	-0.45867900
H	0.32717500	6.41786100	3.39087100	C	-1.61594300	-3.99327900	-1.57919600
H	0.02815800	5.57909800	4.90276500	C	-1.91888700	-5.06968100	-2.61181600
C	-0.58345900	8.28182200	5.25464400	O	-0.30431600	-4.22827300	-1.01568800
H	1.18636900	7.42830900	6.15942300	O	-1.82069700	-6.36905900	-2.04365400
H	1.49261700	8.26591500	4.64772800	H	-1.57225400	-3.00505600	-2.03895600
H	-0.51315000	9.23119400	5.79516200	H	-2.36254400	-4.00865700	-0.77376200
H	-0.99667000	8.49340800	4.26204300	H	-2.94214300	-4.95634200	-2.98216400
H	-1.30518800	7.64984700	5.78411200	H	-1.22404700	-4.96776500	-3.46037900
C	1.70736700	-0.42073700	-0.23436600	H	-0.84825400	-5.65073000	0.40236600
C	2.13867800	-1.10420000	0.93879200	H	0.86702900	-5.64117400	-0.13782400
C	1.30253700	-1.25955200	-3.31679400	H	0.23337300	-6.54093600	-2.33066000
O	0.13062600	-1.54808000	-3.17900800	H	-0.50445300	-7.59154800	-1.09170900
O	2.19879600	-2.01162900	-3.96345500	H	-0.06628100	1.56226600	3.12675700
C	3.03051800	0.48933800	-3.77167300	H	1.58421800	-0.86811400	1.84080400
O	4.19726700	0.68212700	-3.51558600	E-INT-4bb^{PH}			
O	2.47909700	0.71606900	-4.98082400	C	1.69539200	-1.85165500	-1.72313500
C	1.73472900	-3.28152300	-4.46142500	C	1.35750400	-0.61876500	-2.59213400
H	0.84179600	-3.14202200	-5.07510900	H	2.26188900	-0.30604500	-3.13162500
H	2.55689800	-3.67528100	-5.05800700	H	0.63201400	-0.89175200	-3.36026300
H	1.52594500	-3.94279000	-3.61914400	C	2.13793600	-1.43509400	-0.30137400
C	3.38883900	1.16043900	-6.00228800	H	2.28051600	-2.32724700	0.30533200
H	2.77992900	1.30551600	-6.89418600	H	3.12249700	-0.95903000	-0.40323400
H	3.87068900	2.09578400	-5.70760900	C	0.84825400	0.57447700	-1.82862000
H	4.15842700	0.40546900	-6.18013300	C	0.77296500	0.70703400	-0.48117100
S	-1.01351000	2.58099000	-1.31677200	C	0.31132300	1.97177000	0.16208400
O	-1.63064800	2.50151700	-2.65260900	H	-0.68372100	2.31607300	-0.09408000
O	-1.84903000	2.51067300	-0.10947200	C	1.06767200	2.71395500	0.97945900
C	-0.06952300	4.11511400	-1.26121500	C	0.58946900	3.98884700	1.64006500
C	0.13707000	4.82237000	-2.44752200	H	1.20488500	4.83513000	1.29868400
C	0.43025900	4.57210400	-0.03925100	H	-0.43780300	4.20561200	1.32233900
C	0.86738600	6.01142500	-2.40629400	C	0.66293400	3.90173900	3.10342500
H	-0.28707400	4.44798200	-3.37288900	C	0.73955600	3.80339500	4.30752400
C	1.16734000	5.75533900	-0.01458700	C	0.81782300	3.67340900	5.76351200
H	0.24118600	4.02034000	0.87475800	C	0.59582900	2.23048600	6.26500000
C	1.38496400	6.47306500	-1.19413100	H	0.07369600	4.33621900	6.22671000
H	1.02955000	6.57619000	-3.31948500	H	1.79709000	4.03179500	6.11056400
H	1.57112800	6.11099100	0.92797300	C	0.67922800	2.11505900	7.79124300
H	1.95716400	7.39594800	-1.16768700	H	-0.38421900	1.88000600	5.91777800
Rh	0.87754300	-2.50632700	-0.13697800	H	1.34144600	1.57262700	5.80090000
Cl	2.74052200	-3.71268100	-1.08531800	C	0.45861500	0.68564100	8.29611300
C	-0.65543100	-2.03021800	0.79303900	H	1.66015300	2.47620800	8.12946000
O	-1.64368700	-1.94325000	1.38686600	H	-0.06418000	2.78383500	8.24626000
C	3.55389300	-1.54555700	1.22584600	H	0.52232900	0.63345000	9.38777800
H	4.10667200	-1.85944700	0.34318500	H	-0.52781600	0.30973100	8.00179600
H	4.08979900	-0.71076000	1.70172800	H	1.20851600	-0.00004300	7.88583200
H	3.55548900	-2.37971000	1.93223500	C	1.21667100	-0.44083300	0.38794100
C	-0.51503100	-6.58640200	-1.52393000	C	1.23143800	-0.31926400	1.80728000

C	0.48019300	-2.79513700	-1.66369600	H	-3.14765500	-5.32342200	1.75243300
O	-0.67335500	-2.45026300	-1.82644000	H	-4.30941600	-4.87572300	3.03040800
O	0.86862800	-4.04874400	-1.40897900	H	2.08609100	2.41275900	1.22080200
C	2.86127900	-2.59711600	-2.39605700	H	0.84335200	0.61042900	2.20614200
O	3.96809100	-2.74159800	-1.92900000	Z-P3			
O	2.50108300	-3.02578200	-3.62254400	C	2.12147700	0.17051700	-2.92929900
C	-0.17765800	-5.02618500	-1.25061300	C	1.11556500	1.33982100	-2.90356200
H	-0.84196800	-5.01026300	-2.11783600	H	1.63045700	2.25956700	-3.21490200
H	0.33296600	-5.98516800	-1.17082300	H	0.32134100	1.16233700	-3.63120900
H	-0.73127300	-4.81512700	-0.33462000	C	2.95496300	0.17735000	-1.63226500
C	3.51572600	-3.73605700	-4.35351800	H	3.70467200	-0.61028900	-1.67736300
H	3.05977900	-3.99900800	-5.30758700	H	3.49802300	1.12926500	-1.59733500
H	4.39312900	-3.10311400	-4.50708600	C	0.49328200	1.55524600	-1.54284400
H	3.81718000	-4.63455600	-3.80983100	C	0.88152000	0.95302100	-0.38859300
S	0.39708900	1.92175500	-2.97811800	C	0.15171400	1.11906300	0.90170000
O	0.04961200	1.26759800	-4.25126900	H	-0.89290700	0.82817200	0.89189000
O	-0.54584100	2.85529300	-2.34162900	C	0.66152200	1.59810300	2.04414300
C	1.94644500	2.80348200	-3.24681100	C	2.06153500	2.13517800	2.26531900
C	2.77535900	2.40895300	-4.30008600	H	2.65911500	1.38597300	2.80771800
C	2.28224100	3.87631100	-2.41727100	H	2.56866100	2.28591900	1.30593100
C	3.97412000	3.09153700	-4.51025500	C	2.05705000	3.38428300	3.03605700
H	2.46498400	1.60148800	-4.95443200	C	2.04098400	4.40021800	3.69449200
C	3.48236900	4.55153200	-2.63935900	C	2.00835900	5.61973500	4.50489800
H	1.60251000	4.18044500	-1.62988500	C	0.58845100	6.19319900	4.69841600
C	4.32844000	4.15663500	-3.67902700	H	2.64960800	6.38451300	4.04450900
H	4.62519500	2.79806100	-5.32816000	H	2.45087700	5.41225400	5.48924000
H	3.75338200	5.39116300	-2.00628200	C	0.57469900	7.45642000	5.56689200
H	5.26094600	4.68717900	-3.84786700	H	0.15225200	6.41209900	3.71546600
Rh	-0.54120100	-1.47610400	1.32272000	H	-0.04806200	5.42292400	5.15106200
Cl	0.48732000	-3.57468300	1.91274500	C	-0.83162800	8.03072400	5.76465500
C	-1.65106200	0.00926100	1.22786100	H	1.01878000	7.22783900	6.54540300
O	-2.47831300	0.81542100	1.27746200	H	1.22161900	8.21832000	5.11056300
C	2.24123300	-0.95850300	2.72915900	H	-0.81141100	8.93060000	6.38782600
H	2.61381300	-1.92046200	2.38449000	H	-1.28835800	8.29980400	4.80559100
H	3.09004500	-0.26743900	2.84069000	H	-1.49140400	7.30348700	6.25105800
H	1.80769100	-1.10710400	3.72132400	C	2.05904700	0.04051000	-0.42346600
C	-3.80547100	-4.52264300	2.12565600	C	2.27488700	-0.85392600	0.56467800
C	-2.97143900	-3.28903400	2.43795500	C	1.37374800	-1.16581800	-3.07465900
C	-3.41595000	-2.48893800	0.21547400	O	0.17564400	-1.30522300	-3.13912500
C	-4.23873100	-3.74482300	-0.03356600	O	2.25370600	-2.19133600	-3.11485400
O	-2.40617500	-2.76958600	1.21350900	C	3.05100600	0.34672900	-4.13764400
O	-4.81810800	-4.22645900	1.17204200	O	4.21449400	0.67630000	-4.08113100
H	-2.87272700	-2.18323000	-0.67987100	O	2.38518800	0.12717600	-5.28829500
H	-4.05816100	-1.67208400	0.57113800	C	1.66795300	-3.49655700	-3.26382700
H	-5.06124700	-3.52391900	-0.72041700	H	1.10009400	-3.55617600	-4.19542000
H	-3.59973000	-4.51891900	-0.48757200	H	2.50460900	-4.19476200	-3.27838600
H	-3.59173700	-2.51042600	2.90331500	H	0.99882900	-3.71319400	-2.42776400
H	-2.12234300	-3.53136700	3.07893800	C	3.15060300	0.30170900	-6.49434900

H	2.46163500	0.08963800	-7.31118200	C	-0.24323500	0.46076600	8.25331200
H	3.52680200	1.32513400	-6.56336800	H	1.23438800	2.04066000	8.25720000
H	3.99655200	-0.38954600	-6.51276900	H	-0.42388400	2.61561200	8.27101100
S	-0.84812700	2.77889400	-1.61080100	H	-0.27118200	0.35800900	9.34289300
O	-1.36721600	2.76012000	-2.99003600	H	-1.25144400	0.25959900	7.87400100
O	-1.76114300	2.61015100	-0.46964400	H	0.41845200	-0.32060100	7.86243600
C	0.02452900	4.34400200	-1.40132100	C	1.89090400	-0.20585900	0.21455700
C	0.32112100	5.10609200	-2.53311100	C	1.65408000	-0.36383100	1.53405100
C	0.39025200	4.76524100	-0.11999800	C	0.79220000	-2.51388700	-1.29253400
C	1.00574600	6.31263900	-2.37611600	O	-0.36816100	-2.28841900	-1.54132000
H	-0.00125800	4.75923600	-3.50893100	O	1.20893700	-3.54206200	-0.51973400
C	1.08242300	5.96717100	0.02158000	C	2.91068400	-2.61475500	-2.60845300
H	0.13410900	4.16782500	0.74781000	O	4.11131100	-2.70176700	-2.48024100
C	1.38972500	6.73870100	-1.10287700	O	2.20111700	-3.29087100	-3.53339400
H	1.23610200	6.91887500	-3.24719100	C	0.16329900	-4.38993400	-0.01322200
H	1.38148500	6.29572800	1.01202600	H	-0.39832700	-4.83675500	-0.83707000
H	1.92640300	7.67581500	-0.98551400	H	0.66590800	-5.15984700	0.57188100
C	3.38643300	-1.85272600	0.68556400	H	-0.52451100	-3.81662500	0.61285400
H	4.05038000	-1.88361000	-0.17979800	C	2.96292600	-4.16039100	-4.39020500
H	3.99886300	-1.63779700	1.57142500	H	2.23896200	-4.60994700	-5.06894200
H	2.97657100	-2.85941600	0.83553900	H	3.71026700	-3.58985500	-4.94671100
H	0.00985600	1.64204400	2.91435700	H	3.46930300	-4.92882900	-3.80115700
H	1.56534100	-0.86182800	1.38822000	S	0.43398700	1.96053600	-3.03769800
E-P3				O	0.01102700	1.26122800	-4.26347900
C	1.99704100	-1.69534900	-1.78688700	O	-0.49995100	2.86026400	-2.33911700
C	1.51709000	-0.53940000	-2.68975800	C	1.89756800	2.92575000	-3.46549700
H	2.33358700	-0.26212700	-3.37075500	C	2.61854200	2.58821100	-4.61300700
H	0.69071900	-0.87881800	-3.31696400	C	2.27895100	3.99744800	-2.65449500
C	2.78189200	-1.12215700	-0.58866600	C	3.75294500	3.33115400	-4.94341300
H	3.18475400	-1.93730700	0.00911300	H	2.27267400	1.77481700	-5.24167900
H	3.63746100	-0.56787400	-0.99132800	C	3.41426600	4.73212000	-2.99530100
C	1.08520300	0.68802400	-1.91689100	H	1.68499600	4.25276400	-1.78442900
C	1.21777500	0.86829600	-0.57274400	C	4.15175700	4.39733600	-4.13436300
C	0.72500400	2.07462900	0.13444100	H	4.31902700	3.08249300	-5.83613500
H	-0.23225400	2.46558200	-0.19065300	H	3.71931600	5.57084900	-2.37655700
C	1.40412900	2.72213100	1.09191700	H	5.03376800	4.97459700	-4.39619300
C	0.88751600	3.95916300	1.79271000	C	2.22166300	-1.39772900	2.45986400
H	1.53913000	4.81374200	1.55340700	H	2.86219000	-2.13122400	1.96813100
H	-0.10760100	4.21407500	1.40757100	H	2.80697800	-0.91532700	3.25393700
C	0.84082000	3.79322600	3.25055400	H	1.41128300	-1.93850800	2.96469800
C	0.81905900	3.64217800	4.45120200	H	2.38226900	2.36992900	1.41226000
C	0.77210600	3.44519100	5.90111700	H	0.97165500	0.33616000	2.00768400
C	0.28791600	2.03939900	6.31445700	R-INT-2c^H			
H	0.11180400	4.20108700	6.34873300	C	2.49002900	-1.88231000	-1.39492300
H	1.76826300	3.62618200	6.32871300	C	2.20815400	-0.45770900	-1.93078600
C	0.23727800	1.85406800	7.83535700	H	3.14338600	0.11611000	-1.91260200
H	-0.70590000	1.86420500	5.88418400	H	1.89461100	-0.53394400	-2.97548300
H	0.95308000	1.28834100	5.86971200	C	2.48206800	-1.88306200	0.15633400

H	2.72982100	-2.87665900	0.52833400	H	2.12614200	2.17427400	-4.37820800
H	3.26280200	-1.19388100	0.49806700	C	3.88942500	4.12561200	-1.51681800
C	1.14356000	0.28717500	-1.14483100	H	2.28921200	3.39584400	-0.26124600
C	0.59892300	-0.16721700	0.01775600	C	4.42696000	4.14441900	-2.80718700
C	-0.57812000	0.36624700	0.78172000	H	4.21578400	3.46966500	-4.84493100
H	-1.18060000	1.04808000	0.18637900	H	4.37241300	4.67891400	-0.71710300
C	-0.28738100	0.98279000	2.16421100	H	5.33182000	4.71093800	-3.00680500
C	-1.56189600	1.69741500	2.68594600	C	0.88335100	1.98200700	2.11674400
H	-1.77386300	2.54687300	2.02106600	H	0.67986900	2.77475000	1.38987800
H	-2.42638500	1.02730900	2.60235300	H	1.02386500	2.43892300	3.10069500
C	-1.45692900	2.17077700	4.06637800	H	1.81603100	1.48484300	1.83331700
C	-1.36641500	2.55480400	5.21107600	Rh	-1.52034300	-1.53036100	0.65967000
C	-1.27074900	3.06357900	6.58071400	Cl	-2.34519500	-3.79767800	0.06834100
C	-1.28341600	4.60495800	6.65900900	C	-2.37090200	-1.52281400	2.26646300
H	-0.35227500	2.68400300	7.04986500	O	-2.90232300	-1.59945400	3.28519200
H	-2.10071100	2.66273000	7.17919700	C	0.44973000	-3.34112000	2.20927300
C	-1.17807500	5.12888100	8.09591900	H	-0.17874900	-4.17369700	1.87962000
H	-0.45444500	4.99861200	6.05752000	H	1.50107700	-3.64880300	2.21942300
H	-2.20460000	4.97699500	6.19350100	H	0.16392900	-3.10577400	3.24223100
C	-1.19033900	6.65864500	8.17674000	C	-3.14370900	-0.39856700	-3.43916700
H	-2.00693100	4.72337500	8.69219000	C	-2.99839000	-1.38660600	-2.29144200
H	-0.25705400	4.74480800	8.55566900	C	-3.93659300	0.25441100	-0.82817200
H	-1.11140000	7.00483100	9.21237200	C	-4.06659100	1.20466300	-2.01288400
H	-0.35382400	7.09127900	7.61628200	O	-2.83695400	-0.65019000	-1.04862700
H	-2.11553000	7.07018800	7.75780000	O	-4.25053300	0.47575800	-3.21684900
C	1.11917200	-1.42743500	0.60566100	H	-3.71652000	0.79605800	0.09516900
C	0.23717400	-2.15358000	1.33941600	H	-4.85732700	-0.33095300	-0.69851800
C	1.41540300	-2.85575500	-1.92025700	H	-4.94475200	1.84602800	-1.88548500
O	0.46221000	-2.53676100	-2.59657000	H	-3.16864200	1.83884500	-2.07474200
O	1.67158300	-4.10652700	-1.51020900	H	-3.88019900	-2.03134900	-2.20170100
C	3.86646900	-2.33699400	-1.89646300	H	-2.10783100	-2.00608600	-2.40405500
O	4.85056600	-2.47050100	-1.20462900	H	-2.21554500	0.17860700	-3.55666500
O	3.84809700	-2.53318300	-3.22908300	H	-3.34804000	-0.93791100	-4.36912700
C	0.70037500	-5.10695100	-1.90085300	H	-0.01799200	0.19256200	2.87388900
H	0.60361600	-5.12866800	-2.98850700	R-TS2cc^H			
H	1.09834100	-6.05115200	-1.53050700	C	0.84485100	0.50998400	-1.04589000
H	-0.26722600	-4.88446400	-1.44515800	C	0.43345200	-0.88519700	-0.89203000
C	5.09646500	-2.94872400	-3.81395500	Rh	-1.94678400	0.45311100	-1.74762200
H	4.89725200	-3.06079100	-4.87910400	Cl	-3.70006500	-0.97225600	-2.87824900
H	5.86850200	-2.19487600	-3.64254900	C	1.46096200	-1.99255200	-0.92982200
H	5.42275000	-3.89683500	-3.38029600	C	2.14558000	0.80607800	-1.32584300
S	0.59254300	1.78393300	-1.97859600	H	1.18162700	-2.79971000	-0.24785100
O	0.05598500	1.38740500	-3.29590000	H	1.49413800	-2.44610600	-1.92821700
O	-0.23073700	2.61182500	-1.07440400	H	3.95316000	-1.93958300	3.27833400
C	2.11613700	2.69984400	-2.29590000	C	2.90723000	-2.15341600	3.04602300
C	2.63877900	2.71477400	-3.58995800	O	2.72717900	-2.29066600	1.62558000
C	2.72536400	3.40447700	-1.25414600	H	2.60560600	-3.10910300	3.47367600
C	3.80198600	3.44481000	-3.84132900	H	2.28475100	-1.34427700	3.43568900

C	3.06219200	-1.21182400	0.88755500	H	-4.49776400	0.80913300	2.30425100
C	2.88984200	-1.50759300	-0.61019100	C	-6.99281700	-0.01588100	3.23223500
O	3.45045800	-0.17228200	1.37392000	H	-6.83683000	1.25123500	1.48653400
C	3.88995400	-2.61100000	-0.99970800	H	-7.02629700	-0.45341300	1.11352700
O	3.65875500	-3.52115400	-1.76322500	H	-8.07911200	0.08529300	3.32051800
O	5.08737600	-2.40036500	-0.42110400	H	-6.72538900	-1.02717700	3.55892600
C	6.12166300	-3.34070400	-0.76810200	H	-6.53503300	0.69063400	3.93403900
H	6.30316900	-3.32584500	-1.84507400	H	-0.12091200	-0.11667800	1.58781900
H	7.00739900	-3.01427000	-0.22439600	H	-1.46176700	0.79479400	2.32353000
H	5.83381500	-4.35119300	-0.46878000	C	-2.97284700	2.03037600	-2.41163600
C	-0.91403500	-1.14942700	-0.87022100	O	-3.64679000	2.90435600	-2.71756700
C	-0.27950000	1.50036200	-0.86803400	C	-0.51920400	1.60658900	-4.51041100
H	-0.09717500	2.41819400	-1.42422900	C	0.63963000	1.46505300	-5.48715400
C	3.22244100	-0.25115100	-1.44826000	C	0.37509500	-0.85142400	-5.51770700
H	3.33606500	-0.55949700	-2.49652000	C	-0.79472600	-0.75452800	-4.54867600
H	4.18583800	0.15558400	-1.14098900	O	0.47702300	0.31902300	-6.31498200
S	2.71070200	2.46441300	-1.73751100	O	-0.62952500	0.41029500	-3.70539800
O	1.80041300	3.06356300	-2.74201800	H	1.31129200	-1.01613500	-4.95821000
O	4.14480200	2.34317700	-2.05630200	H	0.22483600	-1.69419800	-6.19980200
C	2.57116900	3.48633300	-0.25507600	H	-1.74814200	-0.67609800	-5.08196900
C	1.91292300	4.71292700	-0.35374200	H	-0.84303900	-1.61556200	-3.88164900
C	3.19493300	3.08308700	0.92916300	H	0.68022300	2.33625800	-6.14759400
C	1.87024800	5.55098300	0.76250200	H	1.58171200	1.41110100	-4.92320700
H	1.45134900	4.99506100	-1.29361000	H	-0.33030500	2.43201400	-3.82473000
C	3.13619800	3.92675100	2.03867300	H	-1.46484700	1.75991600	-5.04882500
H	3.69075100	2.12053300	0.99277800	H	0.46515000	2.13241700	1.05668900
C	2.47837800	5.15768800	1.95610400	E-INT-2c^{BH}			
H	1.36400200	6.50956100	0.69724500	C	3.78545700	-1.84034700	-1.26755000
H	3.60906200	3.62277100	2.96779500	C	3.91256500	-0.37442200	-1.73940600
H	2.44157400	5.81094000	2.82319100	H	4.84756800	0.05717200	-1.36380700
C	-0.50325900	1.82831400	0.63573000	H	3.97236400	-0.35625900	-2.83084900
C	-0.96333300	0.54759200	1.37915400	C	3.37855100	-1.87712800	0.22274800
C	-1.48082400	2.98960200	0.83345700	H	3.35060400	-2.90972000	0.56538300
H	-1.54481100	3.26838000	1.89076900	H	4.16808500	-1.37174600	0.79180200
H	-1.14778700	3.87031700	0.27569000	C	2.74466400	0.46841800	-1.27411900
H	-2.48731600	2.73240600	0.48811900	C	1.85731000	0.08393300	-0.32137400
C	-1.47757200	-2.54357700	-0.82339600	C	0.64029600	0.82844700	0.11341200
H	-1.11300700	-3.13293500	-1.67307200	H	0.13770500	1.39778000	-0.66068700
H	-1.17397000	-3.06833700	0.09268600	C	0.64768300	1.49550600	1.45911200
H	-2.56569400	-2.53130000	-0.88148900	C	-0.11479500	2.84354200	1.43232200
C	-1.93818400	-0.08696800	0.44156700	H	0.53342800	3.54988000	0.89854900
C	-3.10232700	0.21663100	-0.01853600	H	-1.01609800	2.72615300	0.82381800
C	-4.55649500	0.36978900	0.17943000	C	-0.47144000	3.36246200	2.75322200
C	-5.00687900	0.10923200	1.62857400	C	-0.77548500	3.78106000	3.84922100
H	-5.06100700	-0.31164600	-0.51745100	C	-1.09825300	4.33536100	5.16629400
H	-4.85301200	1.37909300	-0.13920600	C	-0.04621700	5.34285000	5.67697400
C	-6.52558200	0.24469200	1.79702200	H	-1.20148100	3.51793500	5.89340600
H	-4.69020600	-0.89878300	1.92518700	H	-2.08053800	4.82637500	5.12467900

C	-0.39546400	5.91548500	7.05545500	C	-3.49479100	0.74364900	-0.34467200
H	0.93179400	4.84732600	5.71573800	C	-3.38933800	1.29659200	1.96415600
H	0.04966900	6.15686900	4.94798400	C	-4.21966400	2.54353000	1.68551200
C	0.64365300	6.91876100	7.56576300	O	-2.62596000	0.93970900	0.79411100
H	-1.38061600	6.39955000	7.00844100	O	-5.07057900	2.35077400	0.56502800
H	-0.49552500	5.09203800	7.77591200	H	-2.67022900	1.48159700	2.76515100
H	0.36911400	7.31121500	8.55011200	H	-4.04354800	0.45597900	2.23640300
H	1.63195600	6.45417300	7.65625700	H	-4.86277700	2.76692800	2.54237000
H	0.74063200	7.77014800	6.88283600	H	-3.54846600	3.40165900	1.52039700
C	2.04842900	-1.17962700	0.40051300	H	-4.15556700	-0.10996900	-0.14449000
C	1.01468400	-1.62021700	1.15505800	H	-2.84986800	0.49320100	-1.18700800
C	2.74120700	-2.56678900	-2.14025900	H	-3.63765200	2.83535100	-0.86276100
O	2.23078800	-2.11563300	-3.13985200	H	-5.01972200	1.84672900	-1.40330700
O	2.47168000	-3.78843500	-1.64320200	C	1.98793900	1.60185400	2.19770400
C	5.14149900	-2.53918800	-1.43820600	H	1.84031200	2.06524200	3.17632300
O	5.86816500	-2.88036500	-0.53185700	H	2.45616000	0.62670200	2.33451700
O	5.44147900	-2.69844200	-2.74221300	H	2.66050600	2.23272300	1.60822200
C	1.44242000	-4.52079100	-2.33817400	H	0.00380900	0.81064800	2.20725400
H	1.69965100	-4.63205100	-3.39388300	E-TS2cc^{BH}			
H	1.39531100	-5.49296500	-1.84778700	C	3.65016700	-1.99457500	-1.05993300
H	0.49000800	-3.99364000	-2.24597200	C	3.82064200	-0.45980100	-1.09615200
C	6.71244100	-3.31494800	-3.01649300	H	4.67047700	-0.16358200	-0.47021700
H	6.78168600	-3.37135300	-4.10229800	H	4.05749500	-0.15441500	-2.11855100
H	7.52600900	-2.70983100	-2.60936200	C	3.00707200	-2.42242600	0.27816200
H	6.75637300	-4.31292800	-2.57392700	H	2.93903500	-3.50787100	0.31112200
S	2.68690400	2.07982700	-2.05919700	H	3.68916600	-2.11872300	1.08159400
O	1.76510500	2.96523300	-1.31458200	C	2.57329700	0.25191500	-0.62122600
O	4.08253200	2.51679100	-2.25196300	C	1.55847600	-0.35159800	0.04709500
C	1.99030700	1.78032900	-3.69621500	C	0.28960400	0.31335300	0.46108500
C	0.94326900	0.87429800	-3.87857100	H	-0.17174100	0.99205900	-0.24623600
C	2.50268800	2.52976100	-4.75774900	C	0.01301800	0.55850800	1.83797300
C	0.39553200	0.72909500	-5.15376700	C	-0.92028500	1.74019500	2.11859700
H	0.57919300	0.26471900	-3.05812700	H	-0.28149600	2.62954200	2.00828600
C	1.93912300	2.38058000	-6.02466900	H	-1.67266900	1.80197200	1.32797600
H	3.33354000	3.20533700	-4.58522200	C	-1.56197700	1.74154000	3.43337700
C	0.88651200	1.48343000	-6.22154200	C	-2.09498000	1.74523500	4.52138000
H	-0.40838900	0.01661700	-5.31044300	C	-2.70517800	1.77515000	5.85269000
H	2.32772100	2.95823300	-6.85813400	C	-1.74067000	2.25622800	6.95767600
H	0.45555500	1.36394000	-7.21147400	H	-3.07772200	0.77316000	6.10680900
Rh	-0.66127800	-0.50001100	1.06313700	H	-3.58837700	2.42856600	5.83144300
Cl	-1.21574800	-1.72601900	-0.92847000	C	-2.39464500	2.27548500	8.34399600
C	-1.78193000	-1.66493900	2.25677900	H	-0.85936900	1.60280500	6.97084800
O	-2.42963400	-2.34132200	2.91593800	H	-1.37758100	3.25913300	6.70160700
C	0.98066500	-2.89233900	1.94637200	C	-1.44297300	2.74912700	9.44698700
H	0.22030000	-3.57015100	1.54157500	H	-3.27982400	2.92565700	8.31880700
H	1.94204600	-3.41468700	1.92713800	H	-2.76339000	1.26903400	8.58511400
H	0.72772600	-2.70466800	2.99644100	H	-1.93623400	2.75234800	10.42417800
C	-4.30892200	2.00574800	-0.58690200	H	-0.56491900	2.09755100	9.51957100

H	-1.08439100	3.76593000	9.25162300	H	-4.32893600	2.29394100	1.70734100
C	1.65376200	-1.76354600	0.43690400	H	-4.43062600	-0.59934600	-0.94559500
C	0.53432800	-2.37176400	0.89581000	H	-2.97239500	0.24537900	-1.50397600
C	2.78538200	-2.43578200	-2.26008600	H	-3.91443200	2.42268700	-0.71440800
O	2.46929500	-1.72687700	-3.18753700	H	-5.11498900	1.63694700	-1.77245000
O	2.43851600	-3.73066400	-2.14728700	H	-0.95813300	-0.70411500	2.30541400
C	5.03211300	-2.65221600	-1.18525600	C	1.04988000	0.31205200	2.91736400
O	5.59643800	-3.26114200	-0.30376500	H	1.77851800	1.13017400	2.85554500
O	5.56071300	-2.43584200	-2.40551500	H	0.59287700	0.33372000	3.90837000
C	1.55652300	-4.22181100	-3.17818100	H	1.57924500	-0.62858700	2.77951800
H	1.99901800	-4.06454300	-4.16433400	S-INT-2c^H			
H	1.43584300	-5.28565000	-2.97428500	C	0.74282400	0.52497200	-0.90763300
H	0.59703500	-3.70300800	-3.11693600	C	0.36574800	-0.88779400	-0.77441100
C	6.87565000	-2.97978900	-2.61835100	Rh	-2.01041300	0.42604300	-1.68039000
H	7.13826400	-2.71712100	-3.64256800	Cl	-3.67782100	-0.97668200	-2.96516800
H	7.58777000	-2.54351300	-1.91381800	C	1.41491600	-1.97445500	-0.79535300
H	6.86638300	-4.06450800	-2.48781100	C	2.02326300	0.83994300	-1.26558300
S	2.58694500	2.01093400	-0.97007400	H	1.16517700	-2.76120900	-0.07815900
O	1.50860500	2.67729400	-0.20767900	H	1.43624100	-2.46507800	-1.77617800
O	3.97444900	2.47742000	-0.78911200	H	3.95462400	-1.77251100	3.35409100
C	2.20106200	2.13682000	-2.72696900	C	2.88983900	-1.91808400	3.15765800
C	1.19277100	1.35441200	-3.29524700	O	2.66198000	-2.11092800	1.74996600
C	2.90629900	3.08084200	-3.47617400	H	2.52988000	-2.82638400	3.63993200
C	0.88435200	1.53497400	-4.64381900	H	2.33997900	-1.04590000	3.51907900
H	0.67592200	0.59400800	-2.71802100	C	3.05496900	-1.09685200	0.95238100
C	2.58024400	3.25638100	-4.82096800	C	2.83673800	-1.44770500	-0.52779300
H	3.69866500	3.65366400	-3.00660400	O	3.53097600	-0.06674800	1.37869000
C	1.57045600	2.48617500	-5.40243900	C	3.85210900	-2.53912600	-0.91575100
H	0.11367800	0.92184700	-5.10041100	O	3.62824400	-3.45543900	-1.67400200
H	3.11993100	3.98809800	-5.41484300	O	5.04919100	-2.31384900	-0.34220100
H	1.32463900	2.62010500	-6.45202700	C	6.09179400	-3.24505600	-0.69025500
Rh	-1.15427500	-1.26838600	0.80118900	H	6.27178900	-3.22862300	-1.76741700
Cl	-1.26038300	-1.81069500	-1.61677300	H	6.97502100	-2.91048100	-0.14741900
C	-2.36420300	-2.71694700	1.28969000	H	5.81329600	-4.25797600	-0.39045900
O	-3.09405100	-3.54997500	1.58303100	C	-0.97295200	-1.18976100	-0.83449200
C	0.43829400	-3.79377200	1.35965400	C	-0.40637600	1.47067000	-0.67878800
H	-0.20408900	-4.37532200	0.68804900	H	-0.24074200	2.43264000	-1.15795700
H	1.41573200	-4.28375100	1.39530600	C	3.10637500	-0.21280900	-1.41899600
H	0.00186300	-3.85188700	2.36332900	H	3.16929500	-0.54899700	-2.46199900
C	-4.58710100	1.55526900	-0.81762200	H	4.08395100	0.20521600	-1.17817700
C	-3.77958500	0.26754100	-0.77201900	S	2.53768000	2.45910500	-1.86496100
C	-4.15811900	0.14848100	1.56837900	O	1.40470600	3.13322900	-2.54007700
C	-4.97711000	1.43090900	1.48426400	O	3.77314900	2.21240700	-2.63209100
O	-3.15908600	0.13422400	0.52810500	C	2.97794800	3.51566500	-0.46726600
O	-5.57716600	1.57481400	0.20555200	C	2.48262700	4.82114600	-0.45678600
H	-3.62340500	0.08918000	2.51816000	C	3.86064400	3.06314100	0.51616500
H	-4.81094700	-0.72846100	1.45110700	C	2.87750300	5.68872200	0.56314500
H	-5.78825900	1.40890000	2.21872700	H	1.80185400	5.13856600	-1.23865600

C	4.23973000	3.93817600	1.53431000	H	0.08066500	2.50527000	2.67055800
H	4.21638600	2.03952600	0.51663900	H	-1.60774800	2.35192400	0.85064100
C	3.75367900	5.24814600	1.55705200	S-TS2cc^H			
H	2.50029000	6.70701100	0.57944600	C	0.74282400	0.52497200	-0.90763300
H	4.91588700	3.59362000	2.31095800	C	0.36574800	-0.88779400	-0.77441100
H	4.05671400	5.92474000	2.35094900	Rh	-2.01041300	0.42604300	-1.68039000
C	-0.73422400	1.68787100	0.83025400	Cl	-3.67782100	-0.97668200	-2.96516800
C	-1.19064600	0.36381600	1.48718400	C	1.41491600	-1.97445500	-0.79535300
C	-1.49257900	-2.60071500	-0.87750100	C	2.02326300	0.83994300	-1.26558300
H	-1.07351300	-3.13926700	-1.73598800	H	1.16517700	-2.76120900	-0.07815900
H	-1.21170200	-3.15943400	0.02578000	H	1.43624100	-2.46507800	-1.77617800
H	-2.57719600	-2.61738000	-0.98244100	H	3.95462400	-1.77251100	3.35409100
C	-2.10332900	-0.23332600	0.47303900	C	2.88983900	-1.91808400	3.15765800
C	-3.24980400	0.06808900	-0.02462600	O	2.66198000	-2.11092800	1.74996600
C	-4.71258100	0.20449000	0.10024900	H	2.52988000	-2.82638400	3.63993200
C	-5.24648700	-0.16375000	1.49684500	H	2.33997900	-1.04590000	3.51907900
H	-5.17544700	-0.41939400	-0.67488700	C	3.05496900	-1.09685200	0.95238100
H	-4.99074600	1.23733100	-0.15448700	C	2.83673800	-1.44770500	-0.52779300
C	-6.77172900	-0.02668100	1.58638500	O	3.53097600	-0.06674800	1.37869000
H	-4.95255900	-1.19450400	1.73199100	C	3.85210900	-2.53912600	-0.91575100
H	-4.77427200	0.47747800	2.25294600	O	3.62824400	-3.45543900	-1.67400200
C	-7.32452800	-0.38743500	2.96850500	O	5.04919100	-2.31384900	-0.34220100
H	-7.05857000	1.00306200	1.33378900	C	6.09179400	-3.24505600	-0.69025500
H	-7.23499900	-0.66742800	0.82476300	H	6.27178900	-3.22862300	-1.76741700
H	-8.41362000	-0.28266300	2.99994200	H	6.97502100	-2.91048100	-0.14741900
H	-7.08212300	-1.42236700	3.23511500	H	5.81329600	-4.25797600	-0.39045900
H	-6.90554000	0.26162000	3.74597100	C	-0.97295200	-1.18976100	-0.83449200
H	-0.34139700	-0.28975300	1.70835800	C	-0.40637600	1.47067000	-0.67878800
H	-1.73841000	0.56015500	2.41572100	H	-0.24074200	2.43264000	-1.15795700
C	-3.04492900	2.02734900	-2.26921700	C	3.10637500	-0.21280900	-1.41899600
O	-3.72270800	2.91890100	-2.50948000	H	3.16929500	-0.54899700	-2.46199900
C	-0.73738000	1.66444500	-4.44800300	H	4.08395100	0.20521600	-1.17817700
C	0.39576700	1.66786400	-5.46523500	S	2.53768000	2.45910500	-1.86496100
C	0.51792200	-0.65553200	-5.39351600	O	1.40470600	3.13322900	-2.54007700
C	-0.62129400	-0.71197900	-4.38544000	O	3.77314900	2.21240700	-2.63209100
O	0.39138600	0.47531100	-6.24189500	C	2.97794800	3.51566500	-0.46726600
O	-0.63565000	0.50092800	-3.59403400	C	2.48262700	4.82114600	-0.45678600
H	1.48637500	-0.63112300	-4.86635600	C	3.86064400	3.06314100	0.51616500
H	0.49154200	-1.54385400	-6.03264600	C	2.87750300	5.68872200	0.56314500
H	-1.59055000	-0.82477600	-4.88153600	H	1.80185400	5.13856600	-1.23865600
H	-0.49108900	-1.53568300	-3.68227500	C	4.23973000	3.93817600	1.53431000
H	0.26767900	2.50373900	-6.15978400	H	4.21638600	2.03952600	0.51663900
H	1.35549300	1.78931500	-4.94338400	C	3.75367900	5.24814600	1.55705200
H	-0.65675400	2.53371300	-3.79571200	H	2.50029000	6.70701100	0.57944600
H	-1.71260100	1.64533500	-4.95306900	H	4.91588700	3.59362000	2.31095800
C	0.39335900	2.35385200	1.63081600	H	4.05671400	5.92474000	2.35094900
H	1.30254800	1.74563400	1.63522700	C	-0.73422400	1.68787100	0.83025400
H	0.64771200	3.33216400	1.21563700	C	-1.19064600	0.36381600	1.48718400

C	-1.49257900	-2.60071500	-0.87750100	H	2.87190300	-3.17682900	0.46662900
H	-1.07351300	-3.13926700	-1.73598800	H	3.47666200	-1.84543300	1.44166500
H	-1.21170200	-3.15943400	0.02578000	C	2.30928700	0.65368600	-0.01428400
H	-2.57719600	-2.61738000	-0.98244100	C	1.31232000	-0.07972500	0.54239600
C	-2.10332900	-0.23332600	0.47303900	C	-0.00703900	0.41585300	1.01995100
C	-3.24980400	0.06808900	-0.02462600	H	-0.38433700	1.29944400	0.51958800
C	-4.71258100	0.20449000	0.10024900	C	-0.33890900	0.36092200	2.48361900
C	-5.24648700	-0.16375000	1.49684500	C	0.78740400	-0.00559700	3.49518900
H	-5.17544700	-0.41939400	-0.67488700	H	0.31408100	-0.19189000	4.46875600
H	-4.99074600	1.23733100	-0.15448700	H	1.26131900	-0.94383300	3.19352200
C	-6.77172900	-0.02668100	1.58638500	C	1.78452000	1.05586100	3.61684900
H	-4.95255900	-1.19450400	1.73199100	C	2.59351800	1.95425800	3.67841400
H	-4.77427200	0.47747800	2.25294600	C	3.54223100	3.06810300	3.69977500
C	-7.32452800	-0.38743500	2.96850500	C	2.84401900	4.44476700	3.68452800
H	-7.05857000	1.00306200	1.33378900	H	4.18968900	2.99067600	2.81757400
H	-7.23499900	-0.66742800	0.82476300	H	4.18966300	2.98830800	4.58412000
H	-8.41362000	-0.28266300	2.99994200	C	3.84136300	5.60781200	3.65197800
H	-7.08212300	-1.42236700	3.23511500	H	2.19030900	4.49064100	2.80611700
H	-6.90554000	0.26162000	3.74597100	H	2.19711300	4.53138000	4.56751000
H	-0.34139700	-0.28975300	1.70835800	C	3.15860500	6.97921700	3.64399400
H	-1.73841000	0.56015500	2.41572100	H	4.51447800	5.53858100	4.51820500
C	-3.04492900	2.02734900	-2.26921700	H	4.47565100	5.50896900	2.76127200
O	-3.72270800	2.91890100	-2.50948000	H	3.89243200	7.79164800	3.61553000
C	-0.73738000	1.66444500	-4.44800300	H	2.50554700	7.08905000	2.77104700
C	0.39576700	1.66786400	-5.46523500	H	2.54078500	7.12064200	4.53846100
C	0.51792200	-0.65553200	-5.39351600	C	1.47060800	-1.53414900	0.70111300
C	-0.62129400	-0.71197900	-4.38544000	C	0.34594500	-2.25259100	0.92289500
O	0.39138600	0.47531100	-6.24189500	C	2.78160800	-1.80313400	-1.96052000
O	-0.63565000	0.50092800	-3.59403400	O	2.44212100	-1.00461400	-2.80257200
H	1.48637500	-0.63112300	-4.86635600	O	2.54034400	-3.12609300	-2.03722800
H	0.49154200	-1.54385400	-6.03264600	C	4.98034700	-2.01514300	-0.79038400
H	-1.59055000	-0.82477600	-4.88153600	O	5.54023700	-2.68786500	0.04611300
H	-0.49108900	-1.53568300	-3.68227500	O	5.55233000	-1.62687000	-1.94738000
H	0.26767900	2.50373900	-6.15978400	C	1.75273200	-3.53936200	-3.17168900
H	1.35549300	1.78931500	-4.94338400	H	2.23675100	-3.23698800	-4.10310700
H	-0.65675400	2.53371300	-3.79571200	H	1.69172700	-4.62544600	-3.10391000
H	-1.71260100	1.64533500	-4.95306900	H	0.75852700	-3.09002000	-3.11412800
C	0.39335900	2.35385200	1.63081600	C	6.90779400	-2.06643900	-2.14716300
H	1.30254800	1.74563400	1.63522700	H	7.20013100	-1.67877400	-3.12247600
H	0.64771200	3.33216400	1.21563700	H	7.55765500	-1.66886300	-1.36389000
H	0.08066500	2.50527000	2.67055800	H	6.96164300	-3.15758100	-2.13263600
H	-1.60774800	2.35192400	0.85064100	S	2.26107900	2.44185900	-0.18200200
Z-INT-2c^{pH}				O	1.03514800	3.00171700	0.42186100
C	3.55280100	-1.46282100	-0.66891700	O	3.57271000	2.95469800	0.26785800
C	3.61983800	0.07183600	-0.50361100	C	2.17077700	2.70756500	-1.96440200
H	4.41208300	0.33065600	0.20896900	C	1.20823200	2.04050200	-2.72573500
H	3.89534500	0.51718900	-1.46291000	C	3.04293200	3.63606300	-2.53432600
C	2.86810100	-2.09299800	0.56377100	C	1.11964600	2.32077900	-4.08876000

H	0.56001500	1.29428000	-2.27730600	H	2.07320700	-0.22535700	2.66899900
C	2.93686100	3.91277800	-3.89798500	H	2.19136700	1.52710400	2.70616100
H	3.78789200	4.12050900	-1.91255000	C	1.10909700	0.67458500	4.30643100
C	1.97686600	3.25738300	-4.67193600	C	0.78340400	0.65342200	5.47225700
H	0.38615700	1.79856200	-4.69510000	C	0.37716800	0.61959800	6.87815400
H	3.60750200	4.63441300	-4.35503700	C	-1.09413600	0.19856600	7.07918100
H	1.90197200	3.47005000	-5.73457100	H	0.53761800	1.60861900	7.32915600
Rh	-1.36562600	-1.17923600	0.93203900	H	1.03036600	-0.07254900	7.42708000
Cl	-1.35741100	-1.35050400	-1.46908700	C	-1.50311400	0.15660000	8.55606900
C	-2.60313700	-2.73746300	1.16290900	H	-1.74211300	0.89693900	6.53401200
O	-3.31501400	-3.62895700	1.26691400	H	-1.24757900	-0.78737300	6.62233600
C	0.25883500	-3.74244700	1.05952200	C	-2.96314200	-0.25931200	8.76034000
H	-0.32449200	-4.16682200	0.23427500	H	-0.84477600	-0.53884200	9.09410400
H	1.24581400	-4.21502600	1.05001400	H	-1.33612700	1.14410800	9.00731300
H	-0.23638700	-4.03195700	1.99384700	H	-3.22603600	-0.28387000	9.82262100
C	-4.65458700	1.99872500	-0.24094500	H	-3.64736800	0.43894500	8.26490800
C	-3.79989500	0.75437300	-0.42833100	H	-3.15246700	-1.25668800	8.34753900
C	-4.42392000	0.04003500	1.74888100	C	1.85749300	-1.60971000	0.57138200
C	-5.27932700	1.29344400	1.89698500	C	0.77752200	-2.15283700	1.18076600
O	-3.32354200	0.29451800	0.85784300	C	2.68903500	-2.55968700	-2.14233500
O	-5.74800300	1.73804100	0.63409700	O	2.29373200	-1.93689800	-3.10063800
H	-3.99096600	-0.25723000	2.70762800	O	2.32531700	-3.82390800	-1.86083900
H	-5.02960000	-0.78744400	1.35228500	C	5.03525900	-2.72770700	-1.29205000
H	-6.15985400	1.08081400	2.51123600	O	5.68580400	-3.25374800	-0.41657200
H	-4.69054500	2.08467900	2.38950400	O	5.42749400	-2.65523500	-2.57867700
H	-4.38205000	-0.04785400	-0.89933700	C	1.32566400	-4.38428300	-2.73764900
H	-2.91478900	0.94270800	-1.03552800	H	1.66394700	-4.34419700	-3.77540600
H	-4.03760800	2.82191200	0.15408900	H	1.20016500	-5.41685200	-2.41209200
H	-5.08119000	2.31168500	-1.19842500	H	0.39239500	-3.82645700	-2.63098100
C	-1.16162700	1.56510200	2.95462300	C	6.70200100	-3.25398700	-2.87471100
H	-1.56242900	1.40261100	3.96094300	H	6.85197800	-3.10796500	-3.94387900
H	-0.50589100	2.43911000	2.97710400	H	7.49547800	-2.76562900	-2.30397100
H	-1.98572300	1.76397100	2.26906700	H	6.69048700	-4.31827200	-2.62781300
H	-1.07625500	-0.58053800	2.64877600	S	2.69178800	1.99228800	-1.28206200
Z-TS2cc^{BH}				O	1.72547000	2.75922000	-0.46715200
C	3.68383900	-2.02773100	-1.08813400	O	4.09884000	2.43351000	-1.31652000
C	3.86984800	-0.50781400	-1.29128700	C	2.09917600	1.95156300	-2.98493600
H	4.78704300	-0.17340400	-0.79268200	C	1.00994300	1.15467800	-3.34562100
H	3.99690400	-0.30678400	-2.35807300	C	2.73516600	2.78436000	-3.90785300
C	3.18130200	-2.30778800	0.34542600	C	0.54741600	1.20759200	-4.66073700
H	3.10878100	-3.38275100	0.49725400	H	0.54419600	0.47791800	-2.63586000
H	3.94556300	-1.93682800	1.03920600	C	2.25552500	2.83328300	-5.21675300
C	2.69167700	0.27673200	-0.75728600	H	3.59372000	3.36979700	-3.59713400
C	1.74167200	-0.23637800	0.06457000	C	1.16297800	2.04778300	-5.59136300
C	0.52694300	0.49170500	0.53330300	H	-0.28844200	0.58115200	-4.95613100
H	0.01954500	1.12350300	-0.18549300	H	2.74026300	3.47784100	-5.94404800
C	0.36015900	0.86232300	1.90285300	H	0.79720600	2.08226000	-6.61362400
C	1.51305600	0.68258600	2.90092100	Rh	-0.89736500	-1.02693600	1.14473200

Cl	-1.25493900	-1.75786200	-1.19635600	C	-1.29356400	-5.28558800	3.21254700
C	-2.06762200	-2.39985400	1.88795700	H	-1.02575500	-3.14110000	3.11784200
O	-2.77597000	-3.18161000	2.33524500	H	-2.70811100	-3.64056900	3.27666600
C	0.70614700	-3.52537700	1.77826300	C	-1.10827800	-5.40842900	4.72838800
H	-0.00178400	-4.15139600	1.22255000	H	-2.02485700	-6.02977400	2.87013900
H	1.67712000	-4.02897000	1.76989800	H	-0.34984900	-5.52350600	2.70474500
H	0.36360500	-3.48384300	2.81836100	H	-0.77642700	-6.41388300	5.00621400
C	-4.62423600	1.53603100	-0.29723500	H	-0.35946400	-4.69746600	5.09538400
C	-3.77778800	0.27772200	-0.18996200	H	-2.04474400	-5.20773900	5.26036900
C	-3.75241500	0.53157500	2.16822900	C	-0.96341900	-2.10468600	-1.60978500
C	-4.61404900	1.78173100	2.02820800	C	-2.26924600	-2.44575000	-1.33942600
O	-2.94426100	0.35673400	0.99019700	C	2.24008600	-3.51938800	-3.29734300
O	-5.42658600	1.71186500	0.86719900	O	2.66010300	-3.20676900	-4.38790200
H	-3.06479000	0.61282000	3.01339000	O	2.38145700	-4.74782600	-2.75995100
H	-4.39019900	-0.35364800	2.30548000	C	2.02335700	-2.74138200	-0.94271000
H	-5.28668800	1.87636800	2.88644100	O	1.45750100	-3.23616500	0.00915700
H	-3.96623800	2.67310100	1.99117500	O	3.27701500	-2.25421900	-0.89301300
H	-4.42074200	-0.60935200	-0.11150300	C	3.08664600	-5.70496600	-3.57304500
H	-3.10287200	0.14427600	-1.03535100	H	4.10282700	-5.35835000	-3.77477700
H	-3.97415900	2.41311800	-0.44848400	H	3.10163300	-6.62674600	-2.99260500
H	-5.30994900	1.46031000	-1.14625900	H	2.56736300	-5.85493300	-4.52233100
H	-0.53117100	-0.33339100	2.56408500	C	3.94043500	-2.36262200	0.37972600
C	-0.51512600	2.06665000	2.18071400	H	4.93711200	-1.95075100	0.22565400
H	-0.83869600	2.09905900	3.22330200	H	3.40212000	-1.79158800	1.13957900
H	0.09741000	2.95408900	1.97944100	H	3.99707100	-3.40801400	0.69173500
H	-1.37910500	2.09417300	1.51776500	S	0.93832000	1.46048000	-2.49203400
TS2a'				O	0.82377600	1.49903400	-3.96395800
C	1.43946200	-2.60192600	-2.35814700	O	0.15891600	2.41242400	-1.68054700
C	1.50835600	-1.16438900	-2.87309500	C	2.67804500	1.75013200	-2.09747500
H	2.53821300	-0.80476600	-2.81381400	C	3.63363000	1.62660100	-3.10850600
H	1.24440900	-1.15789600	-3.93529900	C	3.03204300	2.15712000	-0.80869400
C	-0.02969600	-3.04654700	-2.36367500	C	4.97197100	1.88990000	-2.81249300
H	-0.34246300	-3.14366700	-3.41056300	H	3.32094100	1.34859800	-4.10913700
H	-0.08249300	-4.03397100	-1.91588600	C	4.37292500	2.41561200	-0.52432300
C	0.59025100	-0.26870800	-2.06955300	H	2.26829600	2.29331500	-0.05150500
C	-0.50002900	-0.71018500	-1.36357000	C	5.34097500	2.27762800	-1.52269100
C	-1.40646000	0.18958300	-0.54051000	H	5.72289500	1.79918000	-3.59139900
H	-1.51276600	1.13901000	-1.05884100	H	4.65939500	2.73789000	0.47227800
C	-0.96041500	0.53088900	0.96911700	H	6.38303000	2.48511300	-1.29746600
C	-2.01273300	-0.07882100	1.97031600	C	-0.93996700	2.05492500	1.19099700
H	-1.54032100	-0.40259100	2.90497200	H	-1.90219600	2.50602700	0.92764500
H	-2.78018900	0.65712800	2.22057200	H	-0.74982400	2.27640100	2.24840800
C	-2.58457700	-1.21349700	1.21687000	H	-0.17576600	2.54122500	0.58448500
C	-2.34324500	-2.41436100	0.89438800	C	0.41744200	-0.05760600	1.32314000
C	-1.93518400	-3.78592000	1.25266400	H	0.41623200	-1.15077600	1.28020200
C	-1.75895500	-3.88653500	2.78655200	H	1.19424500	0.29534100	0.64031700
H	-0.99164500	-4.02522800	0.74945700	H	0.70202800	0.24676900	2.33718900
H	-2.68073900	-4.51797100	0.93222700	Rh	-3.31356600	-0.67997800	-0.60766100

Cl	-5.94283600	-1.11592200	-0.26697500	C	6.78427200	-3.06835500	-2.26911700
C	-4.19075200	0.97661900	0.00847100	H	6.72550800	-2.73274500	-3.30703300
O	-4.69175700	1.95157100	0.34276000	H	7.75534200	-2.82371900	-1.84021000
C	-5.49114200	0.63615100	-4.55012800	H	6.60506600	-4.14538600	-2.23258800
C	-5.13323700	0.70826800	-3.07445300	C	-0.19088500	-1.51914800	-0.22622900
C	-2.83320800	0.66139700	-3.66740700	C	0.28580200	0.77851600	0.42801900
C	-3.23323200	0.60782400	-5.13667400	H	0.06419700	1.77236500	0.04598800
O	-3.85775600	0.05965200	-2.84885300	C	3.75108000	-0.22628700	-1.28205500
O	-4.48519500	1.24132300	-5.35465600	H	3.69490200	-0.12003500	-2.37274700
H	-1.91652200	0.09733800	-3.49762700	H	4.74503600	0.11093900	-0.97866900
H	-2.67991900	1.70199900	-3.35118100	S	3.10744000	2.37173400	-0.62121900
H	-2.49023400	1.13801000	-5.73969300	O	2.11195000	3.12365700	0.15859300
H	-3.27383100	-0.44244400	-5.46951900	O	3.38671100	2.72469100	-2.02612300
H	-5.05642800	1.75853200	-2.75856600	C	4.68335500	2.49015500	0.25560300
H	-5.85411600	0.18482500	-2.44395100	C	5.83948500	2.76445900	-0.47645700
H	-5.63678500	-0.41539500	-4.84650300	C	4.71689300	2.36250300	1.64578500
H	-6.42115200	1.18177300	-4.73640200	C	7.05292700	2.90651300	0.19929600
C	-3.03125700	-3.65486100	-1.96483100	H	5.77090900	2.87800600	-1.55290000
C	-3.35726900	-3.25269400	-3.43006300	C	5.93425700	2.50143700	2.30991800
C	-2.28488500	-5.02383800	-2.00951100	H	3.80515100	2.16717100	2.19894000
C	-4.38279700	-3.92454400	-1.26977700	C	7.09999500	2.77230900	1.58799300
H	-3.96262400	-2.34556700	-3.45922700	H	7.95817500	3.12605800	-0.35899400
H	-2.45164400	-3.07793900	-4.02053800	H	5.97280900	2.40314000	3.39054900
H	-3.91676600	-4.06147600	-3.91387000	H	8.04555400	2.88351600	2.11091600
H	-1.54463600	-5.08826200	-2.80794100	C	0.26540100	0.82281700	2.00226000
H	-1.79652400	-5.27816400	-1.06586700	C	-1.14004900	0.28267900	2.23412200
H	-3.02504900	-5.80508500	-2.20956900	C	1.27591300	-0.10852000	2.70273100
H	-4.91647500	-4.70357200	-1.82507000	H	1.17661400	-1.14540300	2.37192500
H	-4.26537200	-4.28521500	-0.24434200	H	2.30416800	0.20705400	2.50688000
H	-5.01436000	-3.03961600	-1.22815600	H	1.11366700	-0.08475500	3.78677700
TS4cc'				C	0.39980800	2.24493400	2.56550400
C	1.47799800	0.13977800	-0.25825000	H	0.23442400	2.23162200	3.65038800
C	1.13030100	-1.26237500	-0.51491200	H	1.38992000	2.65567200	2.36559500
C	2.14573200	-2.17431800	-1.15311800	H	-0.32379800	2.91775200	2.09878800
C	2.68769800	0.62987000	-0.62701000	C	-0.86368100	-0.22422100	0.07916100
H	2.03792800	-3.21228900	-0.84485200	C	-2.12903300	0.18993900	-0.36738400
H	1.99287200	-2.16976300	-2.23918100	C	-2.83828900	-0.44997800	-1.52647800
H	5.35356900	-3.34367500	2.36060800	C	-2.92507600	0.53519600	-2.72160600
C	4.30068900	-3.59545000	2.21425700	H	-3.86371700	-0.73169200	-1.25005000
O	3.88384100	-3.24914000	0.88086600	H	-2.31511400	-1.34823500	-1.87159200
H	4.14559800	-4.67050400	2.30018200	C	-3.59012600	-0.10077300	-3.94846200
H	3.70109300	-3.05992500	2.95392600	H	-3.47624500	1.42770700	-2.40667800
C	4.02387500	-1.94604600	0.54852400	H	-1.91605500	0.87868800	-2.98079400
C	3.59916800	-1.71682300	-0.91136500	C	-3.67967900	0.86118600	-5.13766900
O	4.43547700	-1.10327100	1.31214900	H	-3.03031300	-0.99853200	-4.24541100
C	4.53019600	-2.54183500	-1.81602100	H	-4.59770600	-0.44625000	-3.67790200
O	4.17114900	-3.22473700	-2.74848200	H	-4.15752400	0.38529100	-6.00044000
O	5.81801700	-2.37108000	-1.46031500	H	-4.26295300	1.75268000	-4.88199300

H	-2.68487400	1.19777600	-5.44966800	O	4.20410800	-1.44036000	1.61344200
H	-1.26147000	-0.77708100	2.43358100	C	4.88750900	-2.66324900	-1.55943700
H	-1.84697400	0.90003400	2.77821800	O	4.68793900	-3.31266500	-2.56056500
Rh	-3.05263700	1.56368900	0.66767300	O	6.10434000	-2.48371100	-1.00788500
C	-4.28556100	0.27344300	1.28517300	C	7.19766000	-3.12232300	-1.69326500
O	-5.12275500	-0.40479800	1.70581100	H	7.28201900	-2.74119300	-2.71351300
Cl	-1.89218800	3.46238600	-0.19395600	H	8.08841900	-2.87603200	-1.11635100
C	-4.37452500	4.99030300	3.54410200	H	7.04593800	-4.20371700	-1.72842200
C	-3.50313900	3.91125400	2.92055500	C	-0.02677100	-1.76335700	-0.58745200
C	-5.23138100	3.90498600	1.22443000	C	0.30505400	0.52086700	0.19227400
C	-4.89520500	5.38664000	1.24823800	H	0.12704600	1.47139300	-0.30783900
O	-4.26088700	3.12705600	1.97390600	C	4.01006600	-0.38674200	-1.03920800
O	-4.88131700	5.90716800	2.57769400	H	4.16708000	-0.23510400	-2.11335800
H	-6.22061300	3.72727700	1.66502500	H	4.92610800	-0.05069900	-0.54513600
H	-5.22128300	3.52617100	0.19971300	S	3.16839200	2.20193700	-0.74944500
H	-3.92998300	5.54772800	0.75076700	O	1.94425300	2.99258800	-0.54903100
H	-5.66132800	5.94336700	0.69864000	O	3.89060700	2.33087500	-2.03102500
H	-2.63557200	4.34540200	2.41206800	C	4.35213500	2.67288200	0.53639400
H	-3.15335100	3.21392900	3.68750500	C	4.92656000	3.94159300	0.39982500
H	-5.20869800	4.51894900	4.08742300	C	4.67398100	1.84640800	1.61276800
H	-3.78308200	5.56039000	4.27080000	C	5.82283300	4.39062800	1.36677600
C	-0.80868000	-2.93288000	-0.09337900	H	4.67589700	4.56172600	-0.45456400
C	-2.26369100	-2.93291900	0.43313400	C	5.58167200	2.30691100	2.57201500
C	-0.78482300	-3.71076200	-1.43266800	H	4.25190700	0.85090800	1.69782800
C	0.00631500	-3.71972300	0.97368200	C	6.15046800	3.57458800	2.45423100
H	-2.37692800	-2.32083500	1.33176400	H	6.26913100	5.37599600	1.26999200
H	-2.98830700	-2.59086000	-0.30329900	H	5.84254600	1.66556100	3.40873700
H	-2.53910100	-3.95834000	0.70076200	H	6.85283300	3.92704500	3.20418700
H	0.22711400	-3.88137300	-1.80456900	C	0.17771900	0.80170000	1.74087200
H	-1.25576100	-4.69057800	-1.29647000	C	-1.31891200	0.89143100	2.12615600
H	-1.34052400	-3.18243400	-2.21297500	C	0.76376500	-0.35913000	2.58014000
H	-0.36657100	-4.74798800	1.03512500	H	0.30251400	-1.31618700	2.31774000
H	1.07510500	-3.76463900	0.76248700	H	1.84329600	-0.44699000	2.42601900
H	-0.11629700	-3.26569600	1.96272500	H	0.59129300	-0.18360400	3.64815600
INT-4cc				C	0.87699200	2.10992200	2.14547000
C	1.59977100	-0.08422400	-0.33092500	H	0.71879600	2.29458400	3.21531300
C	1.31943100	-1.47855000	-0.67926200	H	1.95374900	2.05689600	1.98410400
C	2.42095300	-2.32114200	-1.27111700	H	0.50186800	2.95931500	1.57228800
C	2.83120400	0.44808800	-0.57167400	C	-0.74496400	-0.50501400	-0.27413700
H	2.28826500	-3.38882000	-1.11668800	C	-2.02684500	-0.10781900	-0.44002000
H	2.42479600	-2.17855800	-2.35910200	C	-3.08173500	-0.64359600	-1.37207300
H	5.03638500	-3.73467100	2.63521700	C	-3.70361800	0.43964400	-2.28222300
C	4.03917700	-3.99951900	2.27616600	H	-3.89687200	-1.13989900	-0.82490400
O	3.86272900	-3.55541500	0.91831900	H	-2.62593100	-1.39516800	-2.02578700
H	3.91448700	-5.08147300	2.24847700	C	-4.67288800	-0.15059500	-3.31399600
H	3.29215900	-3.54206400	2.92866200	H	-4.23882500	1.18100900	-1.67030400
C	3.98688000	-2.22673600	0.71689200	H	-2.90390700	0.99403500	-2.78562300
C	3.81516600	-1.89335700	-0.77171600	C	-5.31257500	0.91436500	-4.21034200

H	-4.13492200	-0.87826300	-3.93699800	H	2.87081600	-5.38003800	1.34021500
H	-5.45961800	-0.71716400	-2.79626800	H	2.45605900	-3.92081400	2.29872600
H	-5.99067500	0.46499200	-4.94319400	C	3.75324800	-2.36184200	0.56614400
H	-5.89098500	1.63406500	-3.61963200	C	3.87774400	-1.68060600	-0.80483500
H	-4.55057000	1.47726700	-4.76041000	O	3.99775700	-1.85932100	1.64240500
H	-1.68182600	-0.08497100	2.44575500	C	4.93545400	-2.44659000	-1.61863400
H	-1.49872400	1.61633700	2.92573700	O	4.81114000	-2.80019700	-2.76882400
Rh	-2.63481700	1.53857900	0.60948600	O	6.05072100	-2.63838400	-0.88730400
C	-3.89280600	0.47245000	1.48985000	C	7.13223300	-3.30486600	-1.56576000
O	-4.70688000	-0.14828500	2.01666600	H	7.44749800	-2.72737800	-2.43769600
Cl	-1.62364600	3.14210300	-0.80481400	H	7.93848000	-3.37063900	-0.83607500
C	-3.22090200	5.67901700	2.86264900	H	6.82206700	-4.30063900	-1.89099600
C	-2.53444800	4.42303600	2.35080400	C	0.12678000	-0.87215200	-1.07563700
C	-4.64936300	4.09447700	1.22542400	C	0.68582100	0.98581900	0.39512500
C	-4.32781000	5.50425200	0.75602500	H	0.61709600	2.02241000	0.06098300
O	-3.50790000	3.46995000	1.86224200	C	4.34508200	-0.21871900	-0.65809500
O	-3.95980000	6.34971000	1.84361600	H	4.68335500	0.14908200	-1.63391700
H	-5.47963900	4.11028900	1.94324900	H	5.21390800	-0.18125900	0.00497800
H	-4.93275700	3.46666400	0.37496400	S	3.81846500	2.36157500	0.12964600
H	-3.53167200	5.46281700	0.00049300	O	2.68545500	3.25738900	0.41237500
H	-5.21575600	5.94823600	0.29387100	O	4.68630800	2.66294700	-1.02575300
H	-1.82728300	4.65448600	1.54759500	C	4.90527300	2.34459600	1.57639400
H	-1.99559000	3.92605800	3.16173200	C	5.65597000	3.50626400	1.78810100
H	-3.88799700	5.41853100	3.69935500	C	4.99739800	1.25637000	2.44454900
H	-2.46576900	6.37709300	3.24248000	C	6.49700100	3.58049700	2.89596100
C	-0.59727300	-3.20485300	-0.62696800	H	5.58422200	4.33402100	1.09022300
C	-2.07386700	-3.33251900	-0.18082700	C	5.85220800	1.34185400	3.54809100
C	-0.47704700	-3.81483700	-2.04437400	H	4.43711300	0.34531100	2.26264800
C	0.18097900	-4.07188700	0.40638200	C	6.59524000	2.49941400	3.77736400
H	-2.28589300	-2.72750400	0.70480100	H	7.07950300	4.48054800	3.06912300
H	-2.78003000	-3.06266500	-0.96239600	H	5.93415100	0.49601800	4.22419900
H	-2.27195100	-4.37853700	0.07433900	H	7.25519000	2.56009500	4.63793300
H	0.55731800	-3.89332100	-2.38580800	C	0.46540300	0.92452100	1.94265800
H	-0.90824700	-4.82232300	-2.05434900	C	-1.02819400	1.25754800	2.13961700
H	-1.02331000	-3.21045000	-2.77627100	C	0.74167000	-0.48809500	2.50004700
H	-0.14945500	-5.11360300	0.32876200	H	0.14010800	-1.24960100	1.99440300
H	1.26247600	-4.05816700	0.28707800	H	1.79489700	-0.75906600	2.39100400
H	-0.04108600	-3.72985900	1.42303500	H	0.49981900	-0.52131000	3.56827200
TS5cc				C	1.28553300	1.94382700	2.75265000
C	1.93049400	0.32463500	-0.15522600	H	0.96336800	1.92281100	3.80084300
C	1.50119200	-0.83774400	-0.92932200	H	2.35049800	1.70719800	2.73965600
C	2.54194500	-1.71452500	-1.57548800	H	1.16782800	2.95663600	2.36341900
C	3.24355600	0.68118900	-0.13163400	C	-0.46091000	0.13593000	-0.17165500
H	2.20427400	-2.74697600	-1.66441400	C	-1.69634700	0.29219200	0.40367200
H	2.76674400	-1.37078400	-2.58986600	C	-2.69589100	-0.82820000	0.64069200
H	4.15388100	-4.43651200	2.16845400	C	-4.16138300	-0.71292600	0.16184300
C	3.19683700	-4.38587600	1.64416000	H	-2.72031300	-1.00619500	1.72689900
O	3.33161500	-3.63358100	0.42445700	H	-2.26380200	-1.74415600	0.22571400

C	-4.87474700	-2.07285500	0.16773000	H	2.41790100	-0.50840300	-2.67970700
H	-4.71674300	-0.02799800	0.80821300	H	4.44899400	-4.41184600	1.11336300
H	-4.20721900	-0.27506900	-0.84122700	C	3.44867600	-4.33588000	0.68076600
C	-6.35433800	-1.97493500	-0.21664800	O	3.41212300	-3.30430100	-0.32129300
H	-4.36193500	-2.75748000	-0.52165400	H	3.18189500	-5.25676500	0.16307200
H	-4.78495900	-2.52443300	1.16564200	H	2.73226800	-4.12093100	1.47720500
H	-6.83615500	-2.95804900	-0.20586800	C	3.73951000	-2.06603500	0.10322500
H	-6.90205200	-1.32853900	0.47849900	C	3.69724700	-1.07005100	-1.06703800
H	-6.47573700	-1.55648700	-1.22228000	O	4.02848000	-1.81344200	1.25248900
H	-1.54043200	0.56872300	2.81118200	C	4.74062800	-1.52347400	-2.10413300
H	-1.12713100	2.27027600	2.54631300	O	4.54787600	-1.62673400	-3.29373300
Rh	-2.49601400	2.22402700	0.65708400	O	5.92857100	-1.75705100	-1.51115400
C	-3.72401200	1.82445200	1.99280700	C	6.99672500	-2.14764200	-2.39409100
O	-4.51439000	1.69928700	2.82714000	H	7.18400300	-1.36649200	-3.13436500
Cl	-1.27303000	3.13304600	-1.21920500	H	7.86764800	-2.28850600	-1.75490300
C	-4.30333500	6.38338800	0.66356900	H	6.74292500	-3.07532200	-2.91244100
C	-3.21492600	5.30934600	0.55017100	C	-0.11377200	-0.47408300	-1.00960700
C	-4.56224200	4.01825500	-0.98574700	C	0.43806500	0.95092100	0.92791000
C	-4.93671100	5.44111100	-1.40546600	H	0.33427300	2.03749500	0.93133700
O	-3.83903500	4.03575100	0.27989300	C	4.06668700	0.35056700	-0.59364000
O	-5.35727800	6.19088900	-0.27949800	H	4.28095300	0.97712000	-1.46786700
H	-5.45557300	3.41850800	-0.79191500	H	4.98552300	0.30539400	-0.00238200
H	-3.93942400	3.53661900	-1.74579400	S	3.44481000	2.52287800	0.98054700
H	-4.09841000	5.93087300	-1.92281600	O	2.30235200	3.12895900	1.68687100
H	-5.77857600	5.40578000	-2.10278100	O	4.12158400	3.29667400	-0.07768600
H	-2.47555000	5.51926700	-0.22772100	C	4.72210200	2.12209500	2.19674800
H	-2.68363900	5.19695800	1.49720000	C	5.71239900	3.08582400	2.40641200
H	-4.77003100	6.35499300	1.65343500	C	4.69475700	0.93850400	2.93520800
H	-3.83889700	7.37401500	0.53066800	C	6.67582600	2.86656400	3.39002800
C	-0.60127500	-1.69963000	-2.16577500	H	5.72564600	3.98221100	1.79581000
C	-1.94628500	-1.05134400	-2.55878900	C	5.67279300	0.72537800	3.90922200
C	0.21526700	-1.73024600	-3.48862900	H	3.95574300	0.17387500	2.72723300
C	-0.82506000	-3.16050800	-1.70448700	C	6.65519200	1.68912300	4.14240300
H	-2.68289900	-1.08784900	-1.76535000	H	7.44710100	3.61127600	3.56304900
H	-1.80930600	-0.00362400	-2.84186100	H	5.66735800	-0.19908900	4.47873800
H	-2.36579400	-1.58704700	-3.41666700	H	7.41149200	1.51901500	4.90330700
H	1.08905500	-2.37880400	-3.45133000	C	0.21646600	0.41962800	2.39513000
H	-0.42602700	-2.11598700	-4.28721500	C	-1.33627200	0.41181300	2.44236500
H	0.53700200	-0.72530600	-3.77873700	C	0.73540900	-1.02266000	2.55808200
H	-1.30243500	-3.73534000	-2.50619800	H	0.31297400	-1.69971400	1.80776900
H	0.12109900	-3.65344900	-1.45922200	H	1.82348300	-1.07394200	2.46792700
H	-1.46829200	-3.22575000	-0.82249100	H	0.46157900	-1.40747600	3.54694600
INT-5cc				C	0.77827700	1.29984000	3.51629400
C	1.66924500	0.54306700	0.15794400	H	0.41040700	0.93495900	4.48351700
C	1.25290200	-0.40967000	-0.87811600	H	1.86879000	1.28509300	3.54832800
C	2.30850300	-1.05767700	-1.73972600	H	0.47343200	2.34246800	3.39942900
C	2.95408000	0.97367000	0.22090300	C	-0.70449700	0.26499900	0.14881000
H	2.04295400	-2.07960300	-2.00793100	C	-1.77218300	-0.00727600	1.02652300

C	-2.76876700	-1.14847300	0.95661700	C	0.23096000	-0.89988100	-0.46701200
C	-4.13240400	-0.95759600	1.63945500	Rh	-2.15574700	-0.39654200	-0.74073000
H	-2.25499700	-1.98357200	1.46292200	Cl	-3.01797700	-2.26251900	-2.13800600
H	-2.93655800	-1.47873600	-0.06533600	C	1.18453100	-1.35166600	-1.54851900
C	-4.91235300	-2.27470300	1.75226200	C	1.24126100	1.33219500	-0.66233700
H	-4.00653500	-0.52480400	2.63966600	H	1.26021000	-2.43351900	-1.61392700
H	-4.72687600	-0.23719300	1.06628100	H	0.79454900	-1.00675100	-2.51233900
C	-6.29539600	-2.09822700	2.38651000	H	4.93923000	-2.63960000	1.33522100
H	-5.02123100	-2.71885600	0.75331400	C	3.94322200	-3.06128800	1.18314000
H	-4.32760300	-2.99419500	2.34184600	O	3.34707200	-2.51666400	-0.01025000
H	-6.82634300	-3.05295500	2.45816500	H	4.00047200	-4.13614600	1.01635800
H	-6.21735600	-1.68357200	3.39792400	H	3.32360800	-2.83868600	2.05472900
H	-6.91711600	-1.41461800	1.79767100	C	3.19498400	-1.17905500	-0.03122000
H	-1.71110300	-0.30210300	3.18562900	C	2.57762300	-0.72692600	-1.36183600
H	-1.70880400	1.39418200	2.74111200	O	3.49983000	-0.45849800	0.89538700
Rh	-2.20081500	1.95085800	-0.31509500	C	3.49419500	-1.17671700	-2.51062300
C	-3.45425600	2.08145400	1.03216800	O	3.12055800	-1.71907100	-3.52461600
O	-4.22833300	2.33311600	1.85606500	O	4.77267100	-0.83875300	-2.25644400
Cl	-0.62948500	2.42602200	-2.12498000	C	5.72000300	-1.16385100	-3.29309800
C	-3.49969400	6.15151600	-0.96853900	H	5.45772800	-0.65154400	-4.22136400
C	-2.48535500	5.00584300	-0.88447100	H	6.68575700	-0.82106700	-2.92383400
C	-3.78446400	3.65155500	-2.41045500	H	5.73319100	-2.24149300	-3.47123800
C	-4.03205300	5.04873300	-2.98744500	C	-0.55301600	-1.83082600	0.20482900
O	-3.18679100	3.75804000	-1.08703000	C	-1.08811000	1.04673100	0.39437500
O	-4.48866400	5.92664000	-1.97423600	H	-1.31856500	2.05345200	0.06170500
H	-4.72372100	3.11569100	-2.25270700	C	2.44514900	0.80535200	-1.42195300
H	-3.11725000	3.06928200	-3.05255200	H	2.35342500	1.11167900	-2.47010700
H	-3.12631900	5.43797300	-3.47589000	H	3.36708700	1.26462700	-1.05833500
H	-4.81787800	4.99464300	-3.74624500	S	1.26074300	3.14616600	-0.65734400
H	-1.67623700	5.08532400	-1.61553800	O	-0.08374400	3.71458900	-0.42324300
H	-2.03663200	4.95049300	0.10813700	O	1.95965800	3.52460400	-1.90212900
H	-4.04321200	6.25442100	-0.02420500	C	2.28038000	3.67818300	0.73797600
H	-2.95788900	7.09199400	-1.15922800	C	2.15761300	5.02533900	1.09484300
C	-0.86247600	-1.24028700	-2.12657700	C	3.17493400	2.83128500	1.39402300
C	-2.26866900	-0.66615300	-2.43736000	C	2.95330500	5.53112100	2.12095300
C	-0.12838100	-1.16139300	-3.49374000	H	1.44097000	5.65911500	0.58357200
C	-0.96690400	-2.73479200	-1.72064500	C	3.96128200	3.35309900	2.42504100
H	-2.87504200	-0.43800100	-1.56266800	H	3.25465100	1.78060800	1.13737800
H	-2.17146300	0.26236300	-3.00224500	C	3.85633900	4.69673200	2.78536500
H	-2.81758000	-1.38875300	-3.05206200	H	2.86370500	6.57544600	2.40459400
H	0.75408500	-1.79659000	-3.55951300	H	4.65494300	2.69978400	2.94568900
H	-0.81657100	-1.50040800	-4.27511700	H	4.47259500	5.09402300	3.58657400
H	0.15301200	-0.12993400	-3.72093700	C	-1.27743100	0.98904300	1.93294700
H	-1.43375900	-3.30756200	-2.52987800	C	-1.21084000	-0.45492500	2.49207300
H	0.02320800	-3.16371300	-1.53583600	C	-0.15840400	1.78037600	2.65077400
H	-1.56476900	-2.88375400	-0.81862200	H	0.83144500	1.36812400	2.43690900
TS2b'				H	-0.16736600	2.82616300	2.33234000
C	0.21246000	0.57529200	-0.18252000	H	-0.30565000	1.75788700	3.73700700

C	-2.62067200	1.64874900	2.30006100	H	1.34498500	-2.51630100	-1.21786000
H	-2.75045000	1.68087700	3.38765700	H	0.86127300	-1.22382400	-2.28330100
H	-2.64668700	2.67919400	1.93174500	H	4.96797300	-2.24087300	1.81479000
H	-3.47474100	1.12182300	1.87456200	C	4.01064000	-2.74643500	1.66885900
C	-0.44074800	-3.32512700	0.00474000	O	3.41875200	-2.34508300	0.41889400
H	0.58998800	-3.63464300	-0.17736400	H	4.15174200	-3.82400800	1.59327400
H	-0.80873200	-3.82025800	0.90685300	H	3.34808700	-2.50144800	2.50217600
H	-1.06716300	-3.64315100	-0.83680900	C	3.16442600	-1.02554600	0.29155000
C	-1.71954300	-1.41690300	1.00410300	C	2.57052500	-0.72496300	-1.09304200
C	-2.32152100	-1.88040700	2.09471500	O	3.37353800	-0.21832200	1.16991400
C	-3.75894900	-1.81063100	2.49489600	C	3.55233700	-1.21280200	-2.16878900
C	-4.02992700	-1.98799500	3.99565900	O	3.25360800	-1.86921200	-3.13923500
H	-4.21125600	-2.65210400	1.94850200	O	4.79826300	-0.76706500	-1.91084000
H	-4.27352600	-0.91293400	2.11830900	C	5.80036500	-1.13086900	-2.87946700
C	-5.52530700	-2.06192500	4.32730300	H	5.54166200	-0.73253700	-3.86315800
H	-3.52239800	-2.89578500	4.34490200	H	6.72942400	-0.69117700	-2.51839500
H	-3.58299500	-1.15228400	4.55428900	H	5.88721700	-2.21775000	-2.94720200
C	-5.80205500	-2.22144900	5.82541000	C	-0.54827600	-1.85565400	0.50592900
H	-6.02490300	-1.15686700	3.95619500	C	-1.11678600	0.97192400	0.65241800
H	-5.97412500	-2.90129200	3.77926200	H	-1.36176000	1.97648500	0.32878100
H	-6.87632800	-2.27291700	6.02924200	C	2.35300000	0.78700300	-1.27989700
H	-5.34469800	-3.13662700	6.21829600	H	2.21481000	0.99474000	-2.34822500
H	-5.39573600	-1.37832000	6.39602200	H	3.25603200	1.31936100	-0.96945000
C	-3.88966900	0.27042900	-0.51606300	S	1.12156000	3.10420700	-0.56861800
O	-4.97919700	0.62470500	-0.40900700	O	-0.00366300	3.66218900	0.20949500
C	-1.77611800	2.24782000	-3.16935000	O	1.22619600	3.47039000	-1.99866700
C	-0.88571700	2.80528500	-4.27415200	C	2.66141300	3.65663700	0.19991400
C	-0.89321300	0.72019800	-5.34222300	C	3.31890000	4.73009300	-0.40571900
C	-1.79660000	0.15292600	-4.25637200	C	3.13063200	3.08914600	1.38571600
O	-1.10361500	2.11801800	-5.50213000	C	4.45966300	5.25464400	0.20176500
O	-1.54596800	0.83675300	-3.01475700	H	2.94022800	5.13246600	-1.33878700
H	0.16187500	0.51849100	-5.08998100	C	4.28035500	3.61573500	1.97564400
H	-1.11408200	0.25259600	-6.30697900	H	2.63370100	2.23148500	1.82157100
H	-2.85177100	0.28251800	-4.53468000	C	4.93857500	4.69976000	1.39073800
H	-1.62001800	-0.90733900	-4.07053800	H	4.97700900	6.09141900	-0.25786200
H	-1.11782400	3.85951600	-4.45365900	H	4.66202000	3.17365200	2.89084100
H	0.17005900	2.73255200	-3.96976100	H	5.83056400	5.10716900	1.85774200
H	-1.54706700	2.72084900	-2.21264200	C	-1.28253600	0.99741800	2.23615700
H	-2.83518900	2.41452800	-3.41812800	C	-1.46301000	-0.39570600	2.97908900
H	-0.19559200	-0.82714900	2.61912300	C	-0.04585600	1.66875700	2.87148800
H	-1.69318400	-0.47695000	3.47274200	H	0.85730100	1.07412100	2.69903700
INT-3b'				H	0.11112400	2.67408500	2.47540400
C	0.15661300	0.52473100	0.00804600	H	-0.18845100	1.74844800	3.95612100
C	0.19389400	-0.94080600	-0.27303600	C	-2.50547400	1.89964800	2.51376800
Rh	-2.08826200	-0.44175300	-0.73669500	H	-2.72403200	1.94593600	3.58639800
Cl	-2.57882100	-2.38485600	-2.23151100	H	-2.30386300	2.91889900	2.16938200
C	1.21664600	-1.43747500	-1.26940600	H	-3.40365800	1.54945200	1.99821500
C	1.15246000	1.30490200	-0.51359600	C	-0.21333400	-3.32945700	0.55592500

H	0.86494900	-3.50220600	0.60597100	H	-0.08534700	-6.67815900	5.18501500
H	-0.69830000	-3.77456500	1.42883500	C	2.10861200	-5.68759300	4.05119400
H	-0.61134200	-3.83233500	-0.33332800	C	2.86001900	-4.61843100	3.23881500
C	-1.84323200	-1.49876800	0.97336800	O	2.52640300	-6.24450700	5.04178500
C	-2.42504900	-1.19972800	2.14314100	C	3.22845500	-5.22435600	1.87111200
C	-3.90221300	-1.21258400	2.41817900	O	3.19920200	-4.63276000	0.81555000
C	-4.27585000	-2.37479900	3.36866400	O	3.64557900	-6.49769800	2.00557700
H	-4.45931300	-1.33984400	1.48445200	C	4.05939900	-7.14932400	0.78955700
H	-4.22820300	-0.27258500	2.87856200	H	4.89832100	-6.61530500	0.33753500
C	-5.77399300	-2.41250300	3.69667700	H	4.35675800	-8.15512300	1.08388200
H	-3.97413400	-3.32185600	2.90374100	H	3.23301500	-7.18317000	0.07597300
H	-3.69885900	-2.28894300	4.29970700	C	1.05015900	-1.38440200	4.11838900
C	-6.15393900	-3.57318900	4.62149700	C	2.56448500	-1.92456800	6.71970500
H	-6.06810900	-1.46105700	4.16033800	H	3.44762000	-2.03633600	7.33814600
H	-6.34532800	-2.48535400	2.76176500	C	4.15920100	-4.23653200	3.97296100
H	-7.22697900	-3.57468700	4.83876700	H	4.75321900	-3.59134500	3.31047000
H	-5.90533000	-4.53885900	4.16716600	H	4.74294200	-5.13670400	4.15243800
H	-5.62102000	-3.51053800	5.57728700	S	4.95152400	-3.85853900	6.66773200
C	-3.88510100	0.12535400	-0.61483700	O	4.18312800	-4.44859600	7.77862500
O	-4.98152600	0.46761300	-0.57558200	O	5.76423000	-2.64272300	6.90799200
C	-2.21141600	2.32485100	-2.58653000	C	6.10505200	-5.13376500	6.11924500
C	-1.63181100	3.15496200	-3.72585500	C	5.73866300	-6.47734400	6.23804200
C	-1.38446400	1.24819100	-5.03320600	C	7.37234700	-4.75412100	5.67468200
C	-1.97667400	0.38054200	-3.93441000	C	6.66456200	-7.45776900	5.88203800
O	-1.91888800	2.56357600	-4.98811800	H	4.74827200	-6.73747600	6.59360000
O	-1.70238700	0.97051300	-2.63730400	C	8.28965200	-5.74639700	5.32519300
H	-0.28663500	1.27648700	-4.93710000	H	7.63288900	-3.70247400	5.63042400
H	-1.63881400	0.82826800	-6.01147000	C	7.93479000	-7.09342100	5.42617200
H	-3.06323700	0.29154800	-4.05886800	H	6.39625500	-8.50643200	5.96724500
H	-1.55182000	-0.62242300	-3.91806200	H	9.28208100	-5.46734800	4.98421500
H	-2.09010700	4.14890000	-3.72366800	H	8.65288900	-7.86248200	5.15644900
H	-0.54890800	3.26485700	-3.58166500	C	1.30487500	-2.18792000	7.61413900
H	-1.91396700	2.74337700	-1.62415100	C	0.66022200	-0.79025900	7.80601400
H	-3.30820500	2.29227700	-2.65479000	H	1.08100800	-0.23231000	8.64577200
H	-0.48834400	-0.89395800	3.03838500	C	1.74993300	-2.68187100	9.00690400
H	-1.80715900	-0.20841700	4.00362900	H	0.88827700	-2.76297500	9.68059000
TS3b'				H	2.23532600	-3.65696300	8.93022300
C	2.79448000	-2.64879000	5.41251800	H	2.46893300	-1.99047600	9.46044300
C	1.93906400	-2.41989400	4.21674100	C	0.30521400	-3.20806300	7.04183600
Rh	2.33913600	0.14976700	6.50232300	H	-0.12129500	-2.89269900	6.08763300
C	2.03130500	-3.34786400	3.01648000	H	0.79984200	-4.17378200	6.89467300
C	3.83985200	-3.51785500	5.26313300	H	-0.51964300	-3.36021200	7.74807700
H	1.03114200	-3.63082700	2.67791800	C	0.15684400	-1.19088600	2.90545700
H	2.48988200	-2.81872300	2.17210400	H	0.73249400	-1.21797700	1.97421300
H	0.67562600	-7.91616200	4.15913000	H	-0.60378000	-1.97947500	2.83692000
C	0.13203500	-6.96853900	4.15461400	H	-0.35821900	-0.23069700	2.95377000
O	0.90776100	-5.94899700	3.49793400	C	0.87312500	-0.48624000	5.21585200
H	-0.78775900	-7.05450600	3.57693800	C	0.13690100	0.00386200	6.16794500

C	-1.05147700	0.87762000	6.40719300	O	6.49509100	-0.35250400	-2.10378000
C	-1.55648400	1.60136800	5.15249000	C	7.53133900	-0.15313700	-3.08201700
H	-0.76804800	1.61870600	7.16340500	H	7.52423100	0.88482800	-3.43660400
H	-1.85547200	0.26567800	6.84714200	H	8.46985900	-0.37780900	-2.56683300
C	-2.74847900	2.51998800	5.45102000	H	7.38233500	-0.82321200	-3.93642700
H	-0.72849700	2.18915600	4.74143600	C	0.44621000	-1.13006600	-1.21409200
H	-1.84649400	0.86397600	4.39174900	C	0.62413400	-0.21080700	1.01675900
C	-3.26059100	3.25269800	4.20700800	H	0.23956000	0.66759400	1.52972600
H	-3.56525300	1.93201700	5.89285600	C	4.10100900	0.87492800	-0.62045100
H	-2.45107100	3.25340100	6.21157500	H	3.93153400	1.70345900	-1.31995900
H	-4.10872000	3.90191000	4.44744500	H	5.05518700	1.05958200	-0.12075000
H	-2.47592000	3.87848000	3.76784700	S	3.11671100	2.01911200	1.71754800
H	-3.59091100	2.54566600	3.43702100	O	2.08835200	1.74532000	2.73503600
H	-0.41278600	-0.84680400	8.00776500	O	3.19835600	3.33473400	1.05710900
C	3.66629800	0.74647800	7.92205900	C	4.72279000	1.73807500	2.49094200
O	4.35798500	1.09223200	8.76478500	C	5.79921600	2.55341900	2.13092300
Cl	1.91654300	2.68486200	6.35777400	C	4.85203400	0.75605900	3.47284200
C	5.37923500	0.27623900	5.22193800	C	7.03249700	2.36237600	2.75573300
C	6.26641700	0.06215400	4.00332100	H	5.65412600	3.33322000	1.39133000
C	4.68216200	1.09361800	2.63092000	C	6.08805200	0.57498900	4.09145900
C	3.77239600	1.33410000	3.82742200	H	3.99315800	0.15798400	3.76041600
O	6.04952200	1.06513400	3.02110300	C	7.17666300	1.37341600	3.73073100
O	3.99523000	0.29988300	4.81150900	H	7.87609500	2.99132400	2.48716500
H	4.40809100	0.14492000	2.13906600	H	6.20001300	-0.18380800	4.85997900
H	4.57456700	1.90622400	1.90577000	H	8.13692400	1.22973700	4.21765500
H	3.95697000	2.31099700	4.28643800	C	0.72681400	-1.41577600	2.03321200
H	2.71806400	1.27710600	3.55162300	C	-0.42873500	-2.26922900	1.53285600
H	7.32093900	0.11674900	4.29079900	C	2.01702100	-2.26008400	1.95145100
H	6.06982200	-0.93702300	3.57885800	H	2.20460100	-2.62969800	0.94044500
H	5.48582700	-0.54729200	5.93029700	H	2.88927100	-1.68330400	2.26760400
H	5.62523200	1.23078100	5.70702800	H	1.92777900	-3.12772900	2.61383600
TS4dd'				C	0.51153200	-0.96552900	3.48578800
C	1.87067800	0.06551100	0.19338300	H	0.51458500	-1.83686100	4.15483300
C	1.72478800	-0.67637300	-1.05583400	H	1.30646300	-0.28250800	3.79163200
C	2.84475300	-0.79744300	-2.04643300	H	-0.43409800	-0.42826300	3.59620100
C	2.97854700	0.81770900	0.39955800	C	-0.38305200	-0.73306000	-0.06121600
H	2.87954500	-1.80005100	-2.48812600	C	-1.77314400	-0.52688900	-0.08627200
H	2.68899500	-0.10250300	-2.88456800	C	-2.50358500	-0.28048500	-1.38122000
H	6.26147500	-3.68554300	-0.10025800	C	-2.95847400	1.20556800	-1.42083300
C	5.21388200	-3.86314100	-0.35733400	H	-3.39487300	-0.91677000	-1.46879200
O	4.69135800	-2.76054300	-1.11791600	H	-1.87363600	-0.45848100	-2.25745500
H	5.11875200	-4.73580500	-1.00012600	C	-3.60722700	1.59480100	-2.75426600
H	4.64271300	-3.99741800	0.56198400	H	-3.64909400	1.38585500	-0.59016800
C	4.73509500	-1.56186500	-0.49738600	H	-2.08866500	1.84796800	-1.23378900
C	4.21232900	-0.44643100	-1.42173200	C	-4.01229800	3.07168000	-2.79480600
O	5.14961300	-1.40942800	0.62806100	H	-2.91004200	1.38509800	-3.57728900
C	5.23291000	-0.24086500	-2.55811900	H	-4.48912900	0.96394100	-2.93173300
O	4.94766000	0.02225900	-3.70464900	H	-4.47008900	3.33720700	-3.75266600

H	-4.73277900	3.30440200	-2.00327800	C	0.72415300	-0.66999700	-1.73184800
H	-3.14210900	3.72113400	-2.64881800	C	0.82115300	-0.05329900	0.61060000
H	-0.22914400	-3.00593500	0.76050700	H	0.50450900	0.90606400	1.02089400
H	-1.19017100	-2.58145200	2.23942500	C	4.54851500	0.74229400	-0.64732000
Rh	-2.81659100	-0.74260600	1.54705500	H	4.58524000	1.68784700	-1.20063700
C	-3.67707700	-2.22988300	0.79874100	H	5.46857200	0.70339100	-0.06056000
O	-4.33261300	-3.13804500	0.44914700	S	3.47870700	1.95094200	1.58471200
Cl	-2.18989600	1.33082100	2.54035400	O	2.14105500	2.35085700	2.05271900
C	-4.66812100	-2.60881600	5.42597800	O	4.38702800	2.98377000	1.04886300
C	-3.71755800	-2.40189700	4.25693000	C	4.32421400	1.19649300	2.99674200
C	-4.71922100	-0.19539400	4.29000100	C	4.17840300	1.85584700	4.22180000
C	-4.29530000	-0.27182700	5.74545600	C	5.13080300	0.06389800	2.87499600
O	-4.07338500	-1.22884400	3.50494000	C	4.86097500	1.37635100	5.33818700
O	-4.62887700	-1.52663600	6.34809500	H	3.52690200	2.72027000	4.29445900
H	-5.80520800	-0.31774700	4.19460300	C	5.80273800	-0.40956300	4.00546800
H	-4.41365400	0.75654100	3.85289200	H	5.22090300	-0.46477700	1.93229100
H	-3.21428500	-0.08857100	5.81955000	C	5.67462600	0.24497700	5.23098600
H	-4.80691500	0.50796900	6.31964900	H	4.75200500	1.88219000	6.29308000
H	-2.68543900	-2.30675800	4.62032100	H	6.42552000	-1.29540900	3.92172600
H	-3.76877500	-3.25117900	3.56784400	H	6.20209400	-0.12840100	6.10412400
H	-5.68902600	-2.75516300	5.04023400	C	0.75583500	-1.09883100	1.79898300
H	-4.38755100	-3.51616700	5.97163500	C	-0.64717100	-1.72888000	1.90294200
C	0.00606800	-1.98967000	-2.36901200	C	1.71052000	-2.29399700	1.55078300
H	0.78803500	-2.71547500	-2.62504500	H	1.51761400	-2.76119400	0.57898700
H	-0.18535900	-1.40332500	-3.27567600	H	2.75465600	-1.97181200	1.57427000
H	-0.90424200	-2.54450100	-2.13691100	H	1.57903300	-3.05817000	2.32537100
INT-4dd				C	1.10728300	-0.44154300	3.14464700
C	2.17219300	0.11727500	-0.08487300	H	0.98998100	-1.17181400	3.95486400
C	2.03481000	-0.42038300	-1.43615800	H	2.13989500	-0.09862900	3.16969200
C	3.19022200	-0.47357500	-2.39537800	H	0.46542900	0.41950900	3.34423100
C	3.33240900	0.73522900	0.26801000	C	-0.11669300	-0.42671400	-0.55175200
H	3.14748800	-1.36286500	-3.02952900	C	-1.46065800	-0.48864100	-0.43355800
H	3.16425500	0.38535000	-3.07615700	C	-2.49292200	-0.55663000	-1.53177400
H	6.11763900	-4.09066000	-0.89495900	C	-3.61358700	0.49730900	-1.39485500
C	5.10262800	-4.07824300	-1.29888700	H	-2.95705600	-1.55499700	-1.56822600
O	4.79200700	-2.78035300	-1.83641700	H	-2.01464900	-0.40281900	-2.50221900
H	5.01239100	-4.77081700	-2.13520400	C	-4.61097200	0.45665800	-2.55910000
H	4.40037300	-4.34009600	-0.50399500	H	-4.15855400	0.34494400	-0.45123200
C	4.85646000	-1.75651200	-0.96225100	H	-3.16051600	1.49294700	-1.32005200
C	4.54536800	-0.42437000	-1.66176000	C	-5.73755300	1.48521700	-2.41848900
O	5.13961000	-1.90361800	0.20758600	H	-4.07279100	0.62926600	-3.50124200
C	5.66158300	-0.16144400	-2.68878400	H	-5.04145000	-0.55165400	-2.63567100
O	5.49194000	0.24441600	-3.81587700	H	-6.43080200	1.43701800	-3.26460500
O	6.87336000	-0.40108500	-2.15040500	H	-6.31678300	1.31483400	-1.50368300
C	7.99906900	-0.13253300	-3.00715200	H	-5.33885700	2.50454700	-2.37091100
H	8.01317100	0.92036400	-3.29771600	H	-0.72751000	-2.58707800	1.23579100
H	8.88082900	-0.38009900	-2.41719000	H	-0.86383100	-2.04952400	2.92674100
H	7.94927200	-0.74996400	-3.90711700	Rh	-2.26659300	-0.47600800	1.43537300

C	-3.18840000	-2.06310200	1.08745400	H	4.93277100	0.71481700	0.09968800
O	-3.80968900	-3.01595800	0.90327300	S	3.10645600	2.48707300	1.47057400
Cl	-1.71475600	1.78807100	1.82356500	O	1.84933100	2.85482900	2.14101300
C	-4.20412300	-1.45916600	5.74507700	O	3.81807900	3.50930800	0.67874600
C	-3.34618500	-1.63360600	4.50077800	C	4.27760500	1.92121600	2.72684100
C	-3.82351200	0.73084500	4.31191700	C	4.95510100	2.91906600	3.43523900
C	-3.29119500	0.74627100	5.73293500	C	4.47731500	0.56982000	3.00933300
O	-3.44876000	-0.49081400	3.62967800	C	5.82843500	2.55263300	4.45709300
O	-3.79636600	-0.33927800	6.51822800	H	4.80379700	3.96227400	3.17847700
H	-4.91782800	0.81523800	4.30777700	C	5.36489700	0.21604400	4.02978400
H	-3.39519700	1.54683600	3.72783700	H	3.98589700	-0.19908800	2.42357300
H	-2.19223200	0.71528300	5.71258900	C	6.03225300	1.20212300	4.75644600
H	-3.59042400	1.67660900	6.22783100	H	6.35518800	3.32081800	5.01548900
H	-2.29758700	-1.77751600	4.79335200	H	5.53460600	-0.83400700	4.24847500
H	-3.67046200	-2.50928000	3.92899400	H	6.71801900	0.92084200	5.55046600
H	-5.26254500	-1.37163600	5.45272400	C	0.04235600	-0.20664300	2.13804600
H	-4.10970000	-2.34518500	6.38233900	C	-1.50227600	-0.33428400	2.26724800
C	0.25830100	-1.15099100	-3.07644300	C	0.63425500	-1.62524900	2.00314400
H	1.09290000	-1.53466100	-3.66837900	H	0.20312200	-2.16439000	1.15383600
H	-0.20198100	-0.34379700	-3.65939600	H	1.71868600	-1.59120200	1.86527700
H	-0.48345100	-1.94952700	-2.98379400	H	0.42986800	-2.20561600	2.90960200
TS5dd				C	0.58264400	0.44420500	3.42244300
C	1.61127300	0.56385600	0.11357100	H	0.26780000	-0.14292500	4.29388000
C	1.39038200	-0.17701900	-1.12564800	H	1.67351700	0.47908700	3.43052900
C	2.50182500	-0.40204600	-2.10847100	H	0.22334100	1.46904000	3.53430700
C	2.83140600	1.11142000	0.35327000	C	-0.69270000	-0.02493200	-0.14437600
H	2.36166000	-1.32235600	-2.67902800	C	-1.96155300	-0.30626400	0.26935200
H	2.53490000	0.41414900	-2.84128300	C	-2.81754500	-1.40383000	-0.34053200
H	5.01061400	-4.13288700	-0.14866000	C	-3.94727700	-0.95310000	-1.28791600
C	4.04373200	-4.06611600	-0.65277600	H	-3.26417400	-1.98911600	0.47425400
O	3.91792000	-2.80364200	-1.33177400	H	-2.17062100	-2.10719200	-0.87669100
H	3.96111800	-4.82572800	-1.42946400	C	-4.70445100	-2.13312100	-1.91057400
H	3.24804600	-4.18277500	0.08675700	H	-4.64845900	-0.31243100	-0.73960400
C	4.00534700	-1.70900300	-0.55011700	H	-3.52916600	-0.32080300	-2.08138700
C	3.87152800	-0.43287600	-1.39706300	C	-5.83809700	-1.69303000	-2.84255500
O	4.16379700	-1.76165100	0.65039700	H	-3.99967300	-2.76738300	-2.46604000
C	4.98902100	-0.43808000	-2.45302100	H	-5.11312300	-2.76415500	-1.10937200
O	4.83727300	-0.21426300	-3.63207300	H	-6.35855900	-2.55411900	-3.27424200
O	6.18313000	-0.68490300	-1.87935900	H	-6.58008400	-1.09101800	-2.30580000
C	7.31573000	-0.66601300	-2.76850500	H	-5.45681500	-1.08497600	-3.67075200
H	7.40851800	0.31223400	-3.24554300	H	-1.84485800	-1.36275000	2.38673400
H	8.18273300	-0.87225700	-2.14191500	H	-1.85444300	0.24070300	3.13124500
H	7.20625600	-1.43045900	-3.54135600	Rh	-3.12832200	1.05485400	1.37000400
C	0.06429500	-0.47903100	-1.30155800	C	-4.32636400	-0.21860800	2.00925200
C	0.27225700	0.63561900	0.83332700	O	-5.14005200	-0.92088400	2.43460400
H	0.00363900	1.67434200	1.02874300	Cl	-2.01851800	3.01500200	0.52748800
C	4.03963100	0.83009300	-0.52110500	C	-5.59019200	4.39137500	3.24790300
H	4.22361400	1.69337200	-1.17166300	C	-4.44425300	3.42803100	2.98363100

C	-5.43342300	3.23013500	0.76673200	O	4.17642100	2.35316800	-2.04060500
C	-5.32846200	4.74056900	0.90068000	C	2.56679900	3.47655500	-0.25655300
O	-4.77761200	2.54975800	1.87981800	C	1.87123000	4.68278100	-0.34654900
O	-5.89650900	5.20944500	2.12000900	C	3.19375300	3.07853400	0.92768400
H	-6.48218700	2.91114200	0.77151500	C	1.79269400	5.50502100	0.77915600
H	-4.94862700	2.89967200	-0.15355500	H	1.40730600	4.96088000	-1.28641800
H	-4.27766900	5.04220300	0.80389300	C	3.10042200	3.90672200	2.04636600
H	-5.89305800	5.21165200	0.08972100	H	3.71851900	2.13109700	0.98375700
H	-3.50976500	3.94937700	2.75489500	C	2.40388200	5.11684300	1.97292100
H	-4.28465900	2.77772400	3.84746700	H	1.25598500	6.44736400	0.72144300
H	-6.48551600	3.82200000	3.54004000	H	3.57554400	3.60682000	2.97565800
H	-5.32098400	5.04620100	4.08640300	H	2.33895900	5.75777800	2.84753300
C	-0.48830400	-1.11329000	-2.54853700	C	-0.49358000	1.81571300	0.61282300
H	0.17696600	-0.95102300	-3.40019900	C	-0.94319900	0.55613700	1.37980500
H	-0.61358200	-2.19744800	-2.43731300	C	-1.45350100	-2.53921500	-0.81448800
H	-1.46444900	-0.69629900	-2.80464900	H	-1.09042400	-3.13311000	-1.66168400
TS2bb^H				H	-1.14905700	-3.05968400	0.10375300
C	0.87338000	0.51209500	-1.05725500	H	-2.54169100	-2.52588500	-0.87115900
C	0.45859300	-0.88217300	-0.89579000	C	-1.91998200	-0.08110400	0.44496000
Rh	-1.92250200	0.45611100	-1.75153200	C	-3.07602900	0.24049700	-0.02184900
Cl	-3.69063800	-0.97145700	-2.85667900	C	-4.52261900	0.44423700	0.18301600
C	1.48454000	-1.99100600	-0.93632300	C	-4.98179900	0.16034200	1.62495500
C	2.17309100	0.80485500	-1.34262200	H	-5.05584700	-0.19481100	-0.53223100
H	1.20795200	-2.79573300	-0.25040000	H	-4.77542100	1.47532100	-0.10382200
H	1.51017200	-2.44727900	-1.93369100	C	-6.49280700	0.35666900	1.80233500
H	4.00806600	-1.94069400	3.25332600	H	-4.70860300	-0.86881800	1.89015600
C	2.95960400	-2.15093100	3.02925400	H	-4.44164200	0.81688800	2.32000900
O	2.76833100	-2.28919100	1.61038400	C	-6.96809500	0.07415400	3.23074300
H	2.65775600	-3.10499200	3.46037500	H	-6.76062500	1.38450200	1.52259900
H	2.34317500	-1.33898300	3.42266500	H	-7.02464500	-0.29859500	1.10019600
C	3.10050400	-1.21174400	0.86886800	H	-8.04883000	0.21937300	3.32550500
C	2.91684400	-1.50866100	-0.62729000	H	-6.74383700	-0.95692900	3.52656800
O	3.49476500	-0.17264900	1.35102200	H	-6.47888800	0.73921500	3.95161200
C	3.91115400	-2.61533700	-1.02257700	H	-0.10210100	-0.10693900	1.59917400
O	3.67201600	-3.52563100	-1.78352800	H	-1.44310200	0.81781600	2.31895100
O	5.11313500	-2.40745600	-0.45268800	C	-2.93301300	2.04184500	-2.41488700
C	6.14232700	-3.35111500	-0.80580400	O	-3.59028400	2.93177400	-2.71118600
H	6.31637300	-3.33798300	-1.88403000	C	-0.48173100	1.58704000	-4.51688100
H	7.03273200	-3.02656600	-0.26864500	C	0.67700700	1.42599400	-5.49061100
H	5.85369900	-4.36043900	-0.50332200	C	0.37354100	-0.88594300	-5.52121600
C	-0.88900900	-1.14576000	-0.86898000	C	-0.79673900	-0.76884500	-4.55497200
C	-0.25100000	1.50202200	-0.88289300	O	0.49805700	0.28243600	-6.31837700
H	-0.07166200	2.42173700	-1.43554600	O	-0.61294300	0.39302700	-3.71140500
C	3.24777200	-0.25361600	-1.46841600	H	1.30530300	-1.06700300	-4.95935100
H	3.35589000	-0.56320900	-2.51694000	H	0.21041200	-1.72602500	-6.20366000
H	4.21285900	0.15248800	-1.16557700	H	-1.74737700	-0.67356600	-5.09058600
S	2.73714900	2.46593100	-1.74309900	H	-0.86232700	-1.62903100	-3.88843300
O	1.83773000	3.06311200	-2.75849300	H	0.73388000	2.29619300	-6.15111200

H	1.61673100	1.35690200	-4.92421700	H	1.97432300	5.59440300	3.22585000
H	-0.28104400	2.41021300	-3.83190100	C	-0.87194600	1.83175600	0.66261800
H	-1.42349000	1.75473900	-5.05782500	C	-1.18742800	0.56776200	1.50211300
H	0.41337500	2.23716200	1.06388100	C	-1.32833200	-2.70448400	-0.35972300
H	-1.28424300	2.56959100	0.68926600	H	-0.91847200	-3.23721300	-1.21953700
INT-3bb^H				H	-0.99788600	-3.21544900	0.55532000
C	0.70030200	0.57646900	-0.88750100	H	-2.41501200	-2.77408200	-0.41244200
C	0.36316400	-0.85129300	-0.70561900	C	-1.84921000	-0.36775000	0.49961400
Rh	-1.93591600	0.23434500	-1.86543600	C	-2.94088200	0.08332000	-0.14998900
Cl	-3.37493500	-1.53258300	-2.83892700	C	-4.27383000	0.63845800	0.18611100
C	1.40226200	-1.87325200	-1.10025000	C	-4.74339700	0.42380600	1.63607200
C	1.97145100	0.92834600	-1.23452300	H	-4.98898900	0.16273100	-0.50155700
H	1.21349000	-2.83188000	-0.61764900	H	-4.30304200	1.70836200	-0.07294700
H	1.36190600	-2.05376000	-2.18087100	C	-6.19827900	0.86320700	1.84676800
H	4.05431000	-2.28203200	3.00138100	H	-4.63383000	-0.63677600	1.89380500
C	3.02531700	-2.55358900	2.75465900	H	-4.09554800	0.98069500	2.32473700
O	2.82293500	-2.50667000	1.33073000	C	-6.67800200	0.67148200	3.28885300
H	2.81792600	-3.58257300	3.04650100	H	-6.30446000	1.91890200	1.56215600
H	2.34457100	-1.86522500	3.26119400	H	-6.84671500	0.29740300	1.16484500
C	3.04409600	-1.31133900	0.74821100	H	-7.71848000	0.99018900	3.40714100
C	2.83468900	-1.40680100	-0.77117600	H	-6.61586500	-0.38002200	3.59075500
O	3.35968400	-0.31747500	1.36543400	H	-6.07028700	1.25390000	3.99083200
C	3.83278200	-2.42691500	-1.34313200	H	-0.27509800	0.10782600	1.89797900
O	3.57275500	-3.25142000	-2.19004300	H	-1.84121300	0.81254100	2.34396300
O	5.05802500	-2.24459600	-0.81685000	C	-2.96266400	1.58405500	-2.66601500
C	6.09118600	-3.10902500	-1.32767500	O	-3.64999500	2.39094300	-3.11047600
H	6.21087400	-2.96346800	-2.40357700	C	-0.12962400	1.30005600	-4.59744900
H	6.99905600	-2.82346400	-0.79776400	C	1.07811200	1.10195700	-5.50256700
H	5.84187500	-4.15488300	-1.13434600	C	0.65548600	-1.19442100	-5.59945700
C	-0.90957400	-1.24880000	-0.32228500	C	-0.56300400	-1.02336500	-4.70263600
C	-0.47322900	1.50751000	-0.79820700	O	0.90159800	-0.01931500	-6.36029000
H	-0.30885500	2.42535800	-1.35564600	O	-0.36569400	0.10457500	-3.82470700
C	3.11054200	-0.04484600	-1.43709700	H	1.53818100	-1.44408100	-4.98622100
H	3.26795900	-0.20917400	-2.51171500	H	0.48875200	-2.00821900	-6.31213700
H	4.04162500	0.37338800	-1.05436200	H	-1.46732600	-0.86007400	-5.30190400
S	2.45055800	2.63479500	-1.57507800	H	-0.73064800	-1.89517700	-4.06872600
O	1.51715000	3.25163400	-2.54629200	H	1.21992500	1.97760000	-6.14270300
O	3.88790500	2.60095100	-1.89862100	H	1.98142000	0.97496400	-4.88459000
C	2.25361000	3.53564600	-0.02444000	H	0.05587200	2.10839900	-3.89019500
C	1.58380600	4.75929700	-0.04917500	H	-1.02282200	1.51664900	-5.20178600
C	2.83470000	3.03939800	1.14620300	H	-0.06812400	2.41563500	1.12921500
C	1.48703200	5.50094900	1.12969900	H	-1.76321500	2.46953500	0.64274700
H	1.14845100	5.11077100	-0.97815500	TS3bb^H			
C	2.72333100	3.78844700	2.31782700	C	0.01418000	-1.30982400	0.48741400
H	3.33817200	2.07782800	1.15201700	C	0.20704100	-2.72581400	0.15132000
C	2.05400600	5.01601000	2.30989000	Rh	-0.80479000	-0.41970300	-2.56165700
H	0.96891300	6.45530900	1.12450400	Cl	-0.18938100	-0.27535900	-4.90922800
H	3.16184700	3.41251600	3.23734600	C	1.37678800	-3.48295800	0.72939300

C	0.84346800	-0.69350700	1.36207000	H	-2.12104800	-3.95006000	-3.68718300
H	1.14784700	-4.54165600	0.86540900	H	-1.26554100	-2.80130600	-4.75383300
H	2.21758200	-3.44443600	0.02703700	C	-3.82597000	-3.18153300	-5.74626900
H	0.35951900	-4.70173400	5.36325900	H	-4.13632400	-2.41964800	-3.74408000
C	-0.04408800	-5.03500400	4.40435600	H	-3.23732200	-1.32406600	-4.79646700
O	0.79182500	-4.58234100	3.32419900	C	-5.15123700	-2.67183900	-6.32175000
H	-0.04002500	-6.12276600	4.34225100	H	-3.04757200	-3.13414400	-6.51853400
H	-1.05903000	-4.64648300	4.29160200	H	-3.92670000	-4.24118300	-5.47319000
C	0.93823800	-3.24561900	3.22029300	H	-5.45772500	-3.25788200	-7.19433200
C	1.88683800	-2.89512000	2.06323800	H	-5.95657100	-2.73277500	-5.58051600
O	0.38725300	-2.45873900	3.95809400	H	-5.06795500	-1.62553300	-6.63533500
C	3.26401500	-3.50943500	2.37695900	H	-3.39934600	-3.07991000	-0.25965600
O	3.95530500	-4.11172500	1.58737000	H	-3.76021500	-1.69526700	-1.30953900
O	3.62330100	-3.24567400	3.64671100	C	2.43645500	-0.81705500	-2.52955900
C	4.92495000	-3.72267600	4.03867400	C	3.89835800	-0.46102500	-2.20466900
H	5.69905700	-3.26707900	3.41723200	C	3.34429400	1.52259600	-1.08684100
H	5.04330300	-3.42510600	5.07982200	C	2.12282500	1.48309200	-2.02765100
H	4.97864200	-4.80908900	3.93719900	O	3.95988300	0.23604900	-0.97167900
C	-0.67477300	-3.23076200	-0.74274400	O	1.54596900	0.17399600	-1.98434600
C	-1.18275200	-0.69138600	-0.14825400	H	4.07351300	2.26229900	-1.45674300
H	-1.07152600	0.38288900	-0.22529800	H	3.04170600	1.80455000	-0.07714000
C	2.06061900	-1.36164800	1.95751800	H	1.35579100	2.17348300	-1.67916100
H	2.92238000	-1.14444400	1.31087700	H	2.38678500	1.73480400	-3.06356900
H	2.28593500	-0.94414700	2.93826000	H	4.49791500	-1.36977000	-2.09795800
S	0.62954200	1.04390600	1.84273700	H	4.34785700	0.14020000	-3.01088800
O	0.46809100	1.87968300	0.63254300	H	2.27200800	-0.90838300	-3.61076300
O	1.72190300	1.34461300	2.78342700	H	2.14582200	-1.75525300	-2.04887500
C	-0.93162700	1.14955700	2.74297800	C	-1.59723100	1.40727100	-2.63795100
C	-1.89660000	2.05166400	2.29144600	O	-2.35409800	2.24543200	-2.86267000
C	-1.11491800	0.40153100	3.90896900	H	-2.44739700	-1.55440100	1.42304300
C	-3.07909000	2.19746800	3.01917000	H	-3.23470000	-0.26377500	0.51871000
H	-1.71074700	2.62835800	1.39199400	INT-2d^H			
C	-2.30509800	0.55266500	4.62087500	C	-1.11360300	-4.74176200	-5.54842500
H	-0.35755900	-0.29903800	4.24142600	C	-1.24141200	-3.21616700	-5.76554500
C	-3.28360900	1.44763600	4.17928000	H	-0.27122500	-2.74794900	-5.55492700
H	-3.83579200	2.89892700	2.68073800	H	-1.46735000	-3.03599400	-6.81922400
H	-2.46479000	-0.02754900	5.52474200	C	-1.26009300	-5.08084800	-4.04418400
H	-4.20537300	1.56275700	4.74226300	H	-1.13448100	-6.15221300	-3.89251500
C	-2.56008500	-1.11829200	0.42523200	H	-0.45629700	-4.57051000	-3.50125300
C	-3.01390100	-2.12438600	-0.63614000	C	-2.30581100	-2.55217200	-4.90603300
C	-0.72199000	-4.66009900	-1.21359000	C	-2.95519300	-3.17477000	-3.87761800
H	-0.16071600	-5.32745100	-0.55671900	C	-4.11280700	-2.68133700	-3.04649800
H	-1.75496700	-5.02390800	-1.26348000	H	-4.59555300	-1.83710500	-3.52924600
H	-0.30200800	-4.75738200	-2.22258300	C	-3.88430000	-2.26096600	-1.53978700
C	-1.67118500	-2.28809500	-1.37385600	C	-5.25355600	-1.61510900	-1.12314700
C	-1.55735700	-2.09351800	-2.78688500	H	-5.56210400	-0.95530600	-1.94428800
C	-2.01567300	-2.89154000	-3.96139000	H	-6.01467400	-2.40184400	-1.07528800
C	-3.36510400	-2.37677900	-4.52494800	C	-5.34258400	-0.83233700	0.11251800

C	-5.52582100	-0.16568600	1.10697500	C	-3.61610700	-6.76979700	-2.64951400
C	-5.71651500	0.65198300	2.30659800	H	-4.26692900	-7.40602100	-3.25545400
C	-5.46428100	2.15658800	2.07453800	H	-2.60078100	-7.18027000	-2.63596000
H	-5.05175900	0.29157900	3.10455100	H	-3.99769200	-6.80047900	-1.62133800
H	-6.73919800	0.51052700	2.68355800	C	-7.96821400	-3.83494600	-6.91124100
C	-5.67185500	2.99454600	3.34131900	C	-8.07473200	-3.60895000	-5.40931000
H	-4.44143900	2.29330100	1.70128500	C	-6.55661600	-1.80049500	-5.60853400
H	-6.13154700	2.51143100	1.27923100	C	-6.45711400	-2.06115500	-7.10449600
C	-5.41885200	4.48900300	3.11952200	O	-6.84613600	-3.03228500	-4.90454200
H	-6.69628900	2.84707200	3.70991300	O	-7.67292100	-2.61972400	-7.59149200
H	-5.00789400	2.62402500	4.13446500	H	-5.62681700	-1.39799900	-5.21033800
H	-5.57516300	5.06137900	4.03962300	H	-7.36930500	-1.09098900	-5.40008800
H	-4.39147200	4.67151200	2.78450500	H	-6.29270200	-1.12108700	-7.63820700
H	-6.09167000	4.89572500	2.35613700	H	-5.60738500	-2.72836400	-7.31269300
C	-2.61103500	-4.59253400	-3.59710500	H	-8.89204600	-2.91070900	-5.18026800
C	-3.63007600	-5.37133600	-3.15976600	H	-8.22194800	-4.55105900	-4.88246400
C	-2.20989700	-5.46516200	-6.35652100	H	-7.19364100	-4.59033300	-7.10544400
O	-3.06405100	-4.91273300	-7.01152800	H	-8.92355500	-4.19763000	-7.30397400
O	-2.09822700	-6.79648700	-6.21942600	C	-2.75965900	-1.16821200	-1.57486800
C	0.26271000	-5.20244900	-6.04455000	C	-2.09790700	-0.72308600	-0.25865500
O	1.16312300	-5.59429500	-5.33684100	H	-3.16345300	-0.28770100	-2.08699500
O	0.35451000	-5.07843400	-7.38295900	H	-1.95700800	-1.54631300	-2.22023200
C	-3.11095800	-7.57723900	-6.89730200	C	-1.04958500	0.37028400	-0.50187200
H	-3.09372000	-7.36359600	-7.96826400	H	-2.85038900	-0.35249400	0.44070200
H	-2.84611800	-8.61700800	-6.70750300	H	-1.60636700	-1.57650000	0.22245200
H	-4.09706600	-7.34277700	-6.49011800	H	-0.56986700	0.67479100	0.43436000
C	1.61416000	-5.47082700	-7.95914000	H	-0.25879100	0.02357700	-1.17830500
H	1.50964500	-5.30532800	-9.03083000	H	-1.50281400	1.26454000	-0.94592600
H	2.42633900	-4.86419500	-7.55157600	C	-3.47465400	-3.45168500	-0.62497100
H	1.81712800	-6.52353900	-7.74918800	C	-3.74905400	-3.37563000	0.88843100
S	-2.69368600	-0.89606100	-5.51331300	H	-2.40587300	-3.65145800	-0.78104600
O	-3.14311200	-1.05367700	-6.91010900	H	-3.98191000	-4.35110600	-0.97929600
O	-3.55557300	-0.17201500	-4.55723800	C	-3.22696800	-4.62591700	1.60727200
C	-1.11350200	-0.02862400	-5.56892800	H	-3.29855100	-2.48659600	1.33468200
C	-0.42618900	0.04933400	-6.78214700	H	-4.82595400	-3.28328600	1.06540000
C	-0.62553400	0.58460900	-4.41254000	H	-3.43948200	-4.58428300	2.68047000
C	0.78417300	0.74264700	-6.82959700	H	-3.69249300	-5.53780400	1.21425700
H	-0.85075800	-0.40857000	-7.66883000	H	-2.14234000	-4.73255300	1.48701100
C	0.58646400	1.27181500	-4.47264200	TS2dd^H			
H	-1.19347300	0.53904200	-3.49092000	C	0.70528100	0.62262700	-0.88936600
C	1.29104100	1.34753400	-5.67727000	C	0.31253700	-0.77844800	-0.69267300
H	1.32611400	0.81587300	-7.76764800	Rh	-2.01313500	0.53917600	-1.67988200
H	0.97489100	1.75544800	-3.58149400	Cl	-3.65464400	-0.89438800	-2.95672500
H	2.23271000	1.88702300	-5.71942700	C	1.34202300	-1.88487800	-0.66603300
Rh	-5.26795500	-4.36936300	-3.67939500	C	1.97049700	0.89480700	-1.32976900
Cl	-6.21206100	-6.34551500	-4.86748000	H	1.12357200	-2.58970500	0.14200800
C	-6.21806600	-4.65653000	-2.15850100	H	1.29036100	-2.47338000	-1.58992100
O	-6.84480600	-4.92230600	-1.22958100	H	4.24894600	-1.48043400	3.22883100

C	3.17454800	-1.65702800	3.14034200	H	-4.86991000	0.85942800	2.15214300
O	2.82020700	-1.91648000	1.77022400	C	-7.42973900	0.04283800	2.89293400
H	2.88375100	-2.55054100	3.69202000	H	-7.13751200	1.28770100	1.14826400
H	2.63836200	-0.78222800	3.51601900	H	-7.29762600	-0.42157800	0.78364800
C	3.14335000	-0.94814300	0.88912800	H	-8.51957400	0.14443100	2.89496500
C	2.79008300	-1.37446400	-0.54450700	H	-7.18875300	-0.96403500	3.25204200
O	3.66231800	0.09862600	1.21264400	H	-7.02758400	0.75849600	3.61910500
C	3.75131000	-2.50741800	-0.95376900	H	-0.44794600	-0.10168200	1.76073600
O	3.45128800	-3.45833500	-1.63974400	H	-1.83664600	0.78061500	2.42508000
O	4.99586900	-2.27612900	-0.49506100	C	-3.00725700	2.11504200	-2.39521000
C	5.99035100	-3.24600200	-0.87666800	O	-3.67084700	2.98522800	-2.73294100
H	6.08320400	-3.28723700	-1.96419500	C	-0.70490700	1.64048900	-4.50912700
H	6.92031100	-2.90404200	-0.42395700	C	0.42683000	1.60115600	-5.52740100
H	5.71909600	-4.23640900	-0.50399900	C	0.56751100	-0.71437000	-5.33701300
C	-1.03010900	-1.06052700	-0.74578800	C	-0.56951100	-0.72726300	-4.32451800
C	-0.41302700	1.60096200	-0.65178100	O	0.43012600	0.37017800	-6.24223900
H	-0.22806300	2.54222600	-1.16308000	O	-0.59435900	0.52383000	-3.59668100
C	3.00638700	-0.19720000	-1.52482600	H	1.53743300	-0.65455100	-4.81536000
H	2.95585600	-0.59300200	-2.54773000	H	0.54690900	-1.63473100	-5.92933000
H	4.01346900	0.20082700	-1.40469000	H	-1.53761500	-0.87447300	-4.81396500
S	2.49663200	2.48362300	-1.99595500	H	-0.43220600	-1.51260600	-3.57955500
O	1.34096200	3.19342100	-2.59065100	H	0.29049100	2.39910400	-6.26381000
O	3.65818300	2.17604600	-2.85208900	H	1.38843000	1.75530600	-5.01722400
C	3.09358300	3.54827400	-0.66320600	H	-0.63001300	2.54209600	-3.90164400
C	2.53114300	4.81968200	-0.53564800	H	-1.67984500	1.58853700	-5.01255400
C	4.15833000	3.13958300	0.14404800	C	0.57729700	2.34843300	1.60791500
C	3.04302100	5.69677400	0.42243000	C	0.64329000	2.18336000	3.13980800
H	1.71626500	5.10794200	-1.18994000	H	0.76425400	3.39909500	1.35403600
C	4.65487600	4.02223000	1.10261300	H	1.42487400	1.79059200	1.20026500
H	4.57637200	2.14491800	0.04993200	C	1.99803000	2.64031800	3.69583700
C	4.10239900	5.29882800	1.24028000	H	-0.15806300	2.73711800	3.63756700
H	2.61688500	6.69043800	0.52491200	H	0.49308900	1.12953000	3.40737900
H	5.47738600	3.71264300	1.74023000	H	2.04365800	2.51214200	4.78290800
H	4.50038400	5.98346400	1.98378300	H	2.81749200	2.06763200	3.24864800
C	-0.72455200	1.89172500	0.87400600	H	2.18091600	3.69772400	3.47596200
C	-1.26639600	0.57847700	1.51230400	C	-1.79892500	3.01399100	0.88868100
C	-1.57309900	-2.46252400	-0.73394900	C	-2.22781100	3.62803600	2.22997600
H	-1.15973900	-3.04097600	-1.56911900	H	-2.69721500	2.63570100	0.38852700
H	-1.30328900	-2.98872500	0.19202000	H	-1.42544700	3.82532700	0.24952800
H	-2.65747900	-2.46685300	-0.84202200	C	-3.40903000	4.59172500	2.05886500
C	-2.16169500	-0.01811100	0.48546700	H	-2.50900600	2.84355800	2.94510500
C	-3.29793500	0.26334000	-0.04676400	H	-1.39175100	4.17189900	2.68315000
C	-4.76439300	0.39689200	0.03431800	H	-3.69538400	5.04511600	3.01334600
C	-5.32447300	0.15043100	1.44757600	H	-3.16071500	5.40384900	1.36618300
H	-5.20577300	-0.29883700	-0.69042900	H	-4.28898600	4.07595700	1.65755000
H	-5.04726900	1.39855700	-0.31898200	INT-2e^H			
C	-6.85183500	0.28558500	1.49529200	C	-1.17208100	-4.74299400	-5.62206100
H	-5.03099400	-0.85326300	1.78025900	C	-1.28511000	-3.21375500	-5.81448400

H	-0.30172600	-2.76273100	-5.62842700	C	-0.32341600	0.06312800	-6.59609100
H	-1.54199100	-3.01317800	-6.85717500	C	-0.66980800	0.60680600	-4.24571700
C	-1.26589500	-5.09527900	-4.11699900	C	0.89354300	0.74564900	-6.56759000
H	-1.14356100	-6.16892400	-3.97921300	H	-0.69489700	-0.39095300	-7.50810100
H	-0.43886600	-4.59546100	-3.59967200	C	0.54893100	1.28474700	-4.23020100
C	-2.31402800	-2.54913400	-4.91292400	H	-1.29845700	0.56954600	-3.36387800
C	-2.94633400	-3.18175700	-3.87946100	C	1.33056600	1.34992400	-5.38673100
C	-4.08826900	-2.69818000	-3.01913700	H	1.49478900	0.81212500	-7.46929900
H	-4.58802500	-1.85566900	-3.48761200	H	0.88347700	1.76936900	-3.31800900
C	-3.82156100	-2.27861000	-1.51859200	H	2.27754900	1.88138600	-5.36965400
C	-5.18609500	-1.66507900	-1.04498100	Rh	-5.24559500	-4.39900900	-3.61747300
H	-5.55802700	-1.02974400	-1.85916600	Cl	-6.24298200	-6.42835400	-4.68478200
H	-5.92045100	-2.47137500	-0.94069500	C	-6.17185300	-4.68288200	-2.08009900
C	-5.22686500	-0.86342500	0.18124800	O	-6.77920200	-4.94914000	-1.13898400
C	-5.36638200	-0.18817300	1.17689500	C	-3.54541000	-6.77171200	-2.59763400
C	-5.50506300	0.63756700	2.37810600	H	-4.20214900	-7.42696400	-3.17631200
C	-5.46002500	2.15390400	2.09515800	H	-2.52392400	-7.16678800	-2.60185800
H	-4.71033700	0.37883700	3.09232100	H	-3.90190500	-6.79111900	-1.56030900
H	-6.45043200	0.39129700	2.88167000	C	-7.77961700	-3.98413200	-6.94535600
C	-5.59542800	2.99732900	3.36796200	C	-7.99497700	-3.69119000	-5.46674800
H	-4.51711500	2.39395300	1.58780000	C	-6.47516400	-1.88459000	-5.63885600
H	-6.26155900	2.40946200	1.39097900	C	-6.26264000	-2.21184400	-7.10969100
C	-5.54813600	4.50430000	3.09681400	O	-6.80475800	-3.08809200	-4.90263000
H	-6.53856200	2.74521400	3.87205600	O	-7.43820700	-2.79999000	-7.65799600
H	-4.79470100	2.72577700	4.06958700	H	-5.58439200	-1.44989800	-5.18915500
H	-5.64799300	5.07997100	4.02270500	H	-7.30933200	-1.17897100	-5.52386900
H	-4.60147600	4.79265400	2.62593500	H	-6.06150900	-1.29646300	-7.67259200
H	-6.35745900	4.81149700	2.42491500	H	-5.39811300	-2.88306200	-7.22413100
C	-2.59631400	-4.60111500	-3.61644000	H	-8.82546000	-2.98492800	-5.32826500
C	-3.59210500	-5.38188400	-3.12880300	H	-8.17984600	-4.60842700	-4.90902400
C	-2.31063300	-5.44215600	-6.39146300	H	-6.99064700	-4.74263500	-7.04733600
O	-3.19884700	-4.87099300	-6.98322200	H	-8.70268700	-4.37048800	-7.38937300
O	-2.19580600	-6.77617800	-6.29664400	C	-2.72382200	-1.16128400	-1.59170100
C	0.17696600	-5.21757400	-6.17620900	C	-2.00543100	-0.72567300	-0.30553600
O	1.09792900	-5.63054400	-5.50811400	H	-3.17433100	-0.28444500	-2.06738800
O	0.21891700	-5.07803200	-7.51549100	H	-1.95057400	-1.51285200	-2.28349400
C	-3.24393200	-7.53955900	-6.94004900	H	-1.29835000	0.07638000	-0.54906700
H	-3.29285100	-7.28705100	-8.00145300	H	-2.69440000	-0.34323100	0.44791300
H	-2.96234000	-8.58335100	-6.80453100	H	-1.42311600	-1.53989600	0.13585100
H	-4.20471800	-7.32845100	-6.46503900	C	-3.35715300	-3.46209200	-0.62196000
C	1.44940300	-5.48164100	-8.14471900	C	-3.55064700	-3.36594500	0.90023000
H	1.30804100	-5.29650500	-9.20893100	H	-2.29951400	-3.65979000	-0.83768800
H	2.28646400	-4.89562900	-7.75794900	H	-3.88438800	-4.36189000	-0.94297100
H	1.64161000	-6.54099600	-7.95950000	H	-3.15648600	-4.27742600	1.36409200
S	-2.67238300	-0.86994000	-5.47413500	H	-3.04020300	-2.51543500	1.35217700
O	-3.05839400	-0.97615300	-6.89448100	H	-4.60696100	-3.29092600	1.17120600
O	-3.57357500	-0.17756100	-4.53161500	TS2ee^H			
C	-1.08771100	-0.00746200	-5.42902800	C	0.68758200	0.69502100	-0.83466300

C	0.30071200	-0.71133700	-0.65858800	C	-2.16546500	0.03994500	0.57276700
Rh	-2.04875300	0.57344300	-1.60743800	C	-3.30568700	0.32274100	0.04894600
Cl	-3.71193000	-0.89116000	-2.83045200	C	-4.77108100	0.46449300	0.14623900
C	1.32877500	-1.81826500	-0.70060100	C	-5.35524400	-0.08403400	1.46150800
C	1.96206600	0.98432900	-1.23804100	H	-5.21612300	-0.04622700	-0.71603400
H	1.10431700	-2.57882200	0.05249300	H	-5.02617300	1.52886900	0.02888900
H	1.28040400	-2.33717700	-1.66557600	C	-6.88023800	0.06666600	1.52605200
H	4.20793400	-1.72643400	3.23901300	H	-5.08343000	-1.14291000	1.55459900
C	3.13344300	-1.88460400	3.12024000	H	-4.89867500	0.43187100	2.31665100
O	2.80211000	-2.04693600	1.72943700	C	-7.48002700	-0.49065100	2.82071700
H	2.82468900	-2.81029900	3.60484800	H	-7.14537300	1.12790200	1.42549900
H	2.59994200	-1.03074400	3.54431300	H	-7.32816600	-0.44286600	0.66299300
C	3.10856700	-1.00438200	0.93135400	H	-8.56776000	-0.36968600	2.83871800
C	2.77685700	-1.32468300	-0.53357500	H	-7.26221100	-1.55894600	2.93032000
O	3.59609300	0.02499500	1.34689400	H	-7.07379800	0.02218200	3.70010300
C	3.73786700	-2.43515300	-1.00189900	H	-0.41514900	-0.00960000	1.81014600
O	3.43616600	-3.35663700	-1.72581700	H	-1.80516300	0.84578900	2.50484800
O	4.98507900	-2.21699900	-0.54358300	C	-3.05419900	2.11286100	-2.38678800
C	5.98179800	-3.16346200	-0.97514200	O	-3.71476600	2.95789600	-2.78784400
H	6.06460600	-3.15778800	-2.06423300	C	-0.56339800	1.66494300	-4.39724500
H	6.91391300	-2.83503300	-0.51689700	C	0.61554400	1.52934400	-5.35170900
H	5.71991300	-4.17044200	-0.64233300	C	0.45248900	-0.79422400	-5.27505400
C	-1.04040800	-1.00373400	-0.67534400	C	-0.73492800	-0.70332500	-4.32684100
C	-0.44965500	1.65892400	-0.60834500	O	0.51404600	0.33949700	-6.12701000
H	-0.28136800	2.60009300	-1.12568800	O	-0.63751100	0.50466400	-3.53612200
C	3.01628100	-0.09128700	-1.43571300	H	1.38781400	-0.89056400	-4.69813600
H	3.01729200	-0.42826600	-2.48035400	H	0.34884100	-1.67494000	-5.91686900
H	4.01439400	0.30576200	-1.25006100	H	-1.68176300	-0.69444500	-4.87681300
S	2.49359000	2.58536200	-1.87378600	H	-0.75441800	-1.53536400	-3.62221000
O	1.33651500	3.33830100	-2.41131000	H	0.62381300	2.36931000	-6.05283100
O	3.61511100	2.28067000	-2.78408500	H	1.55791300	1.54164300	-4.78441100
C	3.15049700	3.60322700	-0.53030900	H	-0.42186500	2.52735500	-3.74689200
C	2.79512700	4.95436300	-0.51813600	H	-1.50388900	1.74988900	-4.95918500
C	4.04610700	3.07814800	0.40397400	C	0.55905900	2.43781800	1.59952300
C	3.34767600	5.79343300	0.45047000	C	0.48675300	2.84380600	3.07837400
H	2.09435500	5.32792200	-1.25621000	H	0.94541200	3.28855800	1.02886100
C	4.58279300	3.92707700	1.37270100	H	1.30897200	1.64675600	1.50244200
H	4.29082200	2.02300500	0.41209800	H	1.49846500	3.03789900	3.44934200
C	4.23961900	5.28121700	1.39478900	H	-0.09330800	3.75733000	3.23323700
H	3.07901100	6.84556400	0.46682700	H	0.05339700	2.05788400	3.70735000
H	5.27049400	3.52616400	2.11131000	C	-1.82799200	3.09623700	0.94163100
H	4.66514100	5.93596800	2.14986100	C	-2.72577800	3.24012400	2.18021300
C	-0.75361000	1.96301200	0.91390600	H	-2.48553600	2.97627900	0.07628100
C	-1.25481300	0.65178000	1.57965100	H	-1.29524300	4.04089700	0.77318000
C	-1.57452600	-2.40907600	-0.64594400	H	-3.34931600	4.13459400	2.07653900
H	-1.16700700	-2.99321300	-1.47991000	H	-3.40609300	2.38981700	2.29027200
H	-1.29154000	-2.92519700	0.28172500	H	-2.16701200	3.33899000	3.11311700
H	-2.65992200	-2.42024700	-0.74180800				

INT-2th

C	2.47182900	-2.03585600	-1.18935300	O	-0.35001200	2.42185900	-1.25100900
C	2.23213000	-0.61136600	-1.74189000	C	2.13763900	2.59015500	-2.16958400
H	3.16650000	-0.04022500	-1.66255400	C	2.83072200	2.53368500	-3.38099800
H	1.98738300	-0.68707700	-2.80345300	C	2.56492400	3.40838500	-1.12011100
C	2.37789700	-2.03570200	0.35823000	C	3.98260400	3.30586500	-3.53826700
H	2.57791700	-3.03498200	0.74344700	H	2.45442100	1.90859700	-4.18322500
H	3.15230500	-1.36432500	0.74570400	C	3.71951000	4.17182400	-1.29057100
C	1.13435300	0.16087400	-1.02959500	H	1.99989800	3.45749300	-0.19798400
C	0.57361900	-0.23501000	0.15080500	C	4.42764100	4.11936200	-2.49428700
C	-0.59701700	0.36659000	0.87876400	H	4.52705200	3.27534300	-4.47724900
H	-1.08500600	1.11220200	0.26199200	H	4.06186000	4.81393000	-0.48471300
C	-0.40467100	0.99282000	2.30629300	H	5.32434000	4.71909900	-2.62022000
C	-0.00603000	-0.02173400	3.43091000	C	-1.73886200	1.70325800	2.68260800
H	-0.64669200	-0.89591800	3.31487200	C	0.70691000	2.07927400	2.24365800
H	1.00921800	-0.36331300	3.20835100	Rh	-1.62556300	-1.46023400	0.51213900
C	-0.08294600	0.43228200	4.81870500	Cl	-2.51815500	-3.62078400	-0.31245500
C	-0.15139300	0.73413100	5.98749500	C	-2.71643300	-1.68227000	1.95733500
C	-0.27480300	1.16165400	7.38121800	O	-3.41108100	-1.92465600	2.83944300
C	-1.59088000	1.91842700	7.66212100	C	0.07650700	-3.55494100	2.05187400
H	0.57801000	1.80357100	7.64214600	H	-0.54455100	-4.31518500	1.56970100
H	-0.20814000	0.28636200	8.04208300	H	1.10509500	-3.92036900	2.14247700
C	-1.69750900	2.40181500	9.11279400	H	-0.31544900	-3.41352100	3.06715100
H	-1.66234300	2.77122500	6.97606500	C	-3.12201200	0.00230800	-3.54088100
H	-2.43649700	1.26124300	7.42424600	C	-3.00377300	-1.03907300	-2.43784500
C	-3.00217500	3.15269300	9.39737000	C	-3.85485600	0.57634900	-0.89109000
H	-1.61407700	1.54075600	9.79007700	C	-3.95111200	1.57988300	-2.03303800
H	-0.84257600	3.05267400	9.34193800	O	-2.79579400	-0.36876200	-1.16373600
H	-3.05037800	3.48891700	10.43812500	O	-4.18471200	0.91383000	-3.26591800
H	-3.09730400	4.03662700	8.75679600	H	-3.60197200	1.06879000	0.04883400
H	-3.87445700	2.51577300	9.21234200	H	-4.79790400	0.02361900	-0.77970500
C	1.00460900	-1.54402000	0.72274600	H	-4.79612400	2.25554600	-1.86563600
C	0.01769800	-2.27692700	1.29168600	H	-3.02379000	2.17036000	-2.07708100
C	1.41771100	-2.99257400	-1.78312200	H	-3.91095700	-1.64946500	-2.36449500
O	0.52275000	-2.65904100	-2.52691400	H	-2.14331200	-1.69209800	-2.58896900
O	1.61938200	-4.24775400	-1.35226200	H	-2.16960600	0.53896700	-3.65238600
C	3.86910000	-2.50826600	-1.61253400	H	-3.36384700	-0.49163400	-4.48711600
O	4.80549000	-2.66842900	-0.86269300	F	-2.66563000	0.80115700	3.07701100
O	3.92852300	-2.69055200	-2.94554300	F	-1.59850500	2.58962500	3.67979300
C	0.66605500	-5.22869300	-1.82582200	F	-2.27344300	2.37914400	1.64003400
H	0.69205400	-5.27782100	-2.91670600	F	0.38092000	3.08265100	1.40341500
H	0.98775000	-6.17435500	-1.39062700	F	0.97612600	2.63410800	3.43571400
H	-0.33952100	-4.96293700	-1.49296300	F	1.87045500	1.54086800	1.80357100
C	5.20270700	-3.12389800	-3.45820500	TS2ff[†]			
H	5.06703900	-3.22002200	-4.53479400	C	0.61900800	0.56560400	-0.67931500
H	5.97655200	-2.38718600	-3.23021700	C	0.29713600	-0.86558800	-0.54276200
H	5.48349500	-4.08294500	-3.01691300	Rh	-2.03232400	0.36661800	-1.59801200
S	0.63246100	1.61018300	-1.99046500	Cl	-3.51703100	-1.09883100	-2.98418900
O	0.29538400	1.10767700	-3.33680500	C	1.38443200	-1.91474700	-0.52319700

C	1.85211000	0.91719900	-1.14404100	C	-4.88805700	0.13329300	-0.07850800
H	1.23329900	-2.59909800	0.31740300	C	-5.51363700	-0.12195700	1.30570300
H	1.31645100	-2.53350400	-1.42517200	H	-5.30375300	-0.54585600	-0.83282400
H	4.35859900	-1.46548800	3.27120500	H	-5.13208500	1.14619500	-0.42521800
C	3.26896700	-1.50140700	3.20471200	C	-7.04107900	0.02039900	1.28471400
O	2.85631300	-1.79836000	1.85728700	H	-5.24051000	-1.12935900	1.64465400
H	2.87156000	-2.31049000	3.81705000	H	-5.08814900	0.58312000	2.03171700
H	2.85768100	-0.53986000	3.51859300	C	-7.68157700	-0.23386200	2.65261300
C	3.27541800	-0.92458100	0.92132600	H	-7.30544900	1.02740400	0.93549800
C	2.81332800	-1.34073300	-0.48566900	H	-7.45715100	-0.67794800	0.54671900
O	3.96076600	0.04100700	1.17342500	H	-8.76981000	-0.12629800	2.60671000
C	3.78189300	-2.42191100	-1.01439700	H	-7.46206300	-1.24585200	3.01103600
O	3.47322800	-3.29221800	-1.79814900	H	-7.30867600	0.47214400	3.40320700
O	5.02804600	-2.24670300	-0.54368800	H	-0.74756700	-0.41307400	1.96340900
C	6.01775600	-3.16886600	-1.04032700	H	-2.20097300	0.44748100	2.50645400
H	6.10339000	-3.08521500	-2.12597100	C	-3.03825700	1.92052200	-2.35600300
H	6.95081300	-2.88196200	-0.55704700	O	-3.69902900	2.77433400	-2.73176800
H	5.74594400	-4.19470300	-0.78156300	C	-0.64621800	1.60375900	-4.36330500
C	-1.02107900	-1.22417600	-0.66295700	C	0.51339800	1.63693400	-5.35010700
C	-0.55980300	1.46413300	-0.41764700	C	0.74982300	-0.67336500	-5.21087800
H	-0.40394500	2.45838500	-0.82357900	C	-0.40676500	-0.76027500	-4.22412100
C	2.91061000	-0.12893700	-1.44646800	O	0.58333500	0.42461000	-6.09402100
H	2.79096200	-0.49516700	-2.47376400	O	-0.51108300	0.47167700	-3.47010500
H	3.90967000	0.30135200	-1.38966700	H	1.70616500	-0.58440200	-4.66926500
S	2.27470200	2.55101400	-1.78755500	H	0.78072300	-1.58030400	-5.82312700
O	1.03916200	3.27675000	-2.16275500	H	-1.35498100	-0.94396600	-4.73917900
O	3.28305900	2.28793800	-2.83360900	H	-0.24716300	-1.55504800	-3.49355100
C	3.06724800	3.55021300	-0.51030100	H	0.36175400	2.44667100	-6.07046500
C	2.59743300	4.85279000	-0.33033200	H	1.45637700	1.81519300	-4.81345500
C	4.16329200	3.06462200	0.20621600	H	-0.62996700	2.49381400	-3.73406000
C	3.24299700	5.68580800	0.58357600	H	-1.60214700	1.51837800	-4.89747600
H	1.74090200	5.19483800	-0.89943500	F	1.00854900	2.95374500	1.53217900
C	4.79134800	3.90568200	1.12472100	F	1.14860400	0.85203500	2.05422000
H	4.50360200	2.04352400	0.08872100	F	-0.05091200	2.18027400	3.26519200
C	4.33760800	5.21372600	1.31023000	F	-1.34520100	3.94648600	1.06126100
H	2.88688200	6.70127300	0.72931800	F	-2.45062800	2.79516500	2.54050000
H	5.63659700	3.53426800	1.69611700	F	-2.99314700	2.68607100	0.45467900
H	4.83493100	5.86355600	2.02458600				
C	-0.93456100	1.58385400	1.10954000				
C	-1.54670900	0.25873800	1.65104800				
C	0.30548900	1.91074100	1.99046800				
C	-1.93641200	2.76001600	1.29261500				
C	-1.48128600	-2.65332200	-0.72773000				
H	-0.99866700	-3.17444200	-1.56359200				
H	-1.22073500	-3.19852600	0.18969800				
H	-2.55773200	-2.71604600	-0.88432000				
C	-2.32521100	-0.30250700	0.51629400				
C	-3.42280200	-0.01783200	-0.08458200				