

Supporting Information

Mechanistic Insights into Intermolecular Cyclization of Ring-fused Benzocyclobutenols with Alkynes Catalyzed by $\{\text{Ir}(\text{OMe})\text{COD}\}_2$

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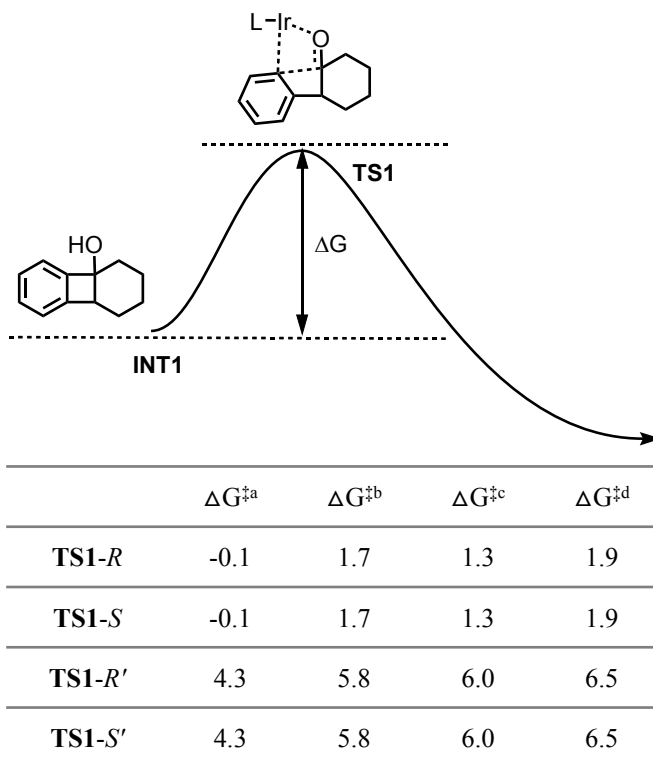
1. Computational Details.

All calculations were carried out with the Gaussian09 package²¹ at the density functional theory (DFT). Geometry optimizations were employed with the dispersion-corrected method B3LYP-D3 with a Becke-Johnson (BJ) damping function^{S1} by using 6-31G(d) basis set for all atoms except for Ir using Lanl2dz basis set without any symmetry constraint. Frequency calculations were employed at the same level of the theory for each transition state. IRC calculations were performed for key transition states to confirm whether it connected the corresponding intermediates. Considering the solvent effect (solvent=toluene), single-point calculations were performed with SMD model and M06L method, using Lanl2dz basis set for Ir and 6-311G(d, p) basis set for other atoms. Actually, we have also carried out full geometry optimizations with solvent effects for **INT1s** and **TS1s** at the SMD-B3LYP-D3/6-31G(d)+LANL2DZ and the SMD-B3LYP-D3/6-311G(d, p)+LANL2DZ level of theory, respectively, to investigate the method effects (see Fig. S2 and Table S1). Through calculations, we can easily find that similar free activation barriers were obtained by the selected four methods. What's more, the dispersion-corrected density functional method B3LYP-D3 is widely used in DFT calculations to describe the mechanism of the organocatalyzed reactions^{S1d-f}. For significantly reduce the computer time, the more economical single-configurational method (SMD-M06L/6-311G(d,p)+Lanl2dz) was employed in the present work.

21. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian 09*, revision D.01 Gaussian, Inc.: Wallingford, CT, 2013.

[S1] (a) S. H. Vosko, L. Wilk and M. Nusair, *Can. J. Phys.* 1980, **58**, 1200. (b) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem.* 1994, **98**, 11623. (c) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648. (d) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B.* 1988, **37**, 785. (d) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104. (e) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.* 2011, **32**, 1456. (f) S. Yu, S. Liu, Y. Lan, B. Wan and X. Li, *J. Am. Chem. Soc.* 2015, **137**, 1623 (g) H. Xiao, Y. Kobayashi, Y. Takemoto and K. Morokuma, *ACS Catal.* 2016, **6**, 2988. (f) J. M. Grandner, R. A. Cacho, Y. Tang and K. N. Houk, *ACS Catal.* 2016, **6**, 4506.

Table S1. The relative free energies (kcal/mol) of the **TS1s** with respect to the corresponding intermediate **INT1s** are calculated at the selected four levels.



^aB3LYP-D3/6-31G(d)+LANL2DZ for full optimization in gas phase

^bSMD-M06L/6-311G(d,p)+LANL2DZ//B3LYP-D3/6-31G(d)+LANL2DZ for single points with solvent effect

^cSMD-B3LYP-D3/6-31G(d)+LANL2DZ for full optimization with solvent effect

^dSMD-B3LYP-D3/6-311G(d,p)+LANL2DZ for full optimization with solvent effect

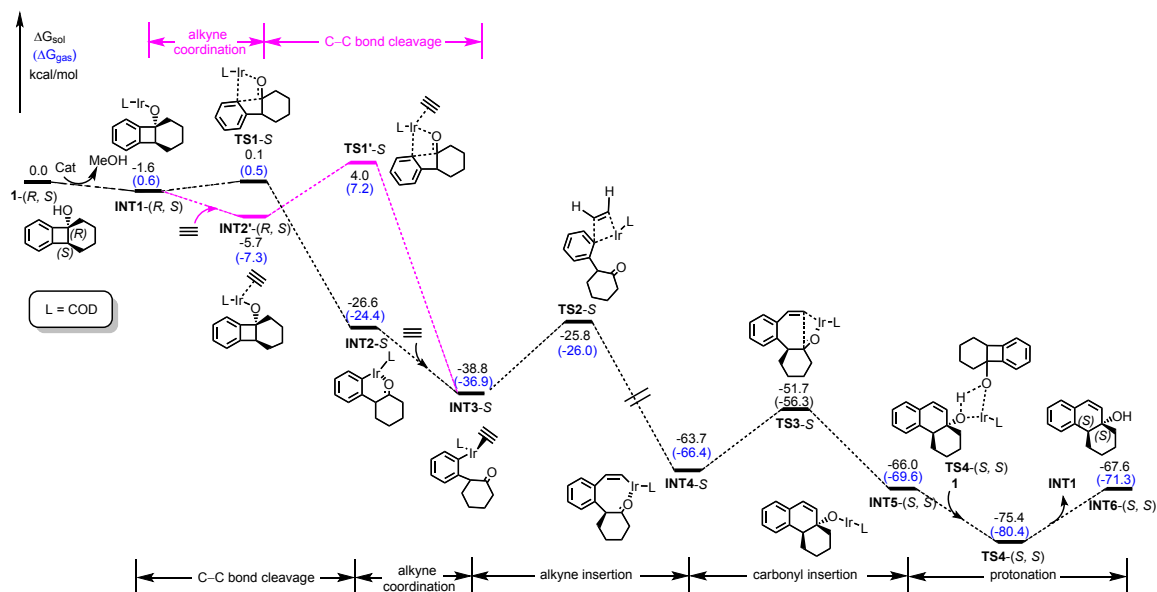


Fig. S1 Free-energy profile diagram for the iridium-catalyzed intermolecular cyclization of ring-fused (*R, S*)-benzocyclobutenols at the level of SMD-M06L/6-311G(d,p)+Lanl2dz (full optimization for gas phase at the level of B3LYP-D3/6-31G(d)+Lanl2dz).

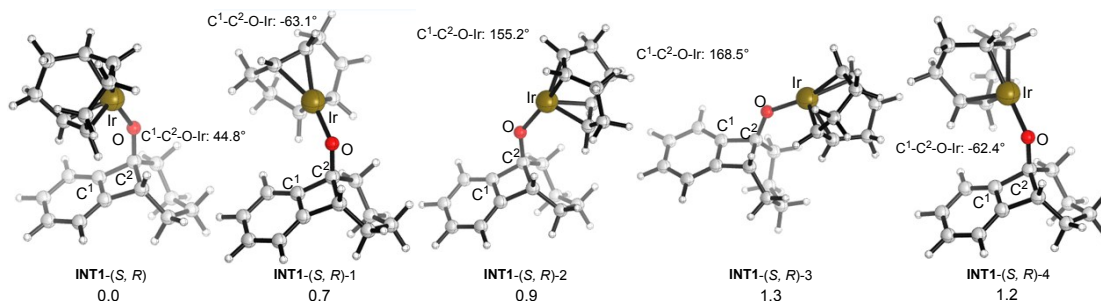


Fig. S2 The relative energies for different INT1-(*S, R*) conformers at the SMD-B3LYP-D3/6-31G(d)+LANL2DZ level of theory. The relative free energies are given in kcal/mol.

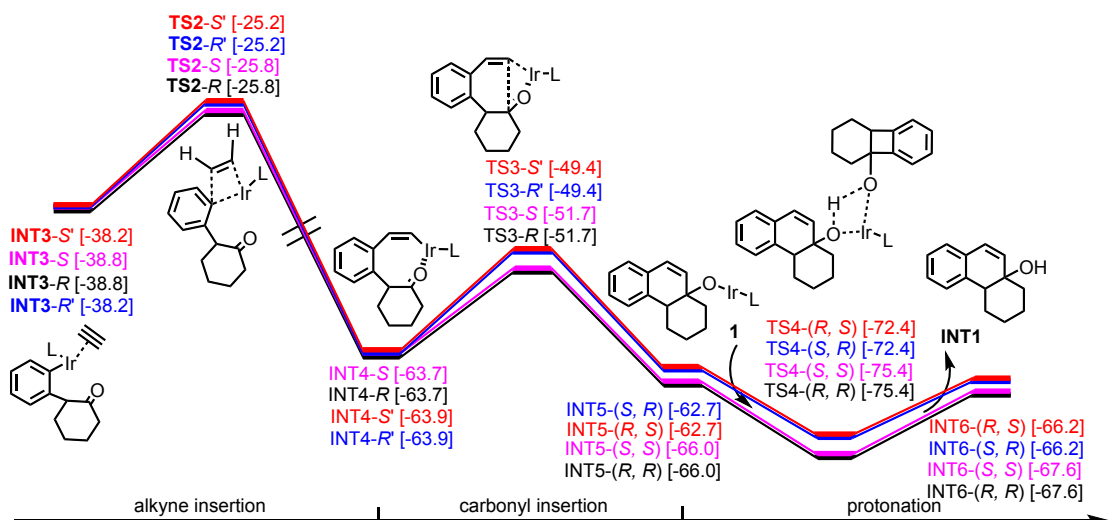


Fig. S3 Free-energy profile diagram for four possible pathways with the different orientation of the coordinated alkyne in INT3 at the level of SMD-M06L/6-311G(d,p)+Lanl2dz. The relative free energies are given in kcal/mol.

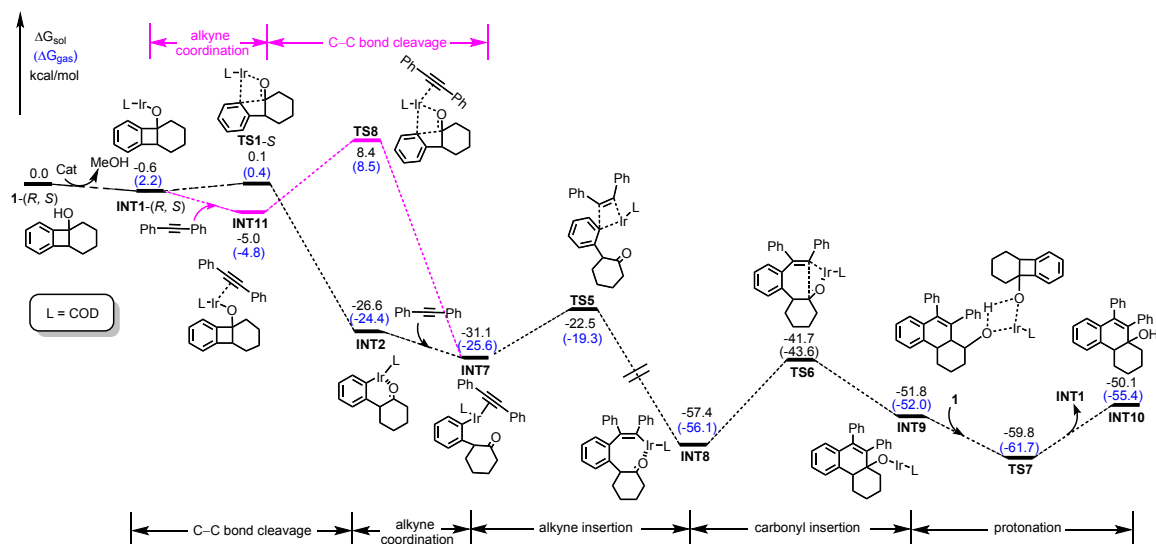


Fig. S4 Free-energy profile diagram for the iridium-catalyzed intermolecular cyclization of ring-fused benzocyclobutenols with diphenylacetylene at the level of SMD-M06L/6-311G(d,p)+Lanl2dz (full optimization for gas phase at the level of B3LYP-D3/6-31G(d)+Lanl2dz).

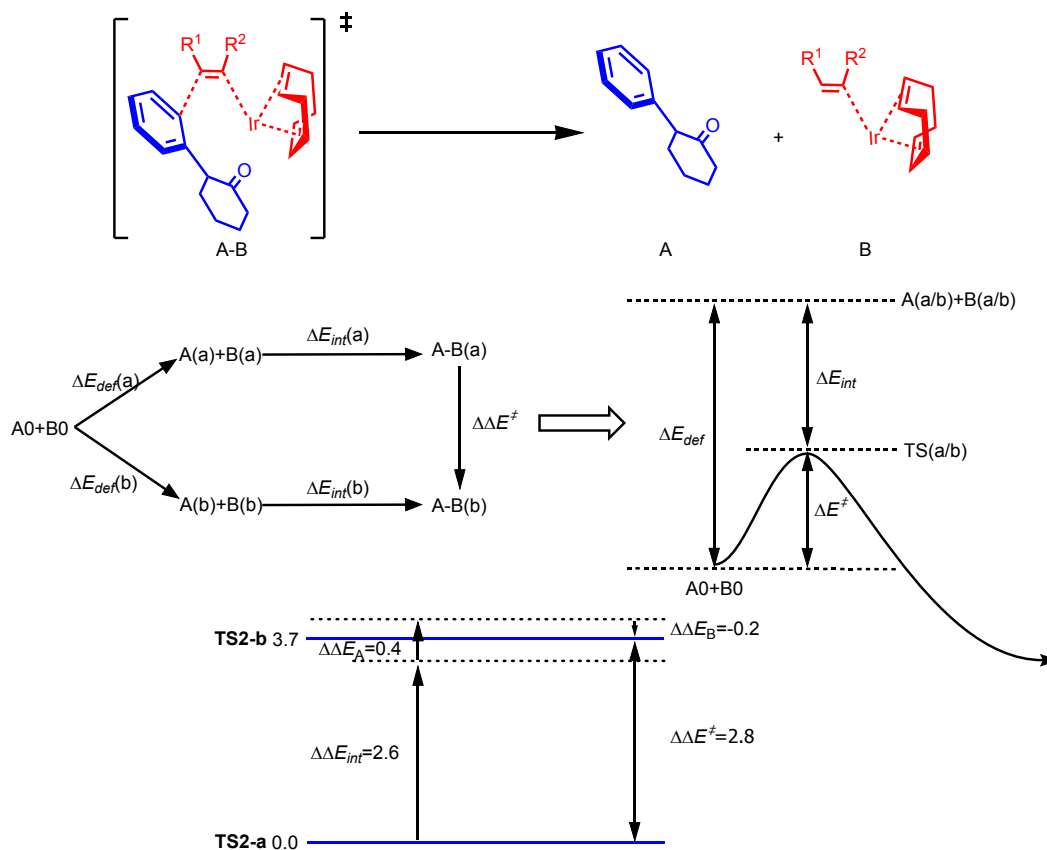


Fig. S5 Schematic diagram for energy decomposition analysis (EDA) for two lowest transition states **TS2-a** and **TS2-b**. The relative free energies are given in kcal/mol.

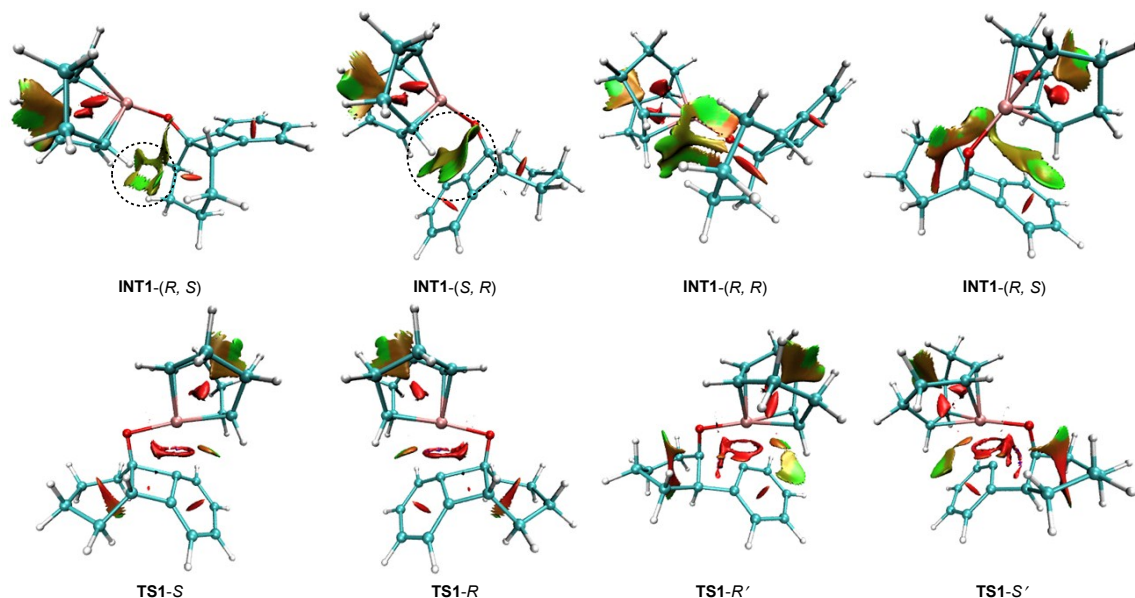
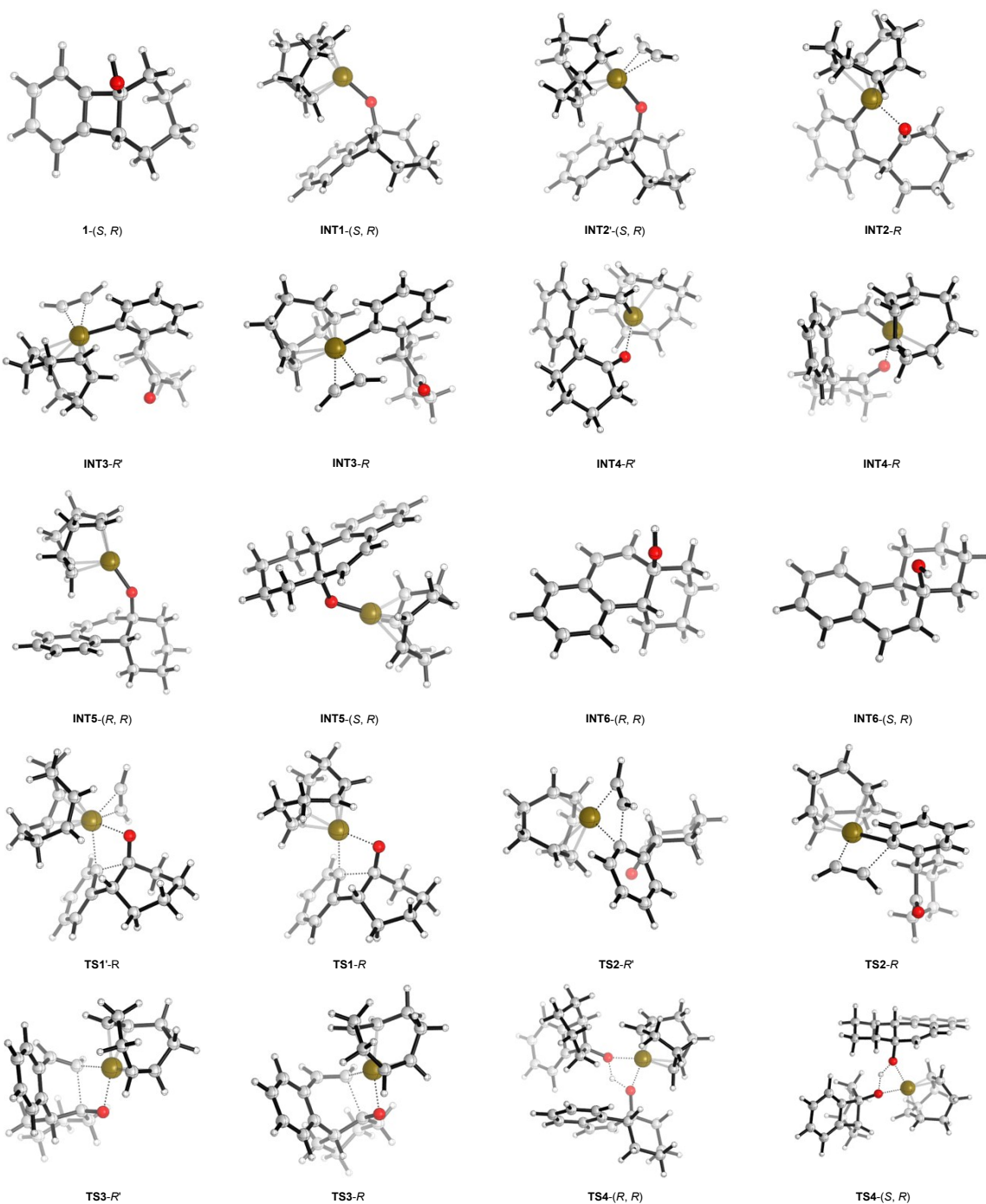
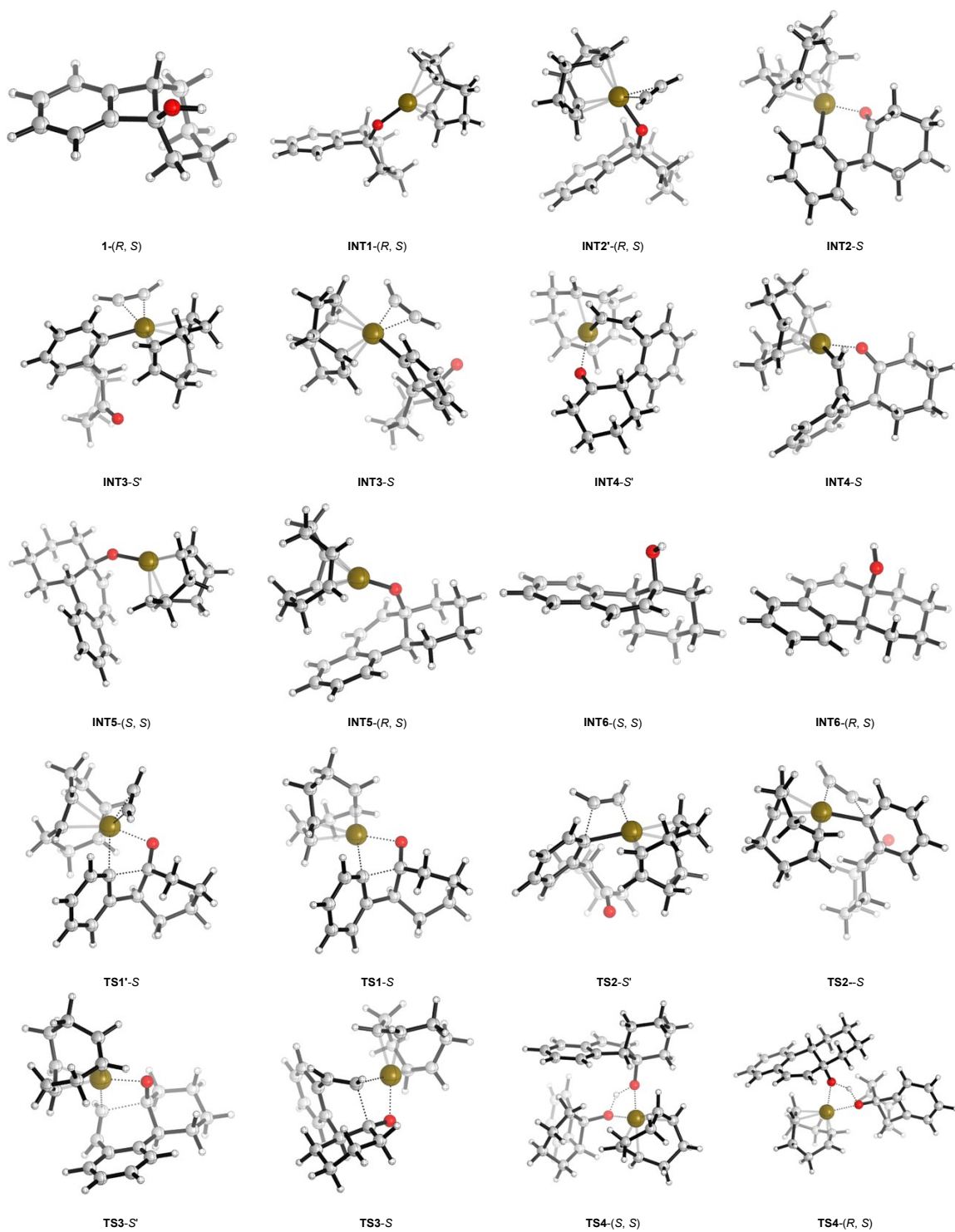


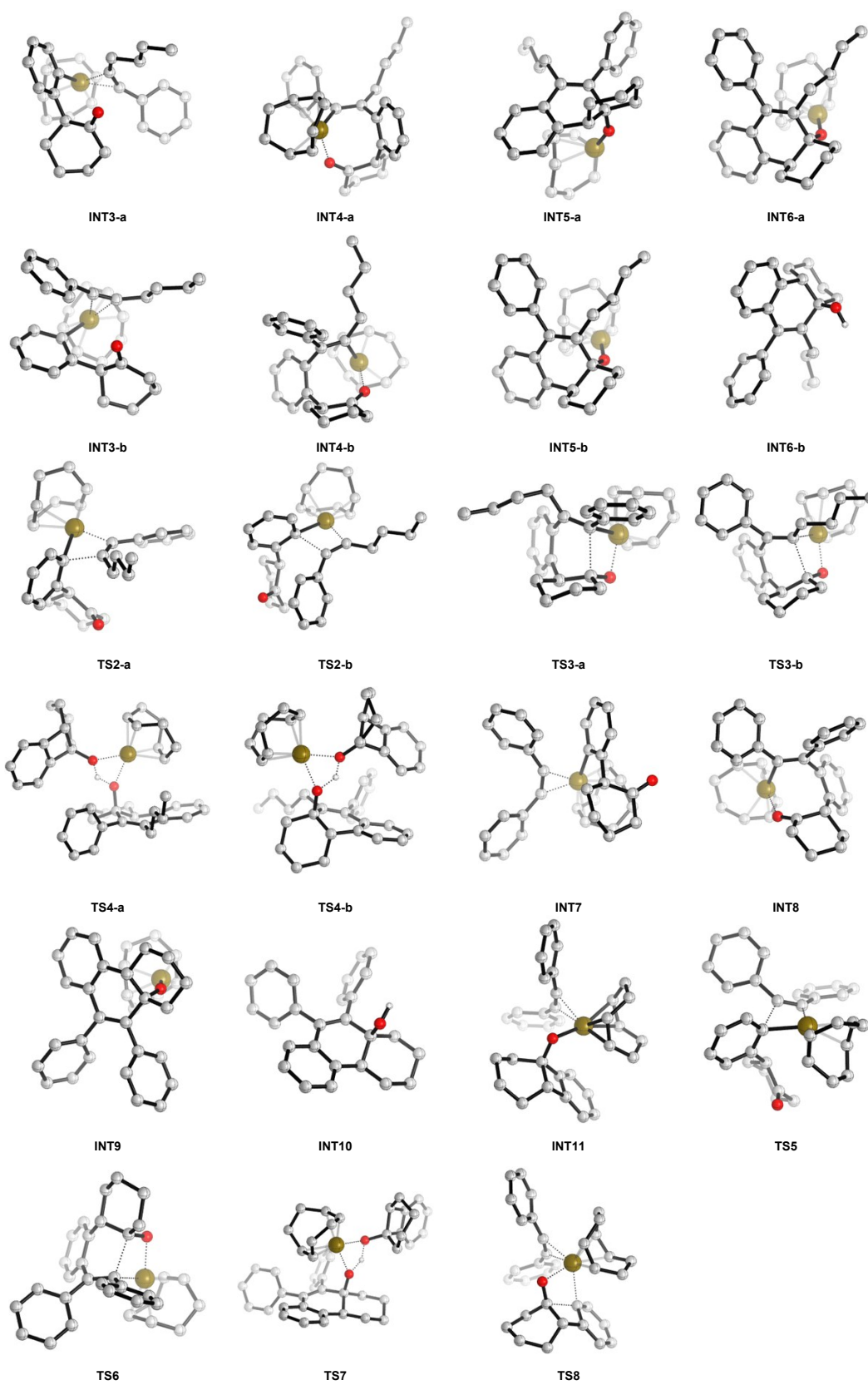
Fig. S6 Schematic diagram for the noncovalent interactions (NCI) for the lowest energy **INT1s** and **TS1s** calculated at the M06L/6-311G(d,p)+Lanl2dz level of theory.



Optimized structures of selected transition states and intermediates



Optimized structures of selected transition states and intermediates



Optimized structures of selected transition states and intermediates

Cartesian coordinates for all of the calculated structures

1-(S, R)	H -3.88468800 -0.84044900 -1.25351000
C 3.00408900 -0.43669900 -0.76897000	H -1.84015600 -2.25008200 -1.01785800
C 1.85814300 -1.23658300 -0.63103800	H -1.98469400 2.48093200 0.74247700
C 0.78317800 -0.64997100 0.02029100	H -3.95404600 1.45779500 -0.39759100
C 0.82336500 0.65227100 0.50905400	C 0.62304100 0.63576200 1.00793900
C 1.94316100 1.45872800 0.36866700	C 1.55949700 1.68033700 0.34956700
C 3.04407800 0.87738500 -0.28160900	H 2.00889200 2.31586800 1.12099000
H 3.88054600 -0.83936400 -1.26977100	H 0.94900800 2.34210800 -0.27709000
H 1.83742600 -2.24962300 -1.02562500	C 1.69740700 -1.23496200 -0.57537500
H 1.98756000 2.48171600 0.73334000	H 2.58153000 -1.61563900 -0.04820300
H 3.95258800 1.45906500 -0.41451900	H 1.31287300 -2.05455300 -1.19882000
C -0.61850600 0.63573300 1.00963600	C 2.66244500 1.07257500 -0.52910000
C -1.55794300 1.67995200 0.35492600	H 3.45747000 0.65079700 0.10183800
H -2.00470500 2.31521900 1.12809500	H 3.12535500 1.86766100 -1.12606900
H -0.95010400 2.34201400 -0.27398800	C 2.11621900 -0.03749400 -1.43331600
C -1.69868900 -1.23539200 -0.56919000	H 1.25998700 0.33606200 -2.01177000
H -2.58078400 -1.61597500 -0.03853300	H 2.87657600 -0.35323400 -2.15723200
H -1.31652200 -2.05510300 -1.19394100	O 0.76725400 -1.74259900 1.62054500
C -2.66401300 1.07182600 -0.51965200	H 0.55049200 -2.63894900 1.31711000
H -3.45658300 0.64988000 0.11426400	H 0.71968700 0.64395400 2.09771200
H -3.12930900 1.86679600 -1.11490600	C 0.65896500 -0.87635900 0.49057200
C -2.12088500 -0.03814700 -1.42577200	INT1-(S, R)
H -1.26681300 0.33544800 -2.00739300	C -2.41636400 0.58002700 2.15793000
H -2.88379700 -0.35416600 -2.14686400	C -1.27249000 0.36057800 1.37242500
O -0.75961100 -1.74252000 1.62306000	C -0.08626000 0.88249000 1.86759100
H -0.54677600 -2.63935900 1.31828600	C -0.01539500 1.57908000 3.07103100
H -0.71071200 0.64410900 2.09979200	C -1.13673000 1.79546200 3.86148500
C -0.65609800 -0.87645900 0.49261300	C -2.34908800 1.28224600 3.37105800
1-(R, S)	H -3.37747800 0.19786100 1.82394100
C -3.00635800 -0.43759100 -0.75615700	H -1.33337300 -0.18134300 0.43247400
C -1.85961600 -1.23712900 -0.62298300	H -1.10179400 2.33289100 4.80584000
C -0.78226000 -0.65030100 0.02420200	H -3.26094000 1.42949300 3.94400200
C -0.82088100 0.65186200 0.51329500	C 1.49264500 1.80313300 2.99756200
C -1.94147200 1.45800400 0.37750000	C 2.30957900 1.14520400 4.13670300
C -3.04481200 0.87640500 -0.26842100	H 2.86459100 1.91174800 4.69047100

H	1.61088200	0.69339000	4.85223700	C	0.08626000	0.88249000	1.86759100
C	2.25134000	-0.19446700	1.37540000	C	0.01539500	1.57908000	3.07103100
H	3.19170200	0.12261800	0.90738200	C	1.13673000	1.79546200	3.86148500
H	1.74900700	-0.86041800	0.66268100	C	2.34908800	1.28224600	3.37105800
C	3.26974900	0.05022600	3.65392000	H	3.37747800	0.19786100	1.82394100
C	2.57067400	-0.91327100	2.68858300	H	1.33337300	-0.18134300	0.43247400
O	1.64039300	1.91220400	0.46846400	H	1.10179400	2.33289100	4.80584000
H	1.79016900	2.84574000	2.84692900	H	3.26094000	1.42949300	3.94400200
C	1.40223200	1.06696200	1.55885700	C	-1.49264500	1.80313300	2.99756200
C	1.48771800	5.65666100	-0.73612400	C	-2.30957900	1.14520400	4.13670300
C	-0.05671200	6.12059900	1.22696300	H	-2.86459100	1.91174800	4.69047100
C	-0.15039400	4.59569600	1.20844200	H	-1.61088200	0.69339000	4.85223700
C	-0.95294600	3.85922700	0.25401900	C	-2.25134000	-0.19446700	1.37540000
C	-1.76297900	4.49606800	-0.85698800	H	-3.19170200	0.12261800	0.90738200
C	0.54311800	5.13070900	-1.66358900	H	-1.74900700	-0.86041800	0.66268100
H	2.52322900	5.73039400	-1.07775400	C	-3.26974900	0.05022600	3.65392000
H	-0.02421300	4.12210400	2.17923700	C	-2.57067400	-0.91327100	2.68858300
H	-1.34958700	2.90597000	0.59901900	O	-1.64039300	1.91220400	0.46846400
H	0.93337400	4.81361800	-2.63154400	H	-1.79016900	2.84574000	2.84692900
C	1.13910400	6.61889000	0.38809500	C	-1.40223200	1.06696200	1.55885700
C	-0.93300700	5.51702600	-1.66005700	C	-1.48771800	5.65666100	-0.73612400
H	-0.99589500	6.55061900	0.86323900	C	0.05671200	6.12059900	1.22696300
H	0.05241700	6.46089400	2.26197600	C	0.15039400	4.59569600	1.20844200
H	0.94649200	7.62948000	-0.00199800	C	0.95294600	3.85922700	0.25401900
H	2.01911400	6.69796500	1.03617900	C	1.76297900	4.49606800	-0.85698800
H	-1.05682800	6.52456800	-1.24968400	C	-0.54311800	5.13070900	-1.66358900
H	-1.30274100	5.56407900	-2.68979200	H	-2.52322900	5.73039400	-1.07775400
H	-2.09101400	3.68992700	-1.52300400	H	0.02421300	4.12210400	2.17923700
H	-2.67749600	4.95376500	-0.44869100	H	1.34958700	2.90597000	0.59901900
Ir	1.07581700	3.63835500	-0.19425800	H	-0.93337400	4.81361800	-2.63154400
H	1.64941400	-1.29723500	3.14945200	C	-1.13910400	6.61889000	0.38809500
H	3.20783100	-1.78186100	2.48327800	C	0.93300700	5.51702600	-1.66005700
H	4.13032600	0.50207100	3.14025500	H	0.99589500	6.55061900	0.86323900
H	3.66888200	-0.48849700	4.52218500	H	-0.05241700	6.46089400	2.26197600
INT1-(R, S)				H	-0.94649200	7.62948000	-0.00199800
C	2.41636400	0.58002700	2.15793000	H	-2.01911400	6.69796500	1.03617900
C	1.27249000	0.36057800	1.37242500	H	1.05682800	6.52456800	-1.24968400

H 1.30274100 5.56407900 -2.68979200
H 2.09101400 3.68992700 -1.52300400
H 2.67749600 4.95376500 -0.44869100
Ir -1.07581700 3.63835500 -0.19425800
H -1.64941400 -1.29723500 3.14945200
H -3.20783100 -1.78186100 2.48327800
H -4.13032600 0.50207100 3.14025500
H -3.66888200 -0.48849700 4.52218500

TS1-R

C -0.72583300 0.18897900 0.03296100
C -1.59126900 0.09972700 1.27620500
H -2.12971000 -0.85172400 1.28358600
H -2.32966400 0.90645000 1.26232800
C -0.68356100 0.24245700 2.52440400
H -1.31927000 0.49826100 3.38025800
H -0.22141200 -0.72341900 2.74959300
C 0.42081000 1.31546700 2.33504900
H 1.36145700 0.82436200 2.05560000
H 0.60918000 1.83605700 3.28052800
C 0.06394200 2.32270200 1.22929000
H 0.81237800 3.12128600 1.17195200
C -0.02348300 1.57916700 -0.11659400
C 1.23655100 -1.75740300 -2.93339700
C 0.67664100 -0.52408300 -5.09324100
C -0.57463000 -0.13163000 -4.30874300
C -1.67278200 -1.01473200 -4.09272700
C -1.73578400 -2.45832400 -4.55838400
C 0.20117000 -2.73316800 -2.93640600
H 1.91336600 -1.76446000 -2.07858600
H -0.80398400 0.93372600 -4.31323000
H -2.65095000 -0.54746400 -3.98581400
H 0.16201100 -3.40559800 -2.08012400
C 1.78830600 -1.06968100 -4.16772200
C -0.45616900 -3.25090200 -4.21089400
H 0.41791800 -1.26375400 -5.85810800
H 1.05519800 0.34954800 -5.63481800
H 2.45864200 -1.74362200 -4.72292300

H 2.40650600 -0.23344600 -3.82156500
H 0.25917300 -3.20705100 -5.03889200
H -0.70660300 -4.30971800 -4.08412100
H -2.58820500 -2.92568200 -4.05065200
H -1.94548700 -2.51983200 -5.63748000
Ir -0.55789800 -0.82506600 -2.29429200
C -3.07372100 0.96170500 -1.89800600
C -1.76405200 0.87169600 -1.39219500
C -1.05900100 2.06050200 -1.10012700
C -1.56483400 3.31625900 -1.41960800
C -2.81392000 3.37616300 -2.04740100
C -3.57222600 2.21442500 -2.25811800
H -3.68090000 0.07318300 -2.04398600
H -1.03216400 4.22752900 -1.15995500
H -3.22864600 4.34035300 -2.32967000
H -4.56224100 2.29645300 -2.69918600
H -0.89433300 2.80789000 1.45430700
O -0.05849700 -0.89982800 -0.30467800
H 0.97714200 1.43210900 -0.53722200

TS1-S

C 0.72583300 0.18897900 0.03296100
C 1.59126900 0.09972700 1.27620500
H 2.12971000 -0.85172400 1.28358600
H 2.32966400 0.90645000 1.26232800
C 0.68356100 0.24245700 2.52440400
H 1.31927000 0.49826100 3.38025800
H 0.22141200 -0.72341900 2.74959300
C -0.42081000 1.31546700 2.33504900
H -1.36145700 0.82436200 2.05560000
H -0.60918000 1.83605700 3.28052800
C -0.06394200 2.32270200 1.22929000
H -0.81237800 3.12128600 1.17195200
C 0.02348300 1.57916700 -0.11659400
C -1.23655100 -1.75740300 -2.93339700
C -0.67664100 -0.52408300 -5.09324100
C 0.57463000 -0.13163000 -4.30874300
C 1.67278200 -1.01473200 -4.09272700

C	1.73578400	-2.45832400	-4.55838400	H	-3.35055700	0.29784500	2.05209600
C	-0.20117000	-2.73316800	-2.93640600	H	-1.41088600	0.08473500	0.48760200
H	-1.91336600	-1.76446000	-2.07858600	H	-0.87228500	2.14322900	5.06543900
H	0.80398400	0.93372600	-4.31323000	H	-3.08349000	1.29382400	4.27974600
H	2.65095000	-0.54746400	-3.98581400	C	1.55954500	1.92603300	2.99810700
H	-0.16201100	-3.40559800	-2.08012400	C	2.52456800	1.40483500	4.08633800
C	-1.78830600	-1.06968100	-4.16772200	H	3.29105300	2.15860000	4.30028400
C	0.45616900	-3.25090200	-4.21089400	H	1.94974300	1.28494700	5.01391100
H	-0.41791800	-1.26375400	-5.85810800	C	2.13098600	-0.18737000	1.50471400
H	-1.05519800	0.34954800	-5.63481800	H	3.11051900	-0.00829400	1.04469100
H	-2.45864200	-1.74362200	-4.72292300	H	1.57357000	-0.84360600	0.82465800
H	-2.40650600	-0.23344600	-3.82156500	C	3.21096800	0.06713200	3.74568800
H	-0.25917300	-3.20705100	-5.03889200	C	2.33528700	-0.83921100	2.87453400
H	0.70660300	-4.30971800	-4.08412100	O	1.79227900	1.88512000	0.43240100
H	2.58820500	-2.92568200	-4.05065200	H	1.73120100	2.99190300	2.80909800
H	1.94548700	-2.51983200	-5.63748000	C	1.41619600	1.17598800	1.56468800
Ir	0.55789800	-0.82506600	-2.29429200	C	1.53064200	5.76189900	-0.49101500
C	3.07372100	0.96170500	-1.89800600	C	-0.28840300	5.77183300	1.29886500
C	1.76405200	0.87169600	-1.39219500	C	-0.32004800	4.26935600	1.02706800
C	1.05900100	2.06050200	-1.10012700	C	-0.91617700	3.67665900	-0.11140700
C	1.56483400	3.31625900	-1.41960800	C	-1.57711800	4.41430300	-1.25315000
C	2.81392000	3.37616300	-2.04740100	C	0.73346100	5.37347700	-1.59598600
C	3.57222600	2.21442500	-2.25811800	H	2.58216000	5.97141600	-0.69421800
H	3.68090000	0.07318300	-2.04398600	H	-0.29076700	3.64209900	1.91069700
H	1.03216400	4.22752900	-1.15995500	H	-1.22693500	2.64099100	-0.00050200
H	3.22864600	4.34035300	-2.32967000	H	1.25553500	5.26915900	-2.54400300
H	4.56224100	2.29645300	-2.69918600	C	0.99828700	6.43627300	0.76131700
H	0.89433300	2.80789000	1.45430700	C	-0.76243600	5.63520700	-1.71678400
O	0.05849700	-0.89982800	-0.30467800	H	-1.17723700	6.25139000	0.87728700
H	-0.97714200	1.43210900	-0.53722200	H	-0.34763200	5.93163500	2.38064000
INT2'-(S, R)				H	0.83700500	7.51000800	0.57914700
C	-2.37102300	0.66149600	2.35187900	H	1.77828800	6.36889900	1.52930600
C	-1.28679200	0.54348500	1.46561000	H	-1.04138700	6.52737200	-1.14848800
C	-0.07195100	1.03929600	1.91595700	H	-1.00601200	5.85817000	-2.76136400
C	0.07943100	1.61233700	3.17680100	H	-1.67664300	3.71025400	-2.08733200
C	-0.97652200	1.71186400	4.07277800	H	-2.60052300	4.70465300	-0.96754900
C	-2.21808100	1.22929800	3.62518400	Ir	1.26393300	3.64286400	-0.34810400

H 1.36928700 -1.02402200 3.36441900
H 2.81656000 -1.81686800 2.74832000
H 4.14217200 0.26305500 3.19637600
H 3.49977900 -0.44107300 4.67381200
C 2.97783500 3.15964400 -1.63956500
C 1.96162000 2.82818600 -2.27912200
H 4.02361800 3.24480400 -1.41717300
H 1.31613300 2.45125500 -3.04712100

INT2'-(R, S)

C 2.37102300 0.66149600 2.35187900
C 1.28679200 0.54348500 1.46561000
C 0.07195100 1.03929600 1.91595700
C -0.07943100 1.61233700 3.17680100
C 0.97652200 1.71186400 4.07277800
C 2.21808100 1.22929800 3.62518400
H 3.35055700 0.29784500 2.05209600
H 1.41088600 0.08473500 0.48760200
H 0.87228500 2.14322900 5.06543900
H 3.08349000 1.29382400 4.27974600
C -1.55954500 1.92603300 2.99810700
C -2.52456800 1.40483500 4.08633800
H -3.29105300 2.15860000 4.30028400
H -1.94974300 1.28494700 5.01391100
C -2.13098600 -0.18737000 1.50471400
H -3.11051900 -0.00829400 1.04469100
H -1.57357000 -0.84360600 0.82465800
C -3.21096800 0.06713200 3.74568800
C -2.33528700 -0.83921100 2.87453400
O -1.79227900 1.88512000 0.43240100
H -1.73120100 2.99190300 2.80909800
C -1.41619600 1.17598800 1.56468800
C -1.53064200 5.76189900 -0.49101500
C 0.28840300 5.77183300 1.29886500
C 0.32004800 4.26935600 1.02706800
C 0.91617700 3.67665900 -0.11140700
C 1.57711800 4.41430300 -1.25315000
C -0.73346100 5.37347700 -1.59598600

H -2.58216000 5.97141600 -0.69421800
H 0.29076700 3.64209900 1.91069700
H 1.22693500 2.64099100 -0.00050200
H -1.25553500 5.26915900 -2.54400300
C -0.99828700 6.43627300 0.76131700
C 0.76243600 5.63520700 -1.71678400
H 1.17723700 6.25139000 0.87728700
H 0.34763200 5.93163500 2.38064000
H -0.83700500 7.51000800 0.57914700
H -1.77828800 6.36889900 1.52930600
H 1.04138700 6.52737200 -1.14848800
H 1.00601200 5.85817000 -2.76136400
H 1.67664300 3.71025400 -2.08733200
H 2.60052300 4.70465300 -0.96754900
Ir -1.26393300 3.64286400 -0.34810400
H -1.36928700 -1.02402200 3.36441900
H -2.81656000 -1.81686800 2.74832000
H -4.14217200 0.26305500 3.19637600
H -3.49977900 -0.44107300 4.67381200
C -2.97783500 3.15964400 -1.63956500
C -1.96162000 2.82818600 -2.27912200
H -4.02361800 3.24480400 -1.41717300
H -1.31613300 2.45125500 -3.04712100

INT2-R

C 0.71085400 0.73638900 1.92082700
C 0.15698800 -0.45981400 2.65303200
H 0.57018800 -1.38164200 2.23852200
H -0.92754100 -0.47439100 2.50357300
C 0.47701800 -0.31321300 4.16980000
H -0.29767600 -0.83931100 4.73915600
H 1.42853800 -0.80642200 4.39365700
C 0.54190500 1.16949900 4.60205500
H 1.56697300 1.54391800 4.47780500
H 0.30318300 1.26185600 5.66730100
C -0.40018300 2.03376000 3.75571100
H -0.45219800 3.05408500 4.15021000
C 0.07721100 2.07504200 2.27915000

C	2.75678500	0.17251300	-1.27521600	H	-0.57018800	-1.38164200	2.23852200
C	1.39710800	0.45619200	-3.41687200	H	0.92754100	-0.47439100	2.50357300
C	0.19493500	0.53539200	-2.47287800	C	-0.47701800	-0.31321300	4.16980000
C	-0.35735900	-0.60043200	-1.80139100	H	0.29767600	-0.83931100	4.73915600
C	0.16076900	-2.02150700	-1.89217200	H	-1.42853800	-0.80642200	4.39365700
C	2.27552000	-1.07221100	-0.86773800	C	-0.54190500	1.16949900	4.60205500
H	3.43638700	0.68591900	-0.59812900	H	-1.56697300	1.54391800	4.47780500
H	-0.47719000	1.35291800	-2.70563300	H	-0.30318300	1.26185600	5.66730100
H	-1.41426500	-0.55344700	-1.54692300	C	0.40018300	2.03376000	3.75571100
H	2.57002800	-1.41042700	0.12161500	H	0.45219800	3.05408500	4.15021000
C	2.73998600	0.69724300	-2.69657400	C	-0.07721100	2.07504200	2.27915000
C	1.69843900	-2.12193300	-1.79671100	C	-2.75678500	0.17251300	-1.27521600
H	1.40107000	-0.51039600	-3.93061600	C	-1.39710800	0.45619200	-3.41687200
H	1.27692900	1.21045000	-4.20173600	C	-0.19493500	0.53539200	-2.47287800
H	3.57098300	0.26833100	-3.27747000	C	0.35735900	-0.60043200	-1.80139100
H	2.92259500	1.77613600	-2.64614600	C	-0.16076900	-2.02150700	-1.89217200
H	2.15110600	-2.03427800	-2.78831500	C	-2.27552000	-1.07221100	-0.86773800
H	1.96976300	-3.11663400	-1.42626000	H	-3.43638700	0.68591900	-0.59812900
H	-0.28482300	-2.58126000	-1.06173300	H	0.47719000	1.35291800	-2.70563300
H	-0.19934200	-2.49861300	-2.81703000	H	1.41426500	-0.55344700	-1.54692300
Ir	0.73320000	0.56644500	-0.40892700	H	-2.57002800	-1.41042700	0.12161500
C	-2.06023400	1.92885900	-0.82539300	C	-2.73998600	0.69724300	-2.69657400
C	-0.96577000	1.70113100	0.03332800	C	-1.69843900	-2.12193300	-1.79671100
C	-1.01971800	2.37657900	1.28071400	H	-1.40107000	-0.51039600	-3.93061600
C	-2.05003800	3.26789500	1.59665300	H	-1.27692900	1.21045000	-4.20173600
C	-3.09008600	3.49662900	0.69906600	H	-3.57098300	0.26833100	-3.27747000
C	-3.09906000	2.80511600	-0.51110000	H	-2.92259500	1.77613600	-2.64614600
H	-2.13251700	1.41126500	-1.77593600	H	-2.15110600	-2.03427800	-2.78831500
H	-2.04814200	3.77821900	2.55630600	H	-1.96976300	-3.11663400	-1.42626000
H	-3.88950700	4.18876600	0.94951900	H	0.28482300	-2.58126000	-1.06173300
H	-3.91518200	2.94720500	-1.21554000	H	0.19934200	-2.49861300	-2.81703000
H	-1.41881000	1.62847300	3.79941100	Ir	-0.73320000	0.56644500	-0.40892700
O	1.87345300	0.70257600	1.38753900	C	2.06023400	1.92885900	-0.82539300
H	0.88421300	2.81633200	2.19257100	C	0.96577000	1.70113100	0.03332800
INT2-S				C	1.01971800	2.37657900	1.28071400
C	-0.71085400	0.73638900	1.92082700	C	2.05003800	3.26789500	1.59665300
C	-0.15698800	-0.45981400	2.65303200	C	3.09008600	3.49662900	0.69906600

C 3.09906000 2.80511600 -0.51110000
H 2.13251700 1.41126500 -1.77593600
H 2.04814200 3.77821900 2.55630600
H 3.88950700 4.18876600 0.94951900
H 3.91518200 2.94720500 -1.21554000
H 1.41881000 1.62847300 3.79941100
O -1.87345300 0.70257600 1.38753900
H -0.88421300 2.81633200 2.19257100

TS1'-R

C -0.72009800 0.21418400 0.09067400
C -1.76833400 0.02576800 1.17296000
H -2.36333000 -0.86451100 0.95557400
H -2.43732300 0.89066300 1.19055500
C -1.04219800 -0.10198900 2.53644600
H -1.77200400 0.08677700 3.33265700
H -0.68794300 -1.12914900 2.66545600
C 0.15210400 0.88024200 2.65776200
H 1.08290000 0.35397700 2.41043100
H 0.25463600 1.22804000 3.69177600
C 0.01010600 2.07352500 1.69937100
H 0.81032500 2.80428000 1.86444200
C 0.05352400 1.56451200 0.24302700
C 1.50926300 0.19319100 -2.54251900
C 0.57920700 1.25612200 -4.64938300
C -0.65462200 0.44243200 -4.26691500
C -0.78656100 -0.94482000 -4.48936600
C 0.29463200 -1.84038700 -5.06325000
C 1.54082100 -1.18089000 -2.94680100
H 1.90823300 0.38545900 -1.54942400
H -1.57711000 1.00960000 -4.20784900
H -1.79671200 -1.32689900 -4.61869500
H 1.92588600 -1.88453700 -2.21135000
C 1.57204900 1.38522300 -3.48008100
C 1.67092900 -1.61768300 -4.40438700
H 1.06003600 0.79642100 -5.51940900
H 0.25733100 2.25208700 -4.97179100
H 2.59469400 1.55082900 -3.85316100

H 1.30609200 2.27111000 -2.89238000
H 2.24920500 -0.87347600 -4.96258600
H 2.24921300 -2.54647300 -4.45560800
H -0.01913600 -2.87633000 -4.88955400
H 0.35391200 -1.71422000 -6.15525400
Ir -0.46453500 -0.63245100 -2.36917700
C -2.72779600 1.60016100 -2.05012200
C -1.56428700 1.26196800 -1.34477100
C -0.79990000 2.29007400 -0.75836300
C -1.10221600 3.63637600 -0.94405100
C -2.20524700 3.95824200 -1.74278500
C -3.02387700 2.94993900 -2.26838500
H -3.37748400 0.83348300 -2.46248100
H -0.52173500 4.41889400 -0.46125900
H -2.45652900 5.00026600 -1.92267000
H -3.90106800 3.22195100 -2.85042600
H -0.93526700 2.59803500 1.88697800
O -0.09084700 -0.86682300 -0.29884800
H 1.09438900 1.42677400 -0.06211900
C -1.40947200 -2.58709900 -2.21512200
C -2.31534300 -1.74327400 -1.99621500
H -0.97364800 -3.56343000 -2.31457700
H -3.32128600 -1.47295600 -1.72959700

TS1'-S

C 0.72009500 0.21418300 0.09067400
C 1.76833300 0.02576900 1.17295900
H 2.36333400 -0.86450600 0.95557000
H 2.43731700 0.89066800 1.19055700
C 1.04219600 -0.10199700 2.53644300
H 1.77200200 0.08675500 3.33265600
H 0.68793400 -1.12915700 2.66543900
C -0.15210100 0.88024000 2.65776900
H -1.08290300 0.35397900 2.41045100
H -0.25462000 1.22804300 3.69178300
C -0.01011000 2.07352000 1.69937400
H -0.81033100 2.80427400 1.86444700
C -0.05353300 1.56450700 0.24303000

C -1.50925100 0.19319800 -2.54252300
 C -0.57917800 1.25612400 -4.64938500
 C 0.65464100 0.44241800 -4.26691800
 C 0.78656500 -0.94483600 -4.48936500
 C -0.29463500 -1.84039600 -5.06324600
 C -1.54081900 -1.18088300 -2.94680200
 H -1.90821900 0.38547300 -1.54942900
 H 1.57713700 1.00957500 -4.20785600
 H 1.79671200 -1.32692500 -4.61869300
 H -1.92588900 -1.88452700 -2.21135100
 C -1.57202700 1.38522700 -3.48008900
 C -1.67093000 -1.61767300 -4.40438800
 H -1.06000500 0.79643600 -5.51941900
 H -0.25728900 2.25208800 -4.97178200
 H -2.59466900 1.55083400 -3.85317600
 H -1.30607200 2.27111500 -2.89238800
 H -2.24919400 -0.87345700 -4.96258800
 H -2.24922900 -2.54645500 -4.45561200
 H 0.01912200 -2.87634000 -4.88954300
 H -0.35391100 -1.71423600 -6.15525100
 Ir 0.46454200 -0.63245600 -2.36917600
 C 2.72778400 1.60017300 -2.05012000
 C 1.56427700 1.26197200 -1.34477000
 C 0.79988200 2.29007300 -0.75836300
 C 1.10218800 3.63637700 -0.94405300
 C 2.20521700 3.95825000 -1.74278900
 C 3.02385500 2.94995200 -2.26838600
 H 3.37747800 0.83349800 -2.46247600
 H 0.52170200 4.41889100 -0.46126300
 H 2.45649100 5.00027600 -1.92267600
 H 3.90104500 3.22197000 -2.85042700
 H 0.93526200 2.59803400 1.88697500
 O 0.09084700 -0.86682700 -0.29884900
 H -1.09439900 1.42676300 -0.06211000
 C 1.40947900 -2.58710300 -2.21511600
 C 2.31534800 -1.74327400 -1.99621200
 H 0.97365900 -3.56343600 -2.31456600

H 3.32129200 -1.47295700 -1.72959600

INT3-R'

C 4.80228000 0.25113100 0.97438600
 C 3.44625100 0.02142400 1.24700400
 C 2.93881800 2.18846100 0.32179600
 C 4.29102300 2.41215700 0.05522700
 C 5.23289200 1.43867800 0.38733300
 H 5.53533100 -0.51286300 1.22703500
 H 4.60550300 3.34318500 -0.41014100
 H 6.28896600 1.59906500 0.18869800
 C 3.02502800 -1.31413000 1.84044600
 H 1.96689200 -1.21294400 2.11900600
 C 3.13146800 -2.47345700 0.83204500
 H 2.41883200 -2.29660100 0.01840300
 H 4.12974500 -2.49235400 0.37519000
 C 2.83520800 -3.80263800 1.53370000
 H 2.78354200 -4.62342000 0.80977600
 H 1.83784400 -3.72873000 1.98866100
 C 3.88284000 -4.12412600 2.62947200
 H 3.39186100 -4.61258200 3.47799400
 H 4.62250200 -4.83682500 2.24822700
 C 4.63421000 -2.86554000 3.13095800
 H 5.06653700 -3.01410500 4.12360300
 H 5.46001900 -2.64683500 2.43824200
 C 3.75161200 -1.63218300 3.15076200
 C -1.17871100 -0.20541000 2.62933700
 C 0.37541500 0.43995300 4.55070900
 C 1.17462400 1.13679000 3.46023500
 C 0.80804100 2.34919300 2.82576000
 C -0.45256600 3.14416300 3.08726900
 C -1.65397500 1.06284100 2.27572800
 H -1.53673600 -1.05035700 2.04520600
 H 2.23240500 0.89892300 3.47922000
 H 1.62681800 2.94959800 2.43641500
 H -2.31314700 1.12401800 1.41489700
 C -0.60687600 -0.59704200 3.97512000
 C -1.70522000 2.25684900 3.21248100

H -0.15256400 1.17687400 5.16459000
 H 1.08064700 -0.06975200 5.21375500
 H -1.42600800 -0.79952100 4.68271900
 H -0.07664200 -1.54654700 3.83879600
 H -1.83116500 1.91317900 4.24315300
 H -2.59558600 2.85096400 2.97966200
 H -0.58882000 3.83467100 2.24667300
 H -0.33073000 3.76784200 3.98642000
 Ir 0.45926700 0.74392200 1.41021800
 O 3.61549100 -0.94434000 4.14843000
 C 2.48924800 1.00662000 0.93052500
 H 2.21371700 2.95236300 0.05066800
 C -0.55325800 -0.10382700 -0.21114300
 C 0.64787100 0.01525400 -0.57524500
 H -1.57300400 -0.40953900 -0.36928200
 H 1.47947400 -0.04797800 -1.24978000

INT3-R

C 4.76358800 0.93394100 0.82990500
 C 3.51532800 0.36546200 1.11673000
 C 2.50922700 2.53861600 0.84752000
 C 3.75511500 3.09884800 0.55973400
 C 4.89248900 2.29172900 0.54852200
 H 5.65167500 0.30566600 0.84011900
 H 3.83551600 4.16276500 0.34984600
 H 5.86954200 2.71534700 0.33294700
 C 3.43431300 -1.11006700 1.44548500
 H 2.36382400 -1.35883200 1.53743800
 C 4.03634500 -2.04404300 0.37546800
 H 3.67075000 -1.74542400 -0.61223000
 H 5.12379600 -1.90266000 0.34744000
 C 3.70547300 -3.52771400 0.64666000
 H 4.48287200 -4.15666400 0.19702200
 H 2.76618600 -3.79439800 0.14719600
 C 3.58028900 -3.83916000 2.15593800
 H 2.53509500 -3.72752700 2.47140500
 H 3.85017900 -4.88178800 2.35565800
 C 4.44327100 -2.89586300 3.00461100

H 4.40485200 -3.13288600 4.07201400
 H 5.49766300 -2.97502600 2.69815700
 C 4.01812100 -1.44419600 2.81998200
 C -1.82786100 0.48384300 1.47538800
 C -1.39016200 1.18437000 -0.93739300
 C 0.06439500 0.88702200 -0.59370600
 C 0.61126900 -0.41908600 -0.47361100
 C -0.14845000 -1.72173700 -0.59904100
 C -1.47298800 -0.86616000 1.39232400
 H -2.13573900 0.85949800 2.44796700
 H 0.76541100 1.66608800 -0.87764000
 H 1.66908200 -0.51103600 -0.70803500
 H -1.48592200 -1.44022400 2.31431900
 C -2.25541800 1.36517000 0.32272200
 C -1.51142100 -1.69368200 0.11877900
 H -1.79484200 0.39365200 -1.57737700
 H -1.43488600 2.10230200 -1.53316300
 H -3.31988400 1.19814200 0.09517000
 H -2.17021700 2.40272300 0.66362800
 H -2.28820600 -1.30959800 -0.54855300
 H -1.80888300 -2.71723700 0.37134200
 H 0.47286200 -2.50628400 -0.14954500
 H -0.27589700 -1.99573000 -1.65789500
 Ir 0.43731300 0.41615300 1.50805600
 O 4.11139700 -0.63004200 3.72123300
 C 2.36069200 1.17032600 1.12429000
 H 1.63239800 3.18104500 0.86320400
 C 0.14872100 0.28471400 3.58255000
 C 1.32838800 0.69513300 3.43988300
 H -0.69648400 -0.01036100 4.17893400
 H 2.33513000 0.95265100 3.70989800

INT3-S'

C -4.80228700 0.25111800 0.97430000
 C -3.44626300 0.02144200 1.24696600
 C -2.93881800 2.18847400 0.32168900
 C -4.29101600 2.41211100 0.05507000
 C -5.23288100 1.43863500 0.38719800

H -5.53532700 -0.51288400 1.22694100
 H -4.60550700 3.34310800 -0.41034800
 H -6.28894500 1.59898600 0.18849100
 C -3.02504200 -1.31409900 1.84044000
 H -1.96691700 -1.21289600 2.11902100
 C -3.13143800 -2.47347600 0.83213000
 H -2.41879100 -2.29665200 0.01849600
 H -4.12969900 -2.49242700 0.37524100
 C -2.83516600 -3.80259600 1.53386400
 H -2.78340500 -4.62342000 0.80999600
 H -1.83784000 -3.72860800 1.98889200
 C -3.88285200 -4.12404100 2.62958200
 H -3.39192200 -4.61248500 3.47813600
 H -4.62250300 -4.83673400 2.24831500
 C -4.63420900 -2.86544700 3.13102000
 H -5.06653200 -3.01395800 4.12367300
 H -5.46002700 -2.64674500 2.43831300
 C -3.75169600 -1.63202900 3.15073200
 C 1.17871600 -0.20537700 2.62923000
 C -0.37540700 0.43976400 4.55065400
 C -1.17460900 1.13666400 3.46022500
 C -0.80804000 2.34911600 2.82586200
 C 0.45253100 3.14410300 3.08741900
 C 1.65398300 1.06289200 2.27571700
 H 1.53677000 -1.05026000 2.04502300
 H -2.23238400 0.89877400 3.47917800
 H -1.62683600 2.94951600 2.43657000
 H 2.31312400 1.12414300 1.41487200
 C 0.60692500 -0.59713800 3.97499100
 C 1.70520800 2.25682500 3.21254100
 H 0.15253600 1.17666300 5.16457600
 H -1.08063600 -0.06998900 5.21366100
 H 1.42608000 -0.79963800 4.68255300
 H 0.07673200 -1.54664500 3.83860200
 H 1.83117000 1.91307800 4.24318000
 H 2.59555300 2.85098400 2.97976900
 H 0.58876000 3.83465300 2.24685700

H 0.33068800 3.76771900 3.98660800
 Ir -0.45928200 0.74397000 1.41020100
 O -3.61541400 -0.94427600 4.14844300
 C -2.48925600 1.00666300 0.93052500
 H -2.21373900 2.95237400 0.05052500
 C 0.55322300 -0.10363900 -0.21120000
 C -0.64791400 0.01546000 -0.57527500
 H 1.57292400 -0.40949700 -0.36932400
 H -1.47953600 -0.04780900 -1.24978100

INT3-S

C -4.76338800 0.93363300 0.82946700
 C -3.51509600 0.36537100 1.11650900
 C -2.50942300 2.53879200 0.84833500
 C -3.75534600 3.09887800 0.56038000
 C -4.89253300 2.29152400 0.54853800
 H -5.65133900 0.30517200 0.83909100
 H -3.83592900 4.16287200 0.35098200
 H -5.86956300 2.71498800 0.33257200
 C -3.43398600 -1.11023200 1.44511200
 H -2.36350100 -1.35876600 1.53684100
 C -4.03602200 -2.04428500 0.37531300
 H -3.67003100 -1.74596600 -0.61236100
 H -5.12341800 -1.90277800 0.34691700
 C -3.70551500 -3.52805600 0.64687100
 H -4.48300500 -4.15691800 0.19726000
 H -2.76625700 -3.79514100 0.14759500
 C -3.58073400 -3.83940800 2.15623300
 H -2.53551800 -3.72848100 2.47186800
 H -3.85131000 -4.88185900 2.35595500
 C -4.44344900 -2.89547300 3.00458100
 H -4.40559500 -3.13237300 4.07202100
 H -5.49773600 -2.97415900 2.69763600
 C -4.01726000 -1.44411300 2.81994900
 C 1.82780100 0.48392200 1.47515500
 C 1.39021900 1.18417200 -0.93763600
 C -0.06445800 0.88751100 -0.59392700
 C -0.61142500 -0.41850900 -0.47402700

C	0.14835400	-1.72120600	-0.59940100	H	2.05489300	-3.47041200	0.10739200
C	1.47324900	-0.86628300	1.39247000	C	0.81278100	-4.08548000	-1.55032600
H	2.13576000	0.85976400	2.44766900	H	1.62017500	-4.64806000	-2.03446100
H	-0.76540000	1.66688000	-0.87713200	H	0.23412900	-3.60695400	-2.35337900
H	-1.66926500	-0.51059400	-0.70825000	C	-0.09614500	-5.03984900	-0.76644500
H	1.48635400	-1.43965800	2.31486700	H	-0.54503700	-5.78495900	-1.43354500
C	2.25517400	1.36544400	0.32257400	H	0.50461600	-5.59407600	-0.03241900
C	1.51114400	-1.69395400	0.11909400	C	-1.20760200	-4.27114900	-0.02178500
H	1.79450500	0.39265000	-1.57684800	H	-1.87400400	-3.79853700	-0.75757500
H	1.43560400	2.10155100	-1.53424200	H	-1.80596100	-4.93182400	0.61171500
H	3.31979500	1.19909000	0.09526800	C	-0.60734200	-3.17371500	0.84403600
H	2.16923200	2.40298400	0.66340800	C	-2.47800600	1.01919200	2.25599200
H	2.28863400	-1.31070200	-0.54793700	C	-4.77025500	1.26838500	1.17519600
H	1.80751200	-2.71780600	0.37176900	C	-4.08897100	0.61857600	-0.01960400
H	-0.47336900	-2.50560400	-0.15026100	C	-3.80036900	-0.76414400	-0.11285900
H	0.27624600	-1.99525400	-1.65821400	C	-4.07426200	-1.77984100	0.98009800
Ir	-0.43718300	0.41601100	1.50794700	C	-2.41117300	-0.38793000	2.31930000
O	-4.10920900	-0.62998800	3.72135600	H	-1.61496700	1.56338600	2.63754900
C	-2.36061300	1.17052800	1.12467700	H	-4.18582300	1.16160400	-0.95763500
H	-1.63270300	3.18140600	0.86448000	H	-3.74928600	-1.19045600	-1.11445900
C	-0.14871200	0.28494500	3.58255100	H	-1.49493500	-0.81998300	2.70885200
C	-1.32826000	0.69498200	3.43956600	C	-3.74960100	1.83763400	2.18513400
H	0.69656900	-0.01020000	4.17876600	C	-3.62222400	-1.31022900	2.37990200
H	-2.33490900	0.95248000	3.70988800	H	-5.42917500	0.54483800	1.66468400
TS2-R'				H	-5.41817300	2.07814800	0.82195900
C	1.82268000	-1.22458100	1.79436300	H	-4.21384900	1.93166000	3.17928700
C	0.76892800	-1.03066000	0.88795800	H	-3.47306700	2.85221500	1.87477700
C	0.72671200	1.30975300	1.55360300	H	-4.44625100	-0.81507900	2.90417000
C	1.78043000	1.10083700	2.43186500	H	-3.35917500	-2.18905200	2.97594100
C	2.32501300	-0.18182100	2.56481900	H	-3.52376300	-2.69103900	0.72481100
H	2.24705300	-2.21770000	1.90575800	H	-5.14089900	-2.05480200	0.98644700
H	2.17354400	1.92782400	3.01713300	Ir	-1.94326800	0.27185800	0.26199900
H	3.14028300	-0.36294600	3.25939600	O	-0.79074500	-3.11944300	2.04531400
C	0.27517100	-2.19611900	0.06506700	C	0.17786800	0.25208800	0.79790600
H	-0.36770300	-1.80718800	-0.73135300	H	0.30454300	2.30482200	1.44431200
C	1.40033200	-3.00187100	-0.63875500	C	-1.28462800	0.36936300	-1.65771300
H	2.02190200	-2.30518100	-1.21224000	C	-0.22729800	0.81510700	-1.04421500

H 0.67415900 1.38752600 -1.20242000
 H -1.62179100 0.33738800 -2.68640000
TS2-R
 C 1.87249600 -0.63382100 1.25629300
 C 0.56680900 -1.02069200 0.95760300
 C -0.22828600 0.94813500 2.15123400
 C 1.08612300 1.33585000 2.41477800
 C 2.13920400 0.54076200 1.96720500
 H 2.70382400 -1.25531900 0.93705600
 H 1.28285700 2.24073800 2.98329200
 H 3.16671300 0.81600800 2.18758900
 C 0.27866900 -2.30766200 0.21633100
 H -0.71575900 -2.20351000 -0.24229300
 C 1.26542900 -2.64674800 -0.92749900
 H 1.33256000 -1.78774500 -1.60403400
 H 2.27222700 -2.80564600 -0.52015600
 C 0.82941200 -3.90566200 -1.68350500
 H 1.52943200 -4.11322400 -2.50157000
 H -0.15384400 -3.73091300 -2.14379700
 C 0.75062000 -5.10963300 -0.73839500
 H 0.40889700 -6.00387600 -1.27219100
 H 1.75591100 -5.33464400 -0.35696400
 C -0.18541300 -4.82608600 0.45136600
 H -1.21813900 -4.73675900 0.08127100
 H -0.16420400 -5.62851700 1.19391700
 C 0.14987600 -3.51691800 1.14920900
 C -1.35928400 0.06658000 -1.59739400
 C -3.69799600 -0.39039300 -2.49924200
 C -4.09817200 -0.28736300 -1.03207700
 C -4.22107100 0.93588900 -0.32671200
 C -3.91709700 2.30751400 -0.89664200
 C -1.55757200 1.37961100 -1.11307300
 H -0.35724100 -0.33932000 -1.47577400
 H -4.68307200 -1.12549400 -0.65807900
 H -4.91721000 0.95200400 0.51090000
 H -0.70613300 1.84658500 -0.62314800
 C -2.17819900 -0.60094100 -2.68164400

C -2.58888100 2.34917600 -1.68047800
 H -4.02484400 0.50692500 -3.03409500
 H -4.23589400 -1.22704800 -2.95852700
 H -1.86697200 -0.26110900 -3.68209300
 H -1.96230200 -1.67602200 -2.64179300
 H -2.76153900 2.13051500 -2.73922600
 H -2.18310900 3.36629800 -1.64733700
 H -3.85210700 3.00090900 -0.05043700
 H -4.75052600 2.66030500 -1.52440000
 Ir -2.40922700 -0.04104600 0.32644400
 O 0.27186900 -3.44359300 2.35881900
 C -0.50531600 -0.19958100 1.38833700
 H -1.05706000 1.53748500 2.53079700
 C -3.20363400 -0.80826300 2.02757800
 C -1.98299000 -1.19772000 2.22260000
 H -1.35037800 -1.87996700 2.76984400
 H -4.16383700 -1.01920700 2.47975000
TS2-S
 C -1.82221800 -1.22390200 1.79491300
 C -0.76865300 -1.03027900 0.88822200
 C -0.72602700 1.31027200 1.55336100
 C -1.77958100 1.10165000 2.43189900
 C -2.32425500 -0.18092500 2.56526800
 H -2.24669600 -2.21694600 1.90658000
 H -2.17248600 1.92880800 3.01706800
 H -3.13938400 -0.36181500 3.26007300
 C -0.27535000 -2.19590300 0.06531000
 H 0.36743700 -1.80728000 -0.73131100
 C -1.40088600 -3.00149000 -0.63813000
 H -2.02250300 -2.30473900 -1.21148900
 H -2.05529200 -3.46984500 0.10826700
 C -0.81376500 -4.08528100 -1.54976500
 H -1.62138600 -4.64771600 -2.03369100
 H -0.23519400 -3.60691900 -2.35297100
 C 0.09516600 -5.03981100 -0.76605600
 H 0.54379500 -5.78497400 -1.43327400
 H -0.50552500 -5.59395400 -0.03191500

C 1.20691800 -4.27127200 -0.02164600
 H 1.87325000 -3.79885500 -0.75761000
 H 1.80525900 -4.93201600 0.61180200
 C 0.60694100 -3.17372800 0.84422100
 C 2.47836600 1.01909800 2.25555900
 C 4.77070800 1.26774200 1.17486400
 C 4.08934200 0.61803700 -0.01995000
 C 3.80048200 -0.76465300 -0.11305100
 C 4.07432000 -1.78022600 0.98004100
 C 2.41121500 -0.38799400 2.31896200
 H 1.61540700 1.56353200 2.63694400
 H 4.18639500 1.16098000 -0.95801100
 H 3.74942100 -1.19104700 -1.11461800
 H 1.49485100 -0.81988300 2.70838900
 C 3.75009000 1.83733600 2.18462400
 C 3.62208600 -1.31051200 2.37976400
 H 5.42934400 0.54402200 1.66447800
 H 5.41891400 2.07728900 0.82166100
 H 4.21428400 1.93157500 3.17878200
 H 3.47368000 2.85186500 1.87398200
 H 4.44611300 -0.81551100 2.90417100
 H 3.35875600 -2.18927300 2.97577000
 H 3.52402500 -2.69155600 0.72475700
 H 5.14100300 -2.05500200 0.98656200
 Ir 1.94360900 0.27175200 0.26153800
 O 0.79016400 -3.11968700 2.04553900
 C -0.17744600 0.25236100 0.79782900
 H -0.30377300 2.30527000 1.44376400
 C 1.28474700 0.36922700 -1.65813500
 C 0.22743000 0.81488100 -1.04457300
 H -0.67434200 1.38680900 -1.20273500
 H 1.62178300 0.33760900 -2.68688000

TS2-S

C -1.87249600 -0.63382100 1.25629300
 C -0.56680900 -1.02069200 0.95760300
 C 0.22828600 0.94813500 2.15123400
 C -1.08612300 1.33585000 2.41477800

C -2.13920400 0.54076200 1.96720500
 H -2.70382400 -1.25531900 0.93705600
 H -1.28285700 2.24073800 2.98329200
 H -3.16671300 0.81600800 2.18758900
 C -0.27866900 -2.30766200 0.21633100
 H 0.71575900 -2.20351000 -0.24229300
 C -1.26542900 -2.64674800 -0.92749900
 H -1.33256000 -1.78774500 -1.60403400
 H -2.27222700 -2.80564600 -0.52015600
 C -0.82941200 -3.90566200 -1.68350500
 H -1.52943200 -4.11322400 -2.50157000
 H 0.15384400 -3.73091300 -2.14379700
 C -0.75062000 -5.10963300 -0.73839500
 H -0.40889700 -6.00387600 -1.27219100
 H -1.75591100 -5.33464400 -0.35696400
 C 0.18541300 -4.82608600 0.45136600
 H 1.21813900 -4.73675900 0.08127100
 H 0.16420400 -5.62851700 1.19391700
 C -0.14987600 -3.51691800 1.14920900
 C 1.35928400 0.06658000 -1.59739400
 C 3.69799600 -0.39039300 -2.49924200
 C 4.09817200 -0.28736300 -1.03207700
 C 4.22107100 0.93588900 -0.32671200
 C 3.91709700 2.30751400 -0.89664200
 C 1.55757200 1.37961100 -1.11307300
 H 0.35724100 -0.33932000 -1.47577400
 H 4.68307200 -1.12549400 -0.65807900
 H 4.91721000 0.95200400 0.51090000
 H 0.70613300 1.84658500 -0.62314800
 C 2.17819900 -0.60094100 -2.68164400
 C 2.58888100 2.34917600 -1.68047800
 H 4.02484400 0.50692500 -3.03409500
 H 4.23589400 -1.22704800 -2.95852700
 H 1.86697200 -0.26110900 -3.68209300
 H 1.96230200 -1.67602200 -2.64179300
 H 2.76153900 2.13051500 -2.73922600
 H 2.18310900 3.36629800 -1.64733700

H 3.85210700 3.00090900 -0.05043700
H 4.75052600 2.66030500 -1.52440000
Ir 2.40922700 -0.04104600 0.32644400
O -0.27186900 -3.44359300 2.35881900
C 0.50531600 -0.19958100 1.38833700
H 1.05706000 1.53748500 2.53079700
C 3.20363400 -0.80826300 2.02757800
C 1.98299000 -1.19772000 2.22260000
H 1.35037800 -1.87996700 2.76984400
H 4.16383700 -1.01920700 2.47975000

INT4-R

C 2.50723400 -1.01416100 1.66174200
C 1.54966500 -0.97263400 0.64065100
C 1.23328900 1.38380400 1.09744900
C 2.20860600 1.33929300 2.09002700
C 2.82957300 0.12639100 2.39472500
H 3.01644800 -1.94639300 1.88860900
H 2.46729800 2.23986300 2.64046000
H 3.57198300 0.07073200 3.18585900
C 1.31409900 -2.18750700 -0.24220500
H 0.80851800 -1.82159800 -1.15204600
C 2.63493600 -2.85999400 -0.69208400
H 3.23455300 -2.10481300 -1.21026500
H 3.21461300 -3.16588800 0.18684600
C 2.40944200 -4.08895200 -1.57429400
H 3.37441800 -4.50751100 -1.88269600
H 1.87902600 -3.80084700 -2.49328900
C 1.59355300 -5.13605300 -0.81336300
H 1.43296700 -6.03415000 -1.42006100
H 2.15062500 -5.45247400 0.07877400
C 0.23703100 -4.55759300 -0.39263600
H -0.38147700 -4.40427300 -1.29214400
H -0.32873900 -5.22662000 0.26209800
C 0.29743800 -3.19559000 0.26658600
C -0.81055200 -1.49765400 3.83704500
C -1.47228900 0.96775500 4.03480900
C -2.00688600 0.76515700 2.61682600

C -3.21126600 0.05158400 2.31032700
C -4.11312400 -0.62891200 3.32374300
C -2.07985800 -2.09160400 3.76908400
H 0.05450600 -2.15348700 3.73079700
H -1.71566600 1.53939900 1.90921500
H -3.73786100 0.36276100 1.40670000
H -2.12243500 -3.16327600 3.58190000
C -0.49744100 -0.15252800 4.46559500
C -3.33345700 -1.46672900 4.36201500
H -2.30874800 1.04495800 4.73830400
H -0.94803300 1.92855900 4.08286200
H -0.46881600 -0.23043900 5.56378500
H 0.51202100 0.12204600 4.14325600
H -3.06602900 -0.84757600 5.22435200
H -3.98646300 -2.25692600 4.74953000
H -4.78281300 -1.29304300 2.76405300
H -4.75700600 0.10819100 3.82963200
Ir -1.55032700 -1.12664200 1.81194700
O -0.57579900 -2.93155000 1.09479900
C 0.85705800 0.23292900 0.38872700
H 0.71193700 2.31371600 0.88839500
C -0.33466000 0.26032800 -0.50871600
C -1.47139800 -0.32025900 -0.07166200
H -2.34951300 -0.24215200 -0.72325400
H -0.26539200 0.81513700 -1.44829100

INT4-R

C -2.39290500 -0.90437500 1.52555600
C -1.34882000 -0.91907100 0.59105600
C -1.04128700 1.44529000 0.99293800
C -2.08595300 1.44946400 1.91395200
C -2.75798800 0.26055400 2.19757900
H -2.93876200 -1.82490300 1.72165300
H -2.36621900 2.37211600 2.41491700
H -3.56925800 0.24149100 2.91968600
C -1.13603400 -2.19984100 -0.19282900
H -1.94235700 -2.89148700 0.10143000
C 0.11580600 -3.02360100 0.05336900

C 0.20249400 -4.31548700 -0.72779100
 H 1.15540500 -4.79746000 -0.49515300
 H -0.60800500 -4.97891300 -0.39217200
 C 0.03870600 -4.05275800 -2.23860600
 H 0.06542300 -5.00678400 -2.77685000
 H 0.89242100 -3.46039800 -2.59246100
 C -1.26335800 -3.29729700 -2.51609700
 H -2.11911800 -3.93202200 -2.24369900
 H -1.35694700 -3.08578900 -3.58784100
 C -1.31867500 -1.98658200 -1.72617600
 C 0.89250800 -1.63772100 3.74447700
 C 1.27866600 0.85926700 4.16882200
 C 1.97195400 0.81519500 2.80728000
 C 3.26418000 0.24373000 2.58396000
 C 4.12532500 -0.43109900 3.63519000
 C 2.21367500 -2.10395700 3.77535500
 H 0.11164100 -2.36212300 3.50943900
 H 1.67408600 1.60924500 2.12576400
 H 3.84261900 0.66877300 1.76241600
 H 2.38384000 -3.14850800 3.52095000
 C 0.38553700 -0.37745000 4.42114400
 C 3.33341000 -1.40893700 4.53265300
 H 2.02684100 0.96560300 4.96212900
 H 0.65399300 1.75774700 4.21857700
 H 0.25863400 -0.54039700 5.50284600
 H -0.61023400 -0.17519300 4.01449800
 H 2.92278800 -0.88028000 5.39904500
 H 4.02042300 -2.16086500 4.93724100
 H 4.90245700 -0.99232900 3.10220700
 H 4.64884300 0.31751500 4.25109500
 Ir 1.78210700 -1.04103000 1.82628500
 C -0.62908700 0.27247000 0.34104200
 H -0.49450600 2.36171300 0.78971000
 C 0.60391100 0.32444800 -0.50283600
 C 1.76289200 -0.14888500 -0.00651100
 H 2.65875300 -0.02810100 -0.62582800
 H 0.53746900 0.84928700 -1.46011000

H -2.27752000 -1.48015400 -1.87651200
 H -0.53410400 -1.30674400 -2.07168800
 O 1.03552300 -2.75105500 0.82828600

INT4-5'

C -2.50723400 -1.01416100 1.66174200
 C -1.54966500 -0.97263400 0.64065100
 C -1.23328900 1.38380400 1.09744900
 C -2.20860600 1.33929300 2.09002700
 C -2.82957300 0.12639100 2.39472500
 H -3.01644800 -1.94639300 1.88860900
 H -2.46729800 2.23986300 2.64046000
 H -3.57198300 0.07073200 3.18585900
 C -1.31409900 -2.18750700 -0.24220500
 H -0.80851800 -1.82159800 -1.15204600
 C -2.63493600 -2.85999400 -0.69208400
 H -3.23455300 -2.10481300 -1.21026500
 H -3.21461300 -3.16588800 0.18684600
 C -2.40944200 -4.08895200 -1.57429400
 H -3.37441800 -4.50751100 -1.88269600
 H -1.87902600 -3.80084700 -2.49328900
 C -1.59355300 -5.13605300 -0.81336300
 H -1.43296700 -6.03415000 -1.42006100
 H -2.15062500 -5.45247400 0.07877400
 C -0.23703100 -4.55759300 -0.39263600
 H 0.38147700 -4.40427300 -1.29214400
 H 0.32873900 -5.22662000 0.26209800
 C -0.29743800 -3.19559000 0.26658600
 C 0.81055200 -1.49765400 3.83704500
 C 1.47228900 0.96775500 4.03480900
 C 2.00688600 0.76515700 2.61682600
 C 3.21126600 0.05158400 2.31032700
 C 4.11312400 -0.62891200 3.32374300
 C 2.07985800 -2.09160400 3.76908400
 H -0.05450600 -2.15348700 3.73079700
 H 1.71566600 1.53939900 1.90921500
 H 3.73786100 0.36276100 1.40670000
 H 2.12243500 -3.16327600 3.58190000

C	0.49744100	-0.15252800	4.46559500	H	2.11911800	-3.93202200	-2.24369900
C	3.33345700	-1.46672900	4.36201500	H	1.35694700	-3.08578900	-3.58784100
H	2.30874800	1.04495800	4.73830400	C	1.31867500	-1.98658200	-1.72617600
H	0.94803300	1.92855900	4.08286200	C	-0.89250800	-1.63772100	3.74447700
H	0.46881600	-0.23043900	5.56378500	C	-1.27866600	0.85926700	4.16882200
H	-0.51202100	0.12204600	4.14325600	C	-1.97195400	0.81519500	2.80728000
H	3.06602900	-0.84757600	5.22435200	C	-3.26418000	0.24373000	2.58396000
H	3.98646300	-2.25692600	4.74953000	C	-4.12532500	-0.43109900	3.63519000
H	4.78281300	-1.29304300	2.76405300	C	-2.21367500	-2.10395700	3.77535500
H	4.75700600	0.10819100	3.82963200	H	-0.11164100	-2.36212300	3.50943900
Ir	1.55032700	-1.12664200	1.81194700	H	-1.67408600	1.60924500	2.12576400
O	0.57579900	-2.93155000	1.09479900	H	-3.84261900	0.66877300	1.76241600
C	-0.85705800	0.23292900	0.38872700	H	-2.38384000	-3.14850800	3.52095000
H	-0.71193700	2.31371600	0.88839500	C	-0.38553700	-0.37745000	4.42114400
C	0.33466000	0.26032800	-0.50871600	C	-3.33341000	-1.40893700	4.53265300
C	1.47139800	-0.32025900	-0.07166200	H	-2.02684100	0.96560300	4.96212900
H	2.34951300	-0.24215200	-0.72325400	H	-0.65399300	1.75774700	4.21857700
H	0.26539200	0.81513700	-1.44829100	H	-0.25863400	-0.54039700	5.50284600
INT4-S				H	0.61023400	-0.17519300	4.01449800
C	2.39290500	-0.90437500	1.52555600	H	-2.92278800	-0.88028000	5.39904500
C	1.34882000	-0.91907100	0.59105600	H	-4.02042300	-2.16086500	4.93724100
C	1.04128700	1.44529000	0.99293800	H	-4.90245700	-0.99232900	3.10220700
C	2.08595300	1.44946400	1.91395200	H	-4.64884300	0.31751500	4.25109500
C	2.75798800	0.26055400	2.19757900	Ir	-1.78210700	-1.04103000	1.82628500
H	2.93876200	-1.82490300	1.72165300	C	0.62908700	0.27247000	0.34104200
H	2.36621900	2.37211600	2.41491700	H	0.49450600	2.36171300	0.78971000
H	3.56925800	0.24149100	2.91968600	C	-0.60391100	0.32444800	-0.50283600
C	1.13603400	-2.19984100	-0.19282900	C	-1.76289200	-0.14888500	-0.00651100
H	1.94235700	-2.89148700	0.10143000	H	-2.65875300	-0.02810100	-0.62582800
C	-0.11580600	-3.02360100	0.05336900	H	-0.53746900	0.84928700	-1.46011000
C	-0.20249400	-4.31548700	-0.72779100	H	2.27752000	-1.48015400	-1.87651200
H	-1.15540500	-4.79746000	-0.49515300	H	0.53410400	-1.30674400	-2.07168800
H	0.60800500	-4.97891300	-0.39217200	O	-1.03552300	-2.75105500	0.82828600
C	-0.03870600	-4.05275800	-2.23860600	TS3-R'			
H	-0.06542300	-5.00678400	-2.77685000	C	-6.41129700	-8.08737000	2.62398800
H	-0.89242100	-3.46039800	-2.59246100	C	-5.08008900	-7.78979700	2.31916000
C	1.26335800	-3.29729700	-2.51609700	C	-4.56483200	-7.74618600	4.68592200

C -5.88934600 -8.08712800 4.98116100
 C -6.81505600 -8.24614800 3.95114900
 H -7.12408600 -8.22940300 1.81581200
 H -6.19613400 -8.21275200 6.01565400
 H -7.84772700 -8.49634100 4.17747000
 C -2.66825700 -12.43947300 1.82804800
 C -3.35550700 -12.66841500 -0.61142400
 C -4.01104000 -11.32112600 -0.36396600
 C -5.08455600 -11.09336900 0.55064900
 C -5.74182300 -12.19580500 1.37839300
 C -3.61986400 -11.97442800 2.76933100
 H -1.62392100 -12.41529100 2.13596500
 H -3.94576500 -10.64090600 -1.21540400
 H -5.72807900 -10.24077100 0.34017300
 H -3.23233400 -11.62881300 3.72805900
 C -2.99937800 -13.40816200 0.69869900
 C -5.09739200 -12.31508300 2.77696200
 H -3.98814500 -13.30329900 -1.25118300
 H -2.43327100 -12.48271600 -1.17496500
 H -3.82064200 -14.06545000 1.00211100
 H -2.13946500 -14.06339100 0.52157900
 H -5.26817800 -13.31760300 3.19872500
 H -5.58502000 -11.60162800 3.45099100
 H -6.80874100 -11.97482400 1.49360200
 H -5.68771200 -13.15068900 0.84542300
 Ir -3.25408500 -10.39215700 1.37475400
 C -4.15243800 -7.58560900 3.36671500
 H -3.85611800 -7.60043200 5.49503300
 C -4.59274400 -7.71813400 0.92598700
 C -3.50515500 -8.42485800 0.53788500
 H -3.11124500 -8.26861400 -0.46883200
 H -5.14772800 -7.08551000 0.22841600
 C -2.75832600 -7.16710400 2.95667500
 C -2.07163100 -8.22606000 2.09853600
 C -0.87538300 -7.68352700 1.34228500
 H -0.46323900 -8.45419500 0.68569400
 H -1.15661900 -6.81456200 0.73825700

C 0.15261800 -7.27651400 2.42856400
 H 1.03216100 -6.82976300 1.95016900
 H 0.48580800 -8.18898500 2.93704700
 C -0.44852800 -6.30252200 3.45536500
 H -0.65474900 -5.34178400 2.96196000
 H 0.28550800 -6.09779800 4.24379300
 C -1.75495000 -6.82826100 4.07680700
 H -2.85977800 -6.27159200 2.32940400
 H -1.55934600 -7.72706200 4.67309600
 H -2.18639900 -6.07434300 4.74595300
 O -1.93632400 -9.41166200 2.62800600

TS3-R

C 6.52135900 -8.11108100 2.63924400
 C 5.22406300 -7.78948800 2.22515400
 C 4.53880500 -7.66615900 4.54369700
 C 5.82615100 -8.03076800 4.94936200
 C 6.82092100 -8.24454700 3.99542300
 H 7.28769400 -8.29456500 1.89058300
 H 6.05169600 -8.13257700 6.00702200
 H 7.82619100 -8.51665900 4.30435700
 C 2.54561100 -12.30324800 1.62378600
 C 3.48122600 -12.65940300 -0.71605800
 C 4.19761100 -11.35142800 -0.42926600
 C 5.17682100 -11.16565700 0.59544100
 C 5.66327500 -12.28580000 1.51339200
 C 3.42046600 -11.88028600 2.65570400
 H 1.47831200 -12.19724300 1.81281100
 H 4.27682800 -10.69820800 -1.30049800
 H 5.89920500 -10.36682800 0.43556900
 H 2.95807000 -11.48459100 3.56037500
 C 2.92975100 -13.32931100 0.56360600
 C 4.85729700 -12.33345700 2.83149800
 H 4.13507900 -13.35666300 -1.26286500
 H 2.64318400 -12.43205300 -1.38599400
 H 3.66389500 -14.03001900 0.97471200
 H 2.05062100 -13.93068800 0.30713800
 H 4.89845600 -13.34124400 3.27320800

H 5.32237700 -11.65501900 3.55595400
 H 6.72224900 -12.12931400 1.74660800
 H 5.60812800 -13.24805600 0.99356200
 Ir 3.32327200 -10.32093400 1.18954900
 C 4.22700500 -7.53661000 3.19290500
 H 3.76991300 -7.47506600 5.28791900
 C 4.85688100 -7.74345100 0.79937800
 C 3.75051200 -8.38053600 0.34766400
 H 3.45733200 -8.22566000 -0.69318300
 H 5.52145600 -7.19251000 0.12806600
 C 2.87266800 -7.04329200 2.72342500
 C 2.98249800 -5.58933400 2.20991000
 H 3.21172200 -4.94346700 3.06536900
 H 3.83755000 -5.51557000 1.52868500
 C 1.72652500 -5.11157300 1.47719700
 H 1.87189000 -4.08245700 1.12750700
 H 0.87061800 -5.09388100 2.16742300
 C 1.41536000 -6.04085200 0.29964100
 H 0.54283400 -5.68393400 -0.25996500
 H 2.26389400 -6.04023800 -0.39590400
 C 1.15148200 -7.46176500 0.80059400
 H 0.22102100 -7.46770800 1.38981300
 H 0.99994200 -8.17547300 -0.01409900
 C 2.20111700 -8.02061600 1.75415000
 O 1.94654700 -9.20439100 2.24233800
 H 2.18896200 -7.04619300 3.58493400

TS3-S

C 6.41129700 -8.08737000 2.62398800
 C 5.08008900 -7.78979700 2.31916000
 C 4.56483200 -7.74618600 4.68592200
 C 5.88934600 -8.08712800 4.98116100
 C 6.81505600 -8.24614800 3.95114900
 H 7.12408600 -8.22940300 1.81581200
 H 6.19613400 -8.21275200 6.01565400
 H 7.84772700 -8.49634100 4.17747000
 C 2.66825700 -12.43947300 1.82804800
 C 3.35550700 -12.66841500 -0.61142400

C 4.01104000 -11.32112600 -0.36396600
 C 5.08455600 -11.09336900 0.55064900
 C 5.74182300 -12.19580500 1.37839300
 C 3.61986400 -11.97442800 2.76933100
 H 1.62392100 -12.41529100 2.13596500
 H 3.94576500 -10.64090600 -1.21540400
 H 5.72807900 -10.24077100 0.34017300
 H 3.23233400 -11.62881300 3.72805900
 C 2.99937800 -13.40816200 0.69869900
 C 5.09739200 -12.31508300 2.77696200
 H 3.98814500 -13.30329900 -1.25118300
 H 2.43327100 -12.48271600 -1.17496500
 H 3.82064200 -14.06545000 1.00211100
 H 2.13946500 -14.06339100 0.52157900
 H 5.26817800 -13.31760300 3.19872500
 H 5.58502000 -11.60162800 3.45099100
 H 6.80874100 -11.97482400 1.49360200
 H 5.68771200 -13.15068900 0.84542300
 Ir 3.25408500 -10.39215700 1.37475400
 C 4.15243800 -7.58560900 3.36671500
 H 3.85611800 -7.60043200 5.49503300
 C 4.59274400 -7.71813400 0.92598700
 C 3.50515500 -8.42485800 0.53788500
 H 3.11124500 -8.26861400 -0.46883200
 H 5.14772800 -7.08551000 0.22841600
 C 2.75832600 -7.16710400 2.95667500
 C 2.07163100 -8.22606000 2.09853600
 C 0.87538300 -7.68352700 1.34228500
 H 0.46323900 -8.45419500 0.68569400
 H 1.15661900 -6.81456200 0.73825700
 C -0.15261800 -7.27651400 2.42856400
 H -1.03216100 -6.82976300 1.95016900
 H -0.48580800 -8.18898500 2.93704700
 C 0.44852800 -6.30252200 3.45536500
 H 0.65474900 -5.34178400 2.96196000
 H -0.28550800 -6.09779800 4.24379300
 C 1.75495000 -6.82826100 4.07680700

H 2.85977800 -6.27159200 2.32940400
H 1.55934600 -7.72706200 4.67309600
H 2.18639900 -6.07434300 4.74595300
O 1.93632400 -9.41166200 2.62800600

TS3-S

C -6.52135900 -8.11108100 2.63924400
C -5.22406300 -7.78948800 2.22515400
C -4.53880500 -7.66615900 4.54369700
C -5.82615100 -8.03076800 4.94936200
C -6.82092100 -8.24454700 3.99542300
H -7.28769400 -8.29456500 1.89058300
H -6.05169600 -8.13257700 6.00702200
H -7.82619100 -8.51665900 4.30435700
C -2.54561100 -12.30324800 1.62378600
C -3.48122600 -12.65940300 -0.71605800
C -4.19761100 -11.35142800 -0.42926600
C -5.17682100 -11.16565700 0.59544100
C -5.66327500 -12.28580000 1.51339200
C -3.42046600 -11.88028600 2.65570400
H -1.47831200 -12.19724300 1.81281100
H -4.27682800 -10.69820800 -1.30049800
H -5.89920500 -10.36682800 0.43556900
H -2.95807000 -11.48459100 3.56037500
C -2.92975100 -13.32931100 0.56360600
C -4.85729700 -12.33345700 2.83149800
H -4.13507900 -13.35666300 -1.26286500
H -2.64318400 -12.43205300 -1.38599400
H -3.66389500 -14.03001900 0.97471200
H -2.05062100 -13.93068800 0.30713800
H -4.89845600 -13.34124400 3.27320800
H -5.32237700 -11.65501900 3.55595400
H -6.72224900 -12.12931400 1.74660800
H -5.60812800 -13.24805600 0.99356200
Ir -3.32327200 -10.32093400 1.18954900
C -4.22700500 -7.53661000 3.19290500
H -3.76991300 -7.47506600 5.28791900
C -4.85688100 -7.74345100 0.79937800

C -3.75051200 -8.38053600 0.34766400
H -3.45733200 -8.22566000 -0.69318300
H -5.52145600 -7.19251000 0.12806600
C -2.87266800 -7.04329200 2.72342500
C -2.98249800 -5.58933400 2.20991000
H -3.21172200 -4.94346700 3.06536900
H -3.83755000 -5.51557000 1.52868500
C -1.72652500 -5.11157300 1.47719700
H -1.87189000 -4.08245700 1.12750700
H -0.87061800 -5.09388100 2.16742300
C -1.41536000 -6.04085200 0.29964100
H -0.54283400 -5.68393400 -0.25996500
H -2.26389400 -6.04023800 -0.39590400
C -1.15148200 -7.46176500 0.80059400
H -0.22102100 -7.46770800 1.38981300
H -0.99994200 -8.17547300 -0.01409900
C -2.20111700 -8.02061600 1.75415000
O -1.94654700 -9.20439100 2.24233800
H -2.18896200 -7.04619300 3.58493400

INT5-(S, R)

C -6.23773800 -9.38333100 2.27303000
C -5.03980100 -8.75629300 1.91321800
C -4.72182900 -8.09252500 4.21580300
C -5.90566400 -8.74937600 4.57317300
C -6.67337800 -9.38464100 3.59831800
H -6.82156300 -9.88856200 1.50713700
H -6.22787500 -8.75248600 5.61073100
H -7.60179400 -9.88092600 3.86650300
C -4.28074000 -8.07361300 2.89378400
H -4.14526300 -7.58951700 4.98470200
C -4.51430700 -8.84932500 0.55047000
C -3.23074200 -8.57524200 0.27392400
H -2.82736100 -8.72818200 -0.72496300
H -5.18085100 -9.22963000 -0.22158700
C -3.06013200 -7.30759700 2.42072100
C -2.27162100 -8.11722900 1.35333300
C -1.15262000 -7.24232000 0.76369900

H	-0.60507300	-7.83828300	0.02294300	C	-1.88049200	4.31960200	-0.42168300
H	-1.60350100	-6.39371600	0.22967700	C	-1.02849200	4.25466500	0.70208700
C	-0.20697900	-6.73594500	1.85671900	C	-1.54003900	3.81163900	1.92071800
H	0.57101400	-6.09978700	1.41714800	C	-2.88020200	3.43309900	2.04219300
H	0.29511700	-7.59802900	2.31036100	H	-4.76214700	3.18964800	1.01436100
C	-0.97736600	-5.96480800	2.93499800	H	-3.87203800	3.98298500	-1.16368000
H	-1.39404600	-5.04629800	2.49485800	H	-0.88259900	3.76752000	2.78586900
H	-0.29892200	-5.64786400	3.73664400	H	-3.26486400	3.09988800	3.00194800
C	-2.12467000	-6.79859100	3.52319800	C	0.43611300	4.57295600	0.51821600
H	-3.44572000	-6.42710100	1.87878600	C	-1.35953700	4.87294500	-1.67234200
H	-1.72014600	-7.65656100	4.07312600	H	-1.98701800	4.79065400	-2.55813400
H	-2.68801300	-6.18887300	4.23927600	C	-0.18938300	5.52787100	-1.72028900
O	-1.65672500	-9.23566100	1.98489800	C	0.65406700	5.73696800	-0.47911700
Ir	-2.24308100	-10.97991100	2.58499300	C	1.15601400	3.27379000	0.07065000
C	-2.00372500	-12.86591800	1.64868200	H	0.64072300	2.87538800	-0.81259800
C	-3.15490800	-12.16771000	1.13331300	H	1.04159400	2.52479800	0.86310100
C	-3.76362400	-11.83450800	3.79619000	C	2.63359300	3.49235800	-0.26287700
C	-2.49373500	-12.32158300	4.23417600	H	3.08074400	2.55154600	-0.60718400
C	-2.10519800	-14.11697000	2.51941500	H	3.17712400	3.78989000	0.64551200
H	-1.09939100	-12.81296500	1.04142500	C	2.78647300	4.58614300	-1.32316300
C	-4.58197200	-12.52647900	1.49653000	H	2.30364100	4.25997000	-2.25521200
H	-3.05707300	-11.67963300	0.16275400	H	3.84430200	4.75646700	-1.55739700
C	-4.77291500	-12.67849600	3.02100900	C	2.14441400	5.88564700	-0.83237200
H	-4.20682500	-11.01996500	4.36636200	H	2.65982000	6.23416300	0.07139000
C	-1.97549000	-13.72923600	4.00130200	H	2.23612800	6.68483300	-1.57812900
H	-2.07546100	-11.83524300	5.11895400	C	-1.92399900	10.17409800	0.28365400
H	-1.31409000	-14.82165200	2.24130000	C	-3.89479400	8.88215400	-0.65153500
H	-3.05162500	-14.63397400	2.32958400	C	-3.00853600	7.71112300	-0.23204800
H	-5.22186100	-11.71686100	1.13436900	C	-2.88063400	7.26488600	1.13674100
H	-4.89461000	-13.43840100	0.96561200	C	-3.56531300	7.91735000	2.31961800
H	-5.78214600	-12.35529300	3.29310200	C	-2.04007400	9.80942900	1.65695200
H	-4.69063200	-13.72855500	3.32123200	H	-1.11450700	10.86020300	0.02316800
H	-2.48174300	-14.45615100	4.65502000	H	-2.86564900	6.95071900	-0.99680100
H	-0.91649000	-13.74243300	4.28403400	H	-2.67644600	6.20727100	1.28155000
INT5-(R, R)				H	-1.28728700	10.21649800	2.33311400
C	-3.72013000	3.48403800	0.92802400	C	-3.08513000	10.19404200	-0.69672700
C	-3.21855000	3.92316300	-0.29645500	C	-3.36473500	9.44473400	2.32189800

H -4.74383900 8.96972300 0.03436200
H -4.32086100 8.67633300 -1.63911900
H -3.73663600 11.06301300 -0.51999900
H -2.66466600 10.31786300 -1.70106000
H -4.19406500 9.94750600 1.81361900
H -3.37252200 9.81834100 3.35139200
H -3.12045900 7.49057800 3.22573700
H -4.63289200 7.64841000 2.34088700
Ir -1.12099300 8.21759400 0.52601300
O 0.28328700 6.96334200 0.13483000
H 0.86434400 4.90038500 1.47384300
H 0.15144700 5.99488300 -2.64152300

INT5-(R, S)

C 6.23806100 -9.38287700 2.27232500
C 5.03994200 -8.75606100 1.91275200
C 4.72202000 -8.09286000 4.21550700
C 5.90599800 -8.74958500 4.57265200
C 6.67379600 -9.38440900 3.59758500
H 6.82192200 -9.88785800 1.50628700
H 6.22825300 -8.75289900 5.61019800
H 7.60235200 -9.88055100 3.86556500
C 4.28086200 -8.07369500 2.89352200
H 4.14540200 -7.59016100 4.98457300
C 4.51420000 -8.84914800 0.55012500
C 3.23050400 -8.57541000 0.27385500
H 2.82688700 -8.72866400 -0.72489200
H 5.18064400 -9.22938000 -0.22206200
C 3.06016900 -7.30773600 2.42067000
C 2.27154000 -8.11734500 1.35336700
C 1.15253800 -7.24236200 0.76381100
H 0.60482500 -7.83831200 0.02315800
H 1.60345700 -6.39385900 0.22965200
C 0.20705800 -6.73583900 1.85690000
H -0.57089000 -6.09958500 1.41737000
H -0.29513700 -7.59786200 2.31056500
C 0.97757300 -5.96481800 2.93515900
H 1.39431100 -5.04631000 2.49505300

H 0.29919400 -5.64784400 3.73685600
C 2.12484700 -6.79871000 3.52325400
H 3.44565400 -6.42721000 1.87868700
H 1.72032500 -7.65666400 4.07322100
H 2.68830000 -6.18904800 4.23929700
O 1.65666300 -9.23574200 1.98499500
Ir 2.24281800 -10.98006600 2.58512700
C 2.00388100 -12.86593300 1.64853500
C 3.15516000 -12.16751200 1.13359300
C 3.76298500 -11.83451300 3.79679900
C 2.49300700 -12.32186900 4.23424900
C 2.10541100 -14.11707200 2.51914000
H 1.09972300 -12.81309500 1.04100300
C 4.58213300 -12.52625500 1.49727800
H 3.05767700 -11.67945200 0.16299000
C 4.77278800 -12.67811300 3.02181900
H 4.20586200 -11.02002700 4.36733300
C 1.97489000 -13.72950200 4.00097700
H 2.07434200 -11.83565100 5.11891500
H 1.31471100 -14.82205500 2.24061300
H 3.05212500 -14.63368300 2.32971000
H 5.22211600 -11.71667900 1.13520800
H 4.89489900 -13.43822000 0.96650700
H 5.78180300 -12.35439900 3.29408900
H 4.69091500 -13.72817700 3.32212000
H 2.48068400 -14.45652300 4.65493000
H 0.91570600 -13.74264500 4.28304400

INT5-(S, S)

C 3.72013000 3.48403800 0.92802400
C 3.21855000 3.92316300 -0.29645500
C 1.88049200 4.31960200 -0.42168300
C 1.02849200 4.25466500 0.70208700
C 1.54003900 3.81163900 1.92071800
C 2.88020200 3.43309900 2.04219300
H 4.76214700 3.18964800 1.01436100
H 3.87203800 3.98298500 -1.16368000
H 0.88259900 3.76752000 2.78586900

H 3.26486400 3.09988800 3.00194800
 C -0.43611300 4.57295600 0.51821600
 C 1.35953700 4.87294500 -1.67234200
 H 1.98701800 4.79065400 -2.55813400
 C 0.18938300 5.52787100 -1.72028900
 C -0.65406700 5.73696800 -0.47911700
 C -1.15601400 3.27379000 0.07065000
 H -0.64072300 2.87538800 -0.81259800
 H -1.04159400 2.52479800 0.86310100
 C -2.63359300 3.49235800 -0.26287700
 H -3.08074400 2.55154600 -0.60718400
 H -3.17712400 3.78989000 0.64551200
 C -2.78647300 4.58614300 -1.32316300
 H -2.30364100 4.25997000 -2.25521200
 H -3.84430200 4.75646700 -1.55739700
 C -2.14441400 5.88564700 -0.83237200
 H -2.65982000 6.23416300 0.07139000
 H -2.23612800 6.68483300 -1.57812900
 C 1.92399900 10.17409800 0.28365400
 C 3.89479400 8.88215400 -0.65153500
 C 3.00853600 7.71112300 -0.23204800
 C 2.88063400 7.26488600 1.13674100
 C 3.56531300 7.91735000 2.31961800
 C 2.04007400 9.80942900 1.65695200
 H 1.11450700 10.86020300 0.02316800
 H 2.86564900 6.95071900 -0.99680100
 H 2.67644600 6.20727100 1.28155000
 H 1.28728700 10.21649800 2.33311400
 C 3.08513000 10.19404200 -0.69672700
 C 3.36473500 9.44473400 2.32189800
 H 4.74383900 8.96972300 0.03436200
 H 4.32086100 8.67633300 -1.63911900
 H 3.73663600 11.06301300 -0.51999900
 H 2.66466600 10.31786300 -1.70106000
 H 4.19406500 9.94750600 1.81361900
 H 3.37252200 9.81834100 3.35139200
 H 3.12045900 7.49057800 3.22573700

H 4.63289200 7.64841000 2.34088700
 Ir 1.12099300 8.21759400 0.52601300
 O -0.28328700 6.96334200 0.13483000
 H -0.86434400 4.90038500 1.47384300
 H -0.15144700 5.99488300 -2.64152300

TS4-(S, R)

C -2.17859200 -4.72056900 5.81265900
 C -0.97554000 -5.39790700 5.55441700
 C -0.10322000 -4.77669900 4.67177500
 C -0.40943300 -3.56747900 4.05490200
 C -1.58884800 -2.88122800 4.30441400
 C -2.47466100 -3.48968400 5.20867600
 H -2.89886100 -5.15535400 6.50087600
 H -0.75688600 -6.34808600 6.03508400
 H -1.83577200 -1.93323600 3.83502900
 H -3.41657800 -3.00113200 5.44437500
 C 0.86970800 -3.56472400 3.20999100
 C 0.60817600 -3.74624600 1.69112900
 H 0.92839000 -2.83317600 1.17995800
 H -0.47274700 -3.83893800 1.52999000
 C 1.60475200 -6.18166900 3.24972300
 H 2.69272900 -6.25935500 3.12983900
 H 1.30186300 -7.04776900 3.85278900
 C 1.28716100 -4.97010800 1.06691100
 C 0.96034400 -6.24038600 1.85971000
 C 1.26625500 -4.89714900 4.01607800
 H -0.13038900 -6.33977000 1.95330200
 H 1.31633700 -7.13115900 1.32830000
 H 2.37465400 -4.82361000 1.03580200
 H 0.95556600 -5.06956400 0.02600700
 O 1.71259900 -2.46470400 3.49171200
 H 2.06851800 -4.64976500 4.72053400
 H 1.47372400 -1.39877700 2.89497200
 C 5.38731500 -0.74745300 2.63405000
 C 6.30574100 -2.59067300 4.12147200
 C 4.91189100 -3.16497300 3.88290500
 C 4.54393200 -3.82043300 2.66888500

C 5.43986700 -3.98391800 1.45535200
 C 5.24136300 -1.45395800 1.40914700
 H 5.08327000 0.29552500 2.63280300
 H 4.37737200 -3.46822900 4.78315600
 H 3.77610400 -4.58556700 2.74964200
 H 4.83310500 -0.89777100 0.56989900
 C 6.36402700 -1.09798500 3.74038700
 C 6.10512300 -2.65593700 1.03650300
 H 7.04407100 -3.16405900 3.55070900
 H 6.57594000 -2.71316000 5.17572200
 H 7.38794100 -0.80220900 3.46529500
 H 6.09077200 -0.49622400 4.61500100
 H 7.09395400 -2.55806900 1.49744600
 H 6.27430600 -2.65541900 -0.04552200
 H 4.80559800 -4.33808200 0.63402800
 H 6.19526500 -4.76612000 1.62594000
 Ir 3.62988600 -1.93270400 2.72749500
 C 1.65336200 1.02269100 0.45515000
 C 1.62963000 0.74325600 1.97905700
 C 0.72601200 0.05698900 -0.28917700
 H 1.10680100 -0.96420900 -0.17268800
 H 0.72898900 0.28433600 -1.36113500
 C -0.71186100 0.15816700 0.24103800
 H -1.35258100 -0.57025700 -0.27044500
 H -1.10948500 1.15375700 -0.00456500
 C -0.78350400 -0.05019400 1.75827700
 H -0.54495700 -1.09352400 1.98974600
 H -1.80563100 0.12280600 2.11727300
 C 0.18695600 0.87755100 2.49871700
 H -0.12994800 1.92170700 2.37691900
 H 0.18250700 0.66486500 3.57551200
 H 1.22521200 2.03485400 0.35389200
 C 3.47340900 0.63429900 -1.31471600
 C 4.77745400 0.83787700 -1.77931600
 C 5.69152400 1.55274700 -1.00639800
 C 5.30293600 2.04212200 0.23981500
 C 4.00750300 1.82200600 0.72193800

C 3.06966500 1.12518400 -0.07403200
 H 2.77261200 0.08296600 -1.93221300
 H 5.07232900 0.44056100 -2.74645400
 H 6.70262200 1.72008400 -1.36609600
 H 6.01553800 2.57768800 0.86255500
 C 3.63012900 2.21870800 2.07939300
 C 2.55059200 1.70733800 2.68943500
 O 2.04569200 -0.60473600 2.22453300
 H 2.33736400 1.92807200 3.73300300
 H 4.31045300 2.87586100 2.61807800

TS4-(R, R)

C -2.31852100 -4.31633400 5.55228500
 C -1.07610800 -4.97011800 5.60431600
 C -0.13060600 -4.55619100 4.67606500
 C -0.40511800 -3.56921400 3.73563600
 C -1.62376300 -2.91078300 3.66911400
 C -2.58478800 -3.30931200 4.61197800
 H -3.09635900 -4.59305300 6.25937500
 H -0.88654900 -5.74742600 6.34013800
 H -1.83547200 -2.13584400 2.93864100
 H -3.56155400 -2.83225400 4.61554800
 C 0.96472400 -3.67891500 3.06708100
 C 0.93198700 -4.11479400 1.58364600
 H 1.64467100 -3.48633100 1.04479900
 H -0.05331500 -3.86329100 1.18348200
 C 1.62117100 -6.20278200 3.68535900
 H 2.69701200 -6.27660700 3.47259900
 H 1.40911600 -6.92199400 4.48741200
 C 1.23631200 -5.59805100 1.28474000
 C 0.83882300 -6.55234500 2.41482200
 C 1.29153800 -4.79179400 4.17522300
 H -0.23970800 -6.48497000 2.61073500
 H 1.04582000 -7.58799400 2.11926500
 H 2.31244300 -5.72587500 1.10270400
 H 0.73655700 -5.87755800 0.34949700
 O 1.72572300 -2.50110000 3.26301400
 H 2.05697100 -4.41930900 4.86469300

H 1.44890900 -1.41144900 2.79430200
 C -1.36817000 -2.76045300 -0.96615800
 C -1.58817800 -1.75382300 -0.02703500
 C -0.55560300 -0.87992000 0.34216400
 C 0.71745600 -1.02242700 -0.24865400
 C 0.92493200 -2.03088100 -1.18843500
 C -0.10691600 -2.90061600 -1.54862600
 H -2.17582100 -3.43282200 -1.24059100
 H -2.56860300 -1.63981900 0.42936300
 H 1.90788700 -2.13667800 -1.64215500
 H 0.07398300 -3.68501900 -2.27798600
 C 1.78044600 0.00921900 0.04765600
 C -0.76261100 0.18279000 1.32748900
 H -1.78357100 0.37200100 1.65369200
 C 0.25836600 0.88459800 1.84303600
 C 1.69594700 0.55325700 1.49359400
 C 1.64655300 1.14042400 -1.00645000
 H 0.61252700 1.50795400 -0.99367100
 H 1.81051800 0.70604600 -1.99944200
 C 2.60169100 2.30939300 -0.75749000
 H 2.44024200 3.08954900 -1.51153900
 H 3.64140900 1.96842700 -0.87026000
 C 2.40427300 2.86786900 0.65394200
 H 1.38583900 3.27059500 0.74766700
 H 3.09276000 3.69978500 0.84433000
 C 2.62401000 1.76087900 1.68682000
 H 3.65735800 1.40166900 1.61335700
 H 2.48974900 2.13063500 2.71025000
 C 5.39044200 -0.72363800 2.66312000
 C 6.34573200 -2.80687600 3.75274300
 C 4.93459200 -3.32205500 3.48429100
 C 4.48821000 -3.75774500 2.20192900
 C 5.31349100 -3.71278000 0.92960900
 C 5.19061500 -1.20950000 1.33823100
 H 5.11350400 0.31487800 2.84835400
 H 4.43129000 -3.75890500 4.34643600
 H 3.71004800 -4.51890800 2.19150500

H 4.79412500 -0.49588300 0.61725600
 C 6.40255400 -1.26923100 3.65309700
 C 6.00549200 -2.34749700 0.72544700
 H 7.05065400 -3.26689700 3.05260700
 H 6.66465000 -3.12172500 4.75209800
 H 7.41882400 -0.92797500 3.40375400
 H 6.16134700 -0.84003700 4.63244800
 H 7.01244500 -2.35702900 1.15492900
 H 6.13695600 -2.16272000 -0.34616500
 H 4.62579400 -3.89223100 0.09458800
 H 6.04933000 -4.53102200 0.90912500
 Ir 3.62023400 -1.88484800 2.61278100
 O 2.10355900 -0.43320600 2.44886900
 H 2.76857000 -0.45195100 -0.05975000
 H 0.08802900 1.64069800 2.60541600

TS4-(R, S)

C 2.17776400 -4.72273600 5.81218200
 C 0.97385700 -5.39902100 5.55519200
 C 0.10165500 -4.77760400 4.67258300
 C 0.40871600 -3.56918300 4.05456900
 C 1.58897300 -2.88394400 4.30289200
 C 2.47471700 -3.49261900 5.20707400
 H 2.89800400 -5.15773100 6.50029600
 H 0.75449600 -6.34859000 6.03674000
 H 1.83661600 -1.93657100 3.83265900
 H 3.41726900 -3.00483600 5.44182800
 C -0.87108400 -3.56567900 3.21060900
 C -0.61087400 -3.74854800 1.69165600
 H -0.93091700 -2.83568700 1.17998100
 H 0.46987000 -3.84203100 1.52977700
 C -1.60867200 -6.18185300 3.25281800
 H -2.69677900 -6.25839800 3.13336400
 H -1.30655300 -7.04780300 3.85648400
 C -1.29104900 -4.97250600 1.06888000
 C -0.96482000 -6.24234700 1.86263100
 C -1.26841100 -4.89710400 4.01797900
 H 0.12587400 -6.34243500 1.95592100

H -1.32166400 -7.13332400 1.33213900
 H -2.37845300 -4.82526600 1.03824500
 H -0.96010400 -5.07309500 0.02787900
 O -1.71267900 -2.46459200 3.49223700
 H -2.06991600 -4.64841900 4.72284200
 H -1.47289900 -1.39963300 2.89412600
 C -5.38588100 -0.74440500 2.63334800
 C -6.30563100 -2.58477600 4.12350700
 C -4.91243100 -3.16071000 3.88520700
 C -4.54560400 -3.81814400 2.67192600
 C -5.44218900 -3.98230800 1.45896600
 C -5.24099300 -1.45259600 1.40929800
 H -5.08084900 0.29825800 2.63067400
 H -4.37786800 -3.46332700 4.78564500
 H -3.77853800 -4.58396500 2.75336200
 H -4.83244600 -0.89781600 0.56923500
 C -6.36261400 -1.09254500 3.74042800
 C -6.10609400 -2.65417300 1.03846900
 H -7.04470400 -3.15821600 3.55375400
 H -6.57557700 -2.70560400 5.17801200
 H -7.38632000 -0.79617900 3.46519500
 H -6.08857900 -0.48984800 4.61415300
 H -7.09470800 -2.55460600 1.49952500
 H -6.27555400 -2.65495100 -0.04351100
 H -4.80867200 -4.33839800 0.63789900
 H -6.19842200 -4.76339300 1.63097000
 Ir -3.62954800 -1.93129100 2.72776500
 C -1.65127800 1.02134000 0.45295100
 C -1.62681500 0.74183800 1.97683400
 C -0.72532800 0.05477900 -0.29201500
 H -1.10692700 -0.96608800 -0.17525200
 H -0.72884200 0.28214300 -1.36396800
 C 0.71298800 0.15465100 0.23723700
 H 1.35267200 -0.57442300 -0.27461800
 H 1.11141400 1.14984100 -0.00868700
 C 0.78540900 -0.05374500 1.75443000
 H 0.54595600 -1.09683300 1.98603600

H 1.80793300 0.11827700 2.11276700
 C -0.18368500 0.87488400 2.49552700
 H 0.13404900 1.91876000 2.37350300
 H -0.17867300 0.66220900 3.57232500
 H -1.22219400 2.03308100 0.35144800
 C -3.47290600 0.63469500 -1.31569000
 C -4.77703100 0.83967500 -1.77945100
 C -5.68980000 1.55563100 -1.00600100
 C -5.29985900 2.04468400 0.23991400
 C -4.00435600 1.82316800 0.72120900
 C -3.06781200 1.12524900 -0.07531500
 H -2.77311800 0.08253900 -1.93359600
 H -5.07298100 0.44259900 -2.74635900
 H -6.70094400 1.72406400 -1.36505900
 H -6.01146600 2.58108300 0.86307600
 C -3.62571800 2.21938400 2.07845900
 C -2.54643900 1.70670400 2.68786500
 O -2.04384900 -0.60587400 2.22237400
 H -2.33248200 1.92697500 3.73138200
 H -4.30504700 2.87716900 2.61763000

TS4-(S,S)

C 2.31885700 -4.31735900 5.55128100
 C 1.07625300 -4.97075200 5.60366800
 C 0.13064600 -4.55658900 4.67563000
 C 0.40521600 -3.56973900 3.73508400
 C 1.62406300 -2.91171900 3.66818800
 C 2.58520600 -3.31049400 4.61082900
 H 3.09678800 -4.59427600 6.25819200
 H 0.88664000 -5.74796200 6.33957900
 H 1.83584600 -2.13691900 2.93758700
 H 3.56213100 -2.83375900 4.61410400
 C -0.96484200 -3.67903600 3.06689500
 C -0.93268100 -4.11490000 1.58344600
 H -1.64536400 -3.48624800 1.04483500
 H 0.05257300 -3.86367300 1.18296300
 C -1.62176600 -6.20274500 3.68538100
 H -2.69769000 -6.27634400 3.47297300

H -1.40961200 -6.92200400 4.48736700
 C -1.23754700 -5.59807200 1.28465800
 C -0.83992900 -6.55249500 2.41458500
 C -1.29167200 -4.79182700 4.17512800
 H 0.23869000 -6.48542200 2.61012700
 H -1.04731400 -7.58808200 2.11908300
 H -2.31378300 -5.72556500 1.10301100
 H -0.73820900 -5.87771500 0.34923200
 O -1.72546100 -2.50101900 3.26300300
 H -2.05686500 -4.41914800 4.86476200
 H -1.44860900 -1.41129200 2.79411500
 C 1.36744500 -2.76156500 -0.96658600
 C 1.58788200 -1.75493600 -0.02756700
 C 0.55561500 -0.88070500 0.34171900
 C -0.71757600 -1.02289000 -0.24888700
 C -0.92546900 -2.03132200 -1.18860000
 C 0.10607200 -2.90137900 -1.54888300
 H 2.17485700 -3.43419600 -1.24108200
 H 2.56840200 -1.64118600 0.42869000
 H -1.90852100 -2.13686700 -1.64217000
 H -0.07515600 -3.68576700 -2.27817900
 C -1.78024400 0.00905700 0.04754700
 C 0.76309200 0.18201200 1.32693400
 H 1.78415800 0.37093400 1.65296900
 C -0.25759000 0.88415300 1.84260700
 C -1.69531600 0.55321600 1.49341900
 C -1.64626400 1.14012000 -1.00670200
 H -0.61212300 1.50733800 -0.99419200
 H -1.81057400 0.70568900 -1.99961400
 C -2.60098100 2.30941500 -0.75766100
 H -2.43944300 3.08944000 -1.51182600
 H -3.64083200 1.96877000 -0.87017100
 C -2.40308900 2.86796400 0.65367800
 H -1.38450500 3.27036100 0.74716600
 H -3.09126900 3.70011900 0.84413300
 C -2.62299800 1.76112300 1.68667600
 H -3.65645900 1.40220700 1.61335700

H -2.48850500 2.13091500 2.71006300
 C -5.38985200 -0.72270100 2.66390500
 C -6.34551500 -2.80560400 3.75384200
 C -4.93458100 -3.32119700 3.48512200
 C -4.48864500 -3.75711800 2.20267900
 C -5.31426200 -3.71196700 0.93058200
 C -5.19046100 -1.20867000 1.33898900
 H -5.11251000 0.31571600 2.84910400
 H -4.43121000 -3.75813100 4.34718400
 H -3.71073000 -4.51853600 2.19210400
 H -4.79391700 -0.49521200 0.61788800
 C -6.40194100 -1.26795500 3.65409300
 C -6.00582900 -2.34645100 0.72645400
 H -7.05070900 -3.26548100 3.05388500
 H -6.66431400 -3.12029400 4.75328500
 H -7.41816200 -0.92645300 3.40489200
 H -6.16045700 -0.83874800 4.63336900
 H -7.01270400 -2.35561100 1.15612600
 H -6.13743300 -2.16171600 -0.34514800
 H -4.62688900 -3.89179100 0.09537500
 H -6.05042100 -4.52992800 0.91041000
 Ir -3.62000300 -1.88444600 2.61320800
 O -2.10309700 -0.43305500 2.44883400
 H -2.76850600 -0.45188000 -0.05959900
 H -0.08690300 1.64023100 2.60493000

INT6-(*S*, *R*)

C -14.72565400 3.60371100 -10.10217500
 C -14.34289100 4.97940300 -10.68701400
 C -13.87352200 2.49091700 -10.72922100
 H -14.11958200 2.41061600 -11.79401000
 H -14.11609200 1.52849300 -10.26467300
 C -12.37484700 2.77174000 -10.55094900
 H -11.78806100 1.98674200 -11.04333800
 H -12.12680000 2.72320700 -9.48003100
 C -11.98187400 4.14953400 -11.09681600
 H -12.12591800 4.16502400 -12.18312300
 H -10.92040100 4.34831500 -10.90561400

C -12.84466500 5.25041300 -10.47300000
 H -12.64679900 5.32491300 -9.39456400
 H -12.59785900 6.22984700 -10.90660900
 H -14.45597400 3.66483400 -9.03391200
 C -16.81563500 2.13851100 -10.36166700
 C -18.20355400 1.97480600 -10.30541100
 C -19.02607400 3.06264700 -10.02054100
 C -18.45423000 4.31555300 -9.80727100
 C -17.06765300 4.49073000 -9.87946900
 C -16.22907600 3.38359600 -10.14717200
 H -16.19316500 1.27741300 -10.57915300
 H -18.63641000 0.99397400 -10.48176200
 H -20.10398300 2.93866500 -9.96843500
 H -19.08565200 5.17528200 -9.59495900
 C -16.46682900 5.81278300 -9.70847000
 C -15.19736900 6.06010700 -10.06264400
 O -14.61439000 4.90058900 -12.10571900
 H -14.67155400 5.81042000 -12.43680700
 H -14.77010300 7.05677300 -9.96382200
 H -17.10023900 6.60755800 -9.31861100

INT6-(R, R)

C -3.25782500 1.77798600 0.14621600
 C -2.60781200 2.18187000 -1.01836900
 C -1.60242800 3.15619800 -0.97485800
 C -1.23635600 3.72477900 0.26373000
 C -1.89027800 3.31053000 1.42133200
 C -2.90038600 2.34654100 1.36925200
 H -4.04020100 1.02584000 0.09973700
 H -2.88422800 1.74769100 -1.97646600
 H -1.60770700 3.74888600 2.37579400
 H -3.40513700 2.04137300 2.28164800
 C -0.06563000 4.68215400 0.31410900
 C -0.92536600 3.61260000 -2.18799300
 H -1.09282600 3.04642300 -3.10244600
 C -0.14573300 4.70459500 -2.19157400
 C 0.00689500 5.55954800 -0.94905200
 C 1.23574200 3.87079300 0.52839400

H 1.30214900 3.10433000 -0.25421100
 H 1.15883400 3.33706600 1.48251400
 C 2.49311600 4.74391700 0.49268500
 H 3.38559800 4.11739700 0.61176600
 H 2.47991700 5.44282600 1.34139400
 C 2.56340500 5.53928500 -0.81419600
 H 2.65988200 4.84354700 -1.65961400
 H 3.45207600 6.18159600 -0.83123600
 C 1.29930000 6.38838900 -0.98096800
 H 1.23704400 7.12398900 -0.16962800
 H 1.33008700 6.95592000 -1.92192700
 H -0.19476500 5.36797800 1.16129000
 H 0.34076800 5.03968500 -3.10618300
 O -1.11923400 6.45906900 -0.84439100
 H -1.27319300 6.82990200 -1.72780700

INT6-(R, S)

C 14.72565400 3.60371100 -10.10217500
 C 14.34289100 4.97940300 -10.68701400
 C 13.87352200 2.49091700 -10.72922100
 H 14.11958200 2.41061600 -11.79401000
 H 14.11609200 1.52849300 -10.26467300
 C 12.37484700 2.77174000 -10.55094900
 H 11.78806100 1.98674200 -11.04333800
 H 12.12680000 2.72320700 -9.48003100
 C 11.98187400 4.14953400 -11.09681600
 H 12.12591800 4.16502400 -12.18312300
 H 10.92040100 4.34831500 -10.90561400
 C 12.84466500 5.25041300 -10.47300000
 H 12.64679900 5.32491300 -9.39456400
 H 12.59785900 6.22984700 -10.90660900
 H 14.45597400 3.66483400 -9.03391200
 C 16.81563500 2.13851100 -10.36166700
 C 18.20355400 1.97480600 -10.30541100
 C 19.02607400 3.06264700 -10.02054100
 C 18.45423000 4.31555300 -9.80727100
 C 17.06765300 4.49073000 -9.87946900
 C 16.22907600 3.38359600 -10.14717200

H 16.19316500 1.27741300 -10.57915300
H 18.63641000 0.99397400 -10.48176200
H 20.10398300 2.93866500 -9.96843500
H 19.08565200 5.17528200 -9.59495900
C 16.46682900 5.81278300 -9.70847000
C 15.19736900 6.06010700 -10.06264400
O 14.61439000 4.90058900 -12.10571900
H 14.67155400 5.81042000 -12.43680700
H 14.77010300 7.05677300 -9.96382200
H 17.10023900 6.60755800 -9.31861100

INT6-(S, S)

C 3.25782500 1.77798600 0.14621600
C 2.60781200 2.18187000 -1.01836900
C 1.60242800 3.15619800 -0.97485800
C 1.23635600 3.72477900 0.26373000
C 1.89027800 3.31053000 1.42133200
C 2.90038600 2.34654100 1.36925200
H 4.04020100 1.02584000 0.09973700
H 2.88422800 1.74769100 -1.97646600
H 1.60770700 3.74888600 2.37579400
H 3.40513700 2.04137300 2.28164800
C 0.06563000 4.68215400 0.31410900
C 0.92536600 3.61260000 -2.18799300
H 1.09282600 3.04642300 -3.10244600
C 0.14573300 4.70459500 -2.19157400
C -0.00689500 5.55954800 -0.94905200
C -1.23574200 3.87079300 0.52839400
H -1.30214900 3.10433000 -0.25421100
H -1.15883400 3.33706600 1.48251400
C -2.49311600 4.74391700 0.49268500
H -3.38559800 4.11739700 0.61176600
H -2.47991700 5.44282600 1.34139400
C -2.56340500 5.53928500 -0.81419600
H -2.65988200 4.84354700 -1.65961400
H -3.45207600 6.18159600 -0.83123600
C -1.29930000 6.38838900 -0.98096800
H -1.23704400 7.12398900 -0.16962800

H -1.33008700 6.95592000 -1.92192700
H 0.19476500 5.36797800 1.16129000
H -0.34076800 5.03968500 -3.10618300
O 1.11923400 6.45906900 -0.84439100
H 1.27319300 6.82990200 -1.72780700

INT3-a

C -6.19453000 -0.33670100 -0.74135200
C -4.79898600 -0.39209600 -0.82736000
C -4.07341300 -1.27119000 0.00407700
C -4.79158800 -2.06273700 0.91158200
C -6.18420900 -1.99565400 1.00002700
C -6.89265100 -1.13003800 0.16802100
H -6.74516900 0.32259100 -1.40781100
H -4.25801900 -2.76539800 1.54705400
H -6.71262700 -2.62592700 1.71152900
H -7.97675600 -1.07834100 0.21864500
Ir -1.98478200 -1.36429600 -0.13696400
C -4.06859000 0.43595900 -1.85837000
C -4.21280200 -0.07955500 -3.28460400
C -4.34921300 1.96227300 -1.80133300
C -3.28775900 0.60754400 -4.28786500
C -3.83736700 2.71513400 -3.05258000
H -2.48906900 -0.10592300 -4.53111500
H -3.86014300 0.75753000 -5.21088200
C -2.72211800 1.93687700 -3.76449000
H -4.66238100 2.85069100 -3.76506400
H -3.49852200 3.71990600 -2.77650900
H -2.30652200 2.52139800 -4.59308400
H -1.89399800 1.75304500 -3.06607100
O -4.96212700 -0.97654900 -3.62552400
H -5.42155100 2.13748100 -1.67076100
H -3.86173600 2.34634000 -0.89767800
H -2.99297600 0.32037800 -1.65186700
C -1.03257800 1.36450100 0.86115200
C 0.32855100 0.70759700 0.56271200
C 0.18558500 -0.61619500 -0.17307200
C 0.15152900 -1.87703100 0.42889900

C 0.19353000 -2.15548000 1.91289100
 C -0.68283600 -1.18719500 2.73064700
 C -1.94932800 -0.80418600 1.97846900
 C -2.11777400 0.35890800 1.18252200
 H -2.86349900 -1.21232300 2.39902200
 H -0.96109100 -1.66892600 3.67431800
 H -0.11871100 -0.29154700 3.00660700
 H -0.16735200 -3.17900500 2.06511700
 H 1.23402300 -2.13511000 2.27282800
 H 0.42382800 -2.72405600 -0.19700400
 H 0.47332500 -0.58849000 -1.21642700
 H -3.12454100 0.76534300 1.12343600
 H -0.93669800 2.09940400 1.67616400
 H -1.35607600 1.92864900 -0.02253700
 H 0.92816100 1.38597800 -0.05452000
 H 0.89640100 0.56295700 1.48579200
 C -2.67739500 -2.72757600 -1.63684200
 C -1.53410700 -2.29743300 -1.98042300
 C -3.90426000 -3.47876900 -1.97564100
 C -3.77572800 -4.16107400 -3.34528000
 H -4.75348400 -2.79149300 -1.99299400
 H -4.11428100 -4.21071300 -1.18496500
 C -5.05514200 -4.90435100 -3.73693600
 H -3.55863300 -3.39120000 -4.09549300
 H -2.92272900 -4.85389600 -3.34261300
 C -4.94599000 -5.58646300 -5.10280800
 H -5.29447600 -5.65244200 -2.96774300
 H -5.88802200 -4.18925000 -3.74509200
 H -5.87442800 -6.10472600 -5.36824500
 H -4.73476600 -4.85317900 -5.89042800
 H -4.13532500 -6.32574900 -5.11225800
 C -0.39713200 -2.36685500 -2.87236200
 C 0.06486600 -1.21987400 -3.54144300
 C 0.24954200 -3.59282800 -3.10219200
 C 1.13514000 -1.30124300 -4.42899800
 H -0.43126300 -0.27142900 -3.36012700
 C 1.32677500 -3.66795500 -3.98339500

H -0.10710300 -4.47926700 -2.58705100
 C 1.77209400 -2.52463900 -4.65007700
 H 1.47457500 -0.40847700 -4.94651000
 H 1.81718000 -4.62241500 -4.15244300
 H 2.61020600 -2.58635300 -5.33804900

TS2-a

C -0.22601900 4.45757200 0.79924200
 C 0.37665800 3.41167200 0.09300600
 C -1.70548300 2.16831600 0.26252100
 C -2.28479400 3.20838100 0.98013200
 C -1.54431800 4.36556300 1.24214600
 H 0.34226600 5.36094100 1.00131300
 H -3.30983100 3.12292500 1.33098200
 H -1.99351100 5.19221300 1.78521700
 C 1.81265500 3.53489100 -0.36349000
 H 2.13598700 2.55139000 -0.72903900
 C 2.81533200 3.89401200 0.75979900
 H 2.69530200 3.17242700 1.57551400
 H 2.58460000 4.88407000 1.17415300
 C 4.25223500 3.87856300 0.22710300
 H 4.95515400 4.13496300 1.02892100
 H 4.50148900 2.85836000 -0.09931600
 C 4.41904100 4.84900700 -0.94888900
 H 5.44066200 4.80734300 -1.34432100
 H 4.26117800 5.87632200 -0.59274200
 C 3.41243400 4.55321900 -2.07887700
 H 3.64451200 3.57567800 -2.52776500
 H 3.45404700 5.30547400 -2.87147700
 C 1.98894200 4.48352300 -1.54839900
 C 1.19054100 0.32924600 1.62258800
 C 3.02344100 -1.25707100 0.84099000
 C 2.37343100 -1.05090800 -0.52438700
 C 1.16370400 -1.67567400 -0.92403000
 C 0.31459300 -2.57518900 -0.05066300
 C 0.06319300 -0.48890400 1.38630400
 H 0.99470100 1.32164100 2.02728100
 H 3.06319600 -0.78935100 -1.32285000

H 1.02409500 -1.83319000 -1.99344100
 H -0.90754900 -0.04809900 1.60413800
 C 2.60435400 -0.16732800 1.84995100
 C 0.09958400 -2.01078400 1.37256000
 H 2.77657200 -2.25203400 1.22439500
 H 4.11307400 -1.24275900 0.72530000
 H 2.73526100 -0.52649100 2.88287800
 H 3.27423200 0.69403000 1.73635500
 H 0.87897100 -2.37441900 2.04985300
 H -0.84593500 -2.39699600 1.76917600
 H -0.65905600 -2.68061200 -0.54326700
 H 0.74867100 -3.58629900 -0.00136100
 Ir 0.75704100 0.40046700 -0.51190400
 O 1.07649600 5.12198900 -2.04001600
 C -0.37221800 2.24330400 -0.19470400
 H -2.28150000 1.27329700 0.05066400
 C 0.80834400 1.03546300 -2.44648700
 C -0.15596000 1.84813700 -2.11901700
 C -1.11443700 2.78299200 -2.78209800
 C -2.51695000 2.19353900 -2.99333800
 H -0.66585100 3.00854900 -3.76102600
 H -1.17135100 3.72754200 -2.23531700
 C -3.44388700 3.16444900 -3.73093800
 H -2.43553600 1.25270900 -3.55495200
 H -2.95579000 1.94046000 -2.02188500
 C -4.84921700 2.59516800 -3.93964100
 H -3.50454500 4.10214800 -3.16196900
 H -3.00144700 3.42420900 -4.70270900
 H -5.49561000 3.30561200 -4.46701100
 H -4.81736000 1.67038600 -4.52873200
 H -5.32424800 2.35893000 -2.97961400
 C 1.44965400 0.67586700 -3.70523900
 C 2.84993000 0.58234100 -3.77890900
 C 0.69725100 0.43101500 -4.86684000
 C 3.48065900 0.27064300 -4.98152000
 H 3.43261800 0.77422300 -2.88303000
 C 1.32919400 0.10381400 -6.06532200

H -0.38593800 0.48839600 -4.81595100
 C 2.72212000 0.02592200 -6.12847200
 H 4.56491100 0.21295300 -5.02307500
 H 0.73285200 -0.08770800 -6.95325300
 H 3.21279700 -0.22611000 -7.06421000

INT4-a

C -0.03301800 0.19226800 1.15233600
 C 0.86177900 -0.64515100 1.83401200
 C 1.03909300 1.05694000 3.54271500
 C 0.14163600 1.87353000 2.85944600
 C -0.39212900 1.44391200 1.64555900
 H -0.46426600 -0.15118400 0.21432600
 H -0.12894600 2.84364100 3.26747600
 H -1.08777700 2.06867600 1.09280600
 C 1.10663200 -2.01288800 1.22208800
 H 0.35646000 -2.13687900 0.42532300
 C 0.86983500 -3.21541700 2.18531500
 H -0.10317700 -3.07277700 2.66614300
 H 1.62936000 -3.19054100 2.96860000
 C 0.93266700 -4.56021200 1.45537400
 H 0.77970900 -5.37501500 2.17265500
 H 0.11719800 -4.62664200 0.72071800
 C 2.27774900 -4.73187700 0.74331800
 H 2.31953100 -5.67890000 0.19408000
 H 3.08662300 -4.75348000 1.48545800
 C 2.52824400 -3.56281500 -0.23409100
 H 1.76691200 -3.59064500 -1.02629600
 H 3.51439500 -3.62397600 -0.70131700
 C 2.42053500 -2.24558800 0.49842000
 C 5.10342000 0.92603500 -0.23869800
 C 6.61978500 1.97956600 1.52727200
 C 5.62411800 1.35847500 2.50653300
 C 4.32988400 1.90571100 2.76675100
 C 3.73637800 3.11447900 2.06699700
 C 3.93679800 1.67927400 -0.03601000
 H 5.05111300 0.11205800 -0.96184100
 H 6.07905900 0.78550500 3.31285400

H	3.91933500	1.73379300	3.76110200
H	3.05128800	1.39580200	-0.60298400
C	6.51070700	1.36832800	0.11257200
C	3.93041800	3.09202100	0.53223800
H	6.47279300	3.06428700	1.48905100
H	7.63676800	1.82686500	1.90502200
H	6.90164000	2.07329200	-0.63790300
H	7.14904800	0.47872400	0.06410500
H	4.85941600	3.60233300	0.25767400
H	3.12231200	3.66409800	0.06291100
H	2.66334800	3.11572200	2.28521200
H	4.14422800	4.04675700	2.48918400
Ir	4.12729800	0.17404800	1.59328100
O	3.38796000	-1.48241000	0.47696900
C	1.43475700	-0.19748700	3.04854100
H	1.48780600	1.40982400	4.46488000
C	3.73829500	-0.93265300	3.28839800
C	2.48344600	-0.97286200	3.78980800
C	2.06522700	-1.68951000	5.06245000
C	1.80615300	-0.77323700	6.27198300
H	2.84576300	-2.40997300	5.33205200
H	1.14655200	-2.26754100	4.88512700
C	1.53491500	-1.56016800	7.55768100
H	2.67248600	-0.11473900	6.42194400
H	0.95151400	-0.11715800	6.06273500
C	1.24200200	-0.65825600	8.75928200
H	0.68737000	-2.24068300	7.39283000
H	2.40162300	-2.19919200	7.77670000
H	1.05744000	-1.24340800	9.66747300
H	2.08437000	0.01492700	8.96095100
H	0.35798400	-0.03473100	8.57736200
C	4.87542700	-1.62942700	3.92941300
C	5.56689900	-2.64030300	3.23611500
C	5.34036800	-1.27522900	5.20761600
C	6.65990900	-3.28729200	3.80769500
H	5.23842900	-2.90423000	2.23426900
C	6.44482900	-1.91258000	5.77606700

H	4.83126600	-0.48412000	5.74999900
C	7.10715200	-2.92522200	5.08191300
H	7.17205600	-4.07103600	3.25493300
H	6.78660600	-1.61649200	6.76474000
H	7.96558800	-3.42336500	5.52389700
TS3-a			
C	-5.66318700	-9.67549500	3.00501900
C	-4.52051900	-9.11072200	2.41549200
C	-3.32308000	-9.54336500	4.48321100
C	-4.45889000	-10.12821900	5.04507800
C	-5.63502300	-10.19002900	4.29891900
H	-6.57997700	-9.75026300	2.43065800
H	-4.42524900	-10.52303900	6.05629300
H	-6.52977300	-10.63986000	4.71999100
C	-2.39961300	-13.18013900	0.50153100
C	-3.89546100	-13.12722200	-1.55134900
C	-4.43534900	-11.86249100	-0.90766100
C	-5.11121300	-11.80426700	0.34937500
C	-5.44178600	-13.02600800	1.20585400
C	-2.95879700	-12.89456700	1.77299600
H	-1.31346400	-13.14922600	0.42473200
H	-4.69083500	-11.08264500	-1.62509900
H	-5.80069200	-10.97155200	0.47398000
H	-2.26126800	-12.65662300	2.57611000
C	-3.11521400	-14.01390900	-0.55581000
C	-4.33525700	-13.32090400	2.24401500
H	-4.70281500	-13.70257700	-2.03066200
H	-3.21764100	-12.81693000	-2.35672800
H	-3.79080200	-14.72535000	-0.07010100
H	-2.38204300	-14.61740900	-1.10231200
H	-4.34054400	-14.38656500	2.52116600
H	-4.54963700	-12.75682200	3.15828400
H	-6.38544800	-12.84908300	1.73386100
H	-5.61359000	-13.89715100	0.56439200
Ir	-3.10897400	-11.13218500	0.56650400
C	-3.33755700	-9.03073100	3.18633000
H	-2.40524400	-9.48123500	5.06226400

C -4.54693400 -8.60455900 1.01339900
 C -3.54406600 -8.99740900 0.16399800
 C -2.10668300 -8.35944200 2.62118600
 C -2.26153000 -6.82855500 2.53162600
 C -1.04844900 -6.17028100 1.87128100
 C -0.86311300 -6.70929400 0.45022100
 C -0.68412700 -8.23095500 0.44076500
 C -1.61836600 -9.02218000 1.33600500
 C -3.33959100 -8.47673500 -1.20214300
 C -2.72136300 -9.29313400 -2.17230100
 C -3.64483600 -7.15357000 -1.58626400
 C -2.47156000 -8.83545700 -3.46389900
 H -2.43629300 -10.30271400 -1.88890700
 C -3.39603300 -6.69241700 -2.87734400
 H -4.05953600 -6.46679000 -0.85897700
 C -2.81564800 -7.53272800 -3.82867800
 H -2.00085400 -9.49795300 -4.18532400
 H -3.64904400 -5.66777000 -3.13689500
 H -2.62043100 -7.17211300 -4.83459100
 H -1.27721600 -8.55714400 3.31902800
 H -3.16011200 -6.58918000 1.95440500
 H -2.42295600 -6.43873600 3.54329000
 H -0.14724900 -6.36920900 2.46983500
 H -1.17868500 -5.08154700 1.85014000
 H 0.00660300 -6.24622300 -0.03075500
 H -1.73368000 -6.43896800 -0.15424300
 H 0.31658800 -8.48426600 0.82510400
 H -0.73071000 -8.63776000 -0.57313600
 O -1.40444700 -10.29821200 1.39385000
 C -5.76864600 -7.80108600 0.60707200
 C -5.85449500 -6.36256200 1.16820900
 H -6.66484900 -8.33968500 0.94178600
 H -5.82456900 -7.76343800 -0.48303500
 C -6.06123000 -6.24881000 2.68250500
 H -4.95039600 -5.80421800 0.88983400
 H -6.68805500 -5.85772500 0.65997500
 C -6.19027800 -4.79305500 3.13734600

H -6.96027300 -6.81134400 2.96805300
 H -5.23077700 -6.72413000 3.21331200
 H -6.35033200 -4.72581800 4.21911400
 H -5.28195300 -4.22536100 2.89923400
 H -7.03157400 -4.29296600 2.64178100

INT5-a

C 5.72186100 0.54886500 0.07279900
 C 5.20766000 0.95291900 -1.15831600
 C 3.89085300 1.42797800 -1.27824100
 C 3.08710500 1.47249500 -0.11904800
 C 3.60762400 1.06040900 1.10717800
 C 4.92246000 0.60356900 1.21455200
 H 6.74704000 0.19540100 0.13779900
 H 5.85052900 0.91513500 -2.03063600
 H 2.97112100 1.10152200 1.98811500
 H 5.31665900 0.29415200 2.17835200
 C 1.64366600 1.86980100 -0.25705900
 C 3.35251200 1.93903100 -2.55738900
 C 2.22397700 2.69106300 -2.57353800
 C 1.45995700 3.00918000 -1.28145600
 C 0.81689200 0.61148300 -0.62335000
 H 1.22973200 0.17531100 -1.54204500
 H 0.95461200 -0.13525300 0.16752100
 C -0.66683300 0.92324300 -0.82600800
 H -1.20588800 0.01145500 -1.11239700
 H -1.10239300 1.26461400 0.12421600
 C -0.84347100 2.01287400 -1.88609800
 H -0.51105200 1.63296300 -2.85990500
 H -1.90235800 2.27568700 -1.99951400
 C -0.04415900 3.26299500 -1.51153100
 H -0.43090500 3.67435500 -0.57086200
 H -0.15592800 4.04400300 -2.26874200
 C 4.42208300 7.18235900 -1.13064000
 C 6.30298300 5.56783700 -1.66263900
 C 5.31960200 4.59608300 -1.01842300
 C 5.11226400 4.48156100 0.40463500
 C 5.81049200 5.33155900 1.44498200

C 4.47808600 7.12867800 0.29299200
 H 3.67984100 7.85327100 -1.56975300
 H 5.13880400 3.69315900 -1.58848700
 H 4.80822900 3.49846000 0.76272800
 H 3.74329100 7.73069000 0.82893100
 C 5.59669700 6.88322300 -2.04749100
 C 5.74947100 6.82703600 1.08115900
 H 7.14240700 5.75457700 -0.98519600
 H 6.72826300 5.10359100 -2.55863200
 H 6.30806800 7.72232900 -2.06462300
 H 5.20221500 6.78718100 -3.06579200
 H 6.63245500 7.12584900 0.50757000
 H 5.76589300 7.43191000 1.99405800
 H 5.29699800 5.16861200 2.39944200
 H 6.84781800 4.99030600 1.58661900
 Ir 3.45443900 5.39626600 -0.49724500
 O 1.95302800 4.22229500 -0.72640300
 H 1.27767800 2.25768000 0.70192900
 C 4.15558300 1.71407400 -3.82622000
 H 3.47418200 1.66895700 -4.67900800
 H 4.65945100 0.74114100 -3.78555800
 C 5.18914900 2.82101500 -4.10662400
 H 4.69078700 3.79472100 -4.02397300
 H 5.97181700 2.80782300 -3.33730200
 C 5.83769500 2.70201800 -5.48735000
 H 5.05299400 2.73871200 -6.25522000
 H 6.31959000 1.71887300 -5.58493000
 C 6.86374100 3.80853800 -5.74498300
 H 7.31337500 3.72042900 -6.74037300
 H 6.39639100 4.79854800 -5.67488600
 H 7.67525700 3.77303600 -5.00732800
 C 1.76205200 3.35253500 -3.82746500
 C 1.98793000 4.72304600 -4.03363400
 C 1.09740500 2.62922700 -4.82912700
 C 1.55723300 5.34800700 -5.20412900
 H 2.51342700 5.28856800 -3.27046400
 C 0.66824800 3.25288500 -6.00079400

H 0.92627800 1.56610500 -4.68599500
 C 0.89506300 4.61661500 -6.19159300
 H 1.74489100 6.40901100 -5.34658400
 H 0.15649400 2.67255700 -6.76373100
 H 0.56146000 5.10432000 -7.10323500

TS4-a

C 3.93412900 -3.50509700 4.84149700
 C 2.71665400 -4.20381600 4.90599400
 C 1.68036700 -3.69341600 4.13582800
 C 1.84394500 -2.56832300 3.33471400
 C 3.03518100 -1.86284800 3.26149300
 C 4.08910800 -2.36143900 4.04336400
 H 4.77999300 -3.85429200 5.42804900
 H 2.61258100 -5.08427700 5.53477100
 H 3.16306900 -0.97295400 2.65196900
 H 5.04776600 -1.84994600 4.03560100
 C 0.40935500 -2.61056300 2.80743000
 C 0.27946600 -2.83855700 1.27972500
 H -0.31184000 -2.01549500 0.86411800
 H 1.27929200 -2.76648900 0.83529600
 C -0.22385400 -5.20886400 3.15675900
 H -1.31852200 -5.29029100 3.19703300
 H 0.17177000 -6.03268800 3.76483600
 C -0.33951900 -4.18341400 0.87043100
 C 0.21966500 -5.34638500 1.69651600
 C 0.20905400 -3.87497900 3.77404400
 H 1.31689400 -5.35312300 1.63486600
 H -0.12889000 -6.30445900 1.29296900
 H -1.42940300 -4.14868300 0.99985800
 H -0.15992100 -4.34532500 -0.19913900
 O -0.33124700 -1.48565300 3.25443300
 H -0.45595200 -3.59376900 4.59831000
 H -0.11886800 -0.46801500 2.69835400
 C -4.00691700 0.43377700 3.05113600
 C -4.76570700 -1.44357700 4.58309900
 C -3.44900300 -2.05557300 4.11042200
 C -3.28885500 -2.66944600 2.83041700

C -4.35822900 -2.74640000 1.75743800
 C -4.07277700 -0.22200000 1.79263500
 H -3.66860900 1.46167100 3.04164600
 H -2.79569000 -2.41378400 4.90628400
 H -2.54908600 -3.46625200 2.76758000
 H -3.77638700 0.36737000 0.92604300
 C -4.81791700 0.06661500 4.27692600
 C -5.02667500 -1.37871600 1.50199100
 H -5.60547000 -1.96329900 4.10941200
 H -4.87703600 -1.60623900 5.66043100
 H -5.85727300 0.41271700 4.17276600
 H -4.39053000 0.61850900 5.12176400
 H -5.92889300 -1.27322600 2.11392700
 H -5.35950500 -1.32266800 0.46006400
 H -3.86745700 -3.08266300 0.83603200
 H -5.11145800 -3.50961500 2.00542500
 Ir -2.30544300 -0.81158800 2.83164300
 C -0.96150900 2.70784000 1.17026000
 C -0.16309800 1.79000200 2.11997400
 C -1.03304500 2.10330300 -0.23895700
 H -1.58869700 1.15903700 -0.19597900
 H -1.57894800 2.77540500 -0.90965300
 C 0.37010200 1.86423800 -0.81050300
 H 0.29689300 1.38891000 -1.79650600
 H 0.86016000 2.83683500 -0.96655600
 C 1.22811600 1.01457600 0.13102400
 H 0.81868900 -0.00027600 0.18084900
 H 2.25105800 0.92971900 -0.25650300
 C 1.25818500 1.60881100 1.54172000
 H 1.76415500 2.58335700 1.53357700
 H 1.83476000 0.96772500 2.21549500
 H -0.35107700 3.62502800 1.10267900
 C -3.42832300 3.33518700 0.99579800
 C -4.61032800 3.82267700 1.55888100
 C -4.64409700 4.14487300 2.91265000
 C -3.50719100 3.95501700 3.69654100
 C -2.32000400 3.43875800 3.15094700

C -2.28103200 3.14591500 1.76587800
 H -3.41140700 3.09791400 -0.06176200
 H -5.49275700 3.95168900 0.93869800
 H -5.55233100 4.53364300 3.36436800
 H -3.56006000 4.18727300 4.75341300
 C -1.14796200 3.14089600 3.99909400
 C -0.13068500 2.38171300 3.53010400
 O -0.73426000 0.47806800 2.16471100
 C 1.02764500 2.00786400 4.39405600
 C 1.11420200 0.74296700 4.99365800
 C 2.08515900 2.91213500 4.58071600
 C 2.23522900 0.38810100 5.74593100
 H 0.31857900 0.02237300 4.84970700
 C 3.19953300 2.56185500 5.34240400
 H 2.02602700 3.89395000 4.11847400
 C 3.28022900 1.29462300 5.92400700
 H 2.29352000 -0.60596900 6.17921400
 H 4.00746400 3.27641800 5.47613800
 H 4.15265400 1.01601500 6.50864100
 C -1.18703800 3.55948600 5.45415800
 H -0.16839500 3.69393100 5.82735200
 H -1.68705000 4.52908200 5.56342800
 C -1.89209400 2.50403300 6.32740200
 H -1.32307900 1.56828700 6.26422100
 H -2.88513300 2.28405600 5.91361600
 C -2.02778400 2.92422900 7.79235100
 H -2.60091400 3.86058500 7.85281100
 H -1.03128100 3.14849200 8.19749700
 C -2.70288800 1.85078700 8.64988800
 H -2.12875500 0.91648100 8.63061100
 H -2.79465900 2.16663400 9.69527700
 H -3.71047700 1.62665800 8.27783600

INT6-a

C 3.17860200 1.72777900 0.07543400
 C 2.50692400 2.11361400 -1.08291800
 C 1.51820900 3.11106500 -1.05401100
 C 1.20990200 3.71006400 0.18447800

C 1.88539200 3.31813800 1.33799700
 C 2.87214400 2.33300300 1.29311300
 H 3.94296200 0.95753400 0.02285800
 H 2.76677600 1.63349700 -2.01945300
 H 1.63333700 3.79401400 2.28300700
 H 3.39568000 2.04267100 2.19967100
 C 0.07265100 4.69394300 0.25373000
 C 0.81868600 3.56624200 -2.27613800
 C 0.08606500 4.70634300 -2.26568200
 C 0.00291200 5.57557900 -1.00157400
 C -1.24774300 3.92092400 0.48962500
 H -1.37435700 3.18903200 -0.31851100
 H -1.14929600 3.34734200 1.41817600
 C -2.46677200 4.84321100 0.54671800
 H -3.38084800 4.25086200 0.67729600
 H -2.38677700 5.50055000 1.42455200
 C -2.55516700 5.69819900 -0.71974300
 H -2.75624300 5.05567000 -1.58523900
 H -3.39161500 6.40444500 -0.65425800
 C -1.24956500 6.46813300 -0.93829200
 H -1.09257200 7.16141600 -0.10189200
 H -1.31348700 7.07464700 -1.84924000
 H 0.23327100 5.37456200 1.09940500
 O 1.16893300 6.42763600 -0.94066000
 H 1.04708500 7.11698200 -1.61260700
 C -0.53814000 5.23927700 -3.50936200
 C -1.70959700 4.68132100 -4.04161200
 C 0.03558400 6.33466700 -4.17421900
 C -2.29370700 5.20432500 -5.19511400
 H -2.15894500 3.82751400 -3.54315100
 C -0.54848300 6.86297900 -5.32501500
 H 0.96653200 6.75248000 -3.80038100
 C -1.71841300 6.30106900 -5.83781300
 H -3.19989700 4.75425800 -5.59125900
 H -0.08384200 7.70751000 -5.82655700
 H -2.17386000 6.71003000 -6.73514300
 C 0.96544200 2.73212300 -3.52958000

H 0.64880300 3.31104600 -4.40026700
 H 2.02202200 2.48826100 -3.69773000
 C 0.14978500 1.42933200 -3.47170900
 H -0.91271000 1.68418500 -3.35645200
 H 0.42472000 0.85922000 -2.57493100
 C 0.33324400 0.55478600 -4.71456000
 H 1.39696300 0.29986700 -4.82342300
 H 0.06611400 1.13591600 -5.60827000
 C -0.49976600 -0.72798300 -4.66604700
 H -0.34977600 -1.33925400 -5.56295200
 H -0.23193800 -1.33881500 -3.79539700
 H -1.56995100 -0.49952100 -4.59189800

INT3-b

C 2.24639700 2.09034400 -1.55413400
 C 1.39676400 1.23795900 -0.83948700
 C -0.20601800 3.02867000 -0.66673500
 C 0.64884500 3.87964100 -1.36883100
 C 1.87896900 3.40700500 -1.82602300
 H 3.20506000 1.71699500 -1.90864900
 H 0.34598300 4.90355400 -1.57399500
 H 2.54482000 4.05496200 -2.38969300
 C 1.84509300 -0.16889300 -0.50758600
 H 1.05081100 -0.59807300 0.13148000
 C 3.15375800 -0.24559100 0.31173400
 H 3.10616000 0.50083000 1.11039400
 H 3.99390400 0.05028900 -0.32819600
 C 3.40102900 -1.65756300 0.89943700
 H 4.47668900 -1.87021400 0.89173200
 H 3.09049600 -1.68688600 1.95050900
 C 2.65212800 -2.76117400 0.12455900
 H 1.62150300 -2.84004100 0.49560900
 H 3.11772000 -3.73636400 0.30559800
 C 2.61191800 -2.45897800 -1.37646700
 H 2.11331300 -3.24532500 -1.95329200
 H 3.63646800 -2.38511900 -1.77221500
 C 1.91687300 -1.13362700 -1.68059200
 C -2.90089500 -0.61852200 1.59843900

C -2.56074800 1.38052400 3.14635500
 C -1.34780000 1.65864200 2.27257100
 C -0.11009200 0.97473800 2.33839500
 C 0.16383700 -0.23551600 3.21028500
 C -1.75194300 -1.34487700 1.92805900
 H -3.53463000 -1.02216300 0.81133600
 H -1.30576200 2.66281600 1.85591600
 H 0.77992800 1.53521600 2.06277200
 H -1.58109700 -2.26813400 1.38411400
 C -3.56557300 0.43498000 2.45412300
 C -1.00566600 -1.24210300 3.25313100
 H -2.24712600 0.97194300 4.11141600
 H -3.06263400 2.32820800 3.37054900
 H -4.22458600 -0.03371600 3.20162800
 H -4.21357500 1.02614600 1.79677700
 H -1.70440200 -0.98164800 4.05294900
 H -0.61278000 -2.23200300 3.51079800
 H 1.04812500 -0.73886100 2.80151000
 H 0.43414700 0.07910600 4.23064800
 Ir -1.14183500 0.34577300 0.53490400
 O 1.43906700 -0.91930400 -2.78182900
 C 0.13549400 1.69509500 -0.40030200
 H -1.18147700 3.40026600 -0.36365100
 C -1.54782100 -0.99549000 -1.06222200
 C -1.67170400 0.13875100 -1.59639300
 C -1.78835100 1.15970500 -2.60374800
 C -2.86994400 2.05507000 -2.56593300
 C -0.80375200 1.29494500 -3.59641800
 C -2.97451500 3.06484500 -3.51796200
 H -3.61151700 1.95276900 -1.77947000
 C -0.91015400 2.31812200 -4.53444100
 H 0.04632900 0.62340000 -3.58471700
 C -1.99160700 3.20149200 -4.50152400
 H -3.81493000 3.75269000 -3.48668900
 H -0.13825700 2.43168600 -5.29036900
 H -2.06590300 3.99874700 -5.23609300
 C -1.60133300 -2.47001200 -1.19239500

H -0.79485000 -2.92206000 -0.59938600
 H -2.54055300 -2.85461400 -0.77032000
 C -1.46167000 -2.90451500 -2.66062200
 H -0.55004000 -2.45553400 -3.07170000
 H -2.30077000 -2.49306700 -3.23635200
 C -1.41320700 -4.42660000 -2.81671300
 H -0.57453300 -4.82294900 -2.22582400
 H -2.32404400 -4.87111100 -2.39071700
 C -1.26053200 -4.86217500 -4.27620200
 H -1.22024400 -5.95342700 -4.36740100
 H -2.10149300 -4.50555500 -4.88291600
 H -0.34171700 -4.45277000 -4.71243800

TS2-b

C -0.89070100 3.82797800 1.27875500
 C -0.01731300 3.12071200 0.45042800
 C -1.73505700 1.41218200 0.19341200
 C -2.58659200 2.12089600 1.04419300
 C -2.16001400 3.33110600 1.58961200
 H -0.58602700 4.79185900 1.67211700
 H -3.58125600 1.73981200 1.25991100
 H -2.82095400 3.90528600 2.23281800
 C 1.31631500 3.71259800 0.06565700
 H 1.85992600 2.96920200 -0.52845100
 C 2.24961300 4.10532500 1.25050800
 H 2.35668000 3.25764700 1.93192200
 H 1.78644800 4.91810200 1.82485300
 C 3.62523500 4.54836600 0.73258100
 H 4.27408600 4.81574400 1.57547500
 H 4.10156800 3.69728300 0.22487800
 C 3.51782800 5.72993400 -0.24174300
 H 4.50115400 5.97993800 -0.65714800
 H 3.16594700 6.61733900 0.30120700
 C 2.52290600 5.42878500 -1.38525400
 H 2.91344200 4.61562700 -2.00903900
 H 2.35407900 6.30639200 -2.01451400
 C 1.20524300 5.00745900 -0.75772000
 C 1.88952700 0.47508500 1.42849500

C 3.67590900 -0.96672600 0.32289000
 C 2.66721600 -1.03239300 -0.81853700
 C 1.50561400 -1.85034500 -0.80220600
 C 1.06178700 -2.71709800 0.35927400
 C 0.87129900 -0.49083400 1.57290500
 H 1.64849900 1.47331900 1.78020600
 H 3.07278100 -0.78510800 -1.79854600
 H 1.13861700 -2.19636400 -1.76689300
 H -0.07329100 -0.14498900 1.98705900
 C 3.36915400 0.17608500 1.31878000
 C 1.13627800 -1.98488500 1.71479800
 H 3.70313600 -1.92855100 0.84522600
 H 4.67911800 -0.82240100 -0.09327000
 H 3.80310700 -0.05721100 2.30399700
 H 3.86559100 1.09132500 0.97371600
 H 2.11281700 -2.14507700 2.18330100
 H 0.40014900 -2.41889200 2.40050000
 H 0.02116700 -3.00355500 0.16683500
 H 1.64142500 -3.65320200 0.39174500
 Ir 0.91276400 0.20320900 -0.51993000
 O 0.22275100 5.72167100 -0.76352700
 C -0.43206300 1.86940600 -0.07516800
 H -2.07318100 0.48914900 -0.26776500
 C 0.39432500 0.49126300 -2.45286700
 C -0.04033800 1.65241100 -2.06055800
 C -0.36849700 2.95454700 -2.63327000
 C 0.52899900 3.49366100 -3.57313100
 C -1.54745100 3.65395500 -2.33717800
 C 0.25006700 4.70503100 -4.20283700
 H 1.44754600 2.95640400 -3.78979100
 C -1.82180400 4.86072200 -2.97144600
 H -2.23160800 3.25357100 -1.59848300
 C -0.92535300 5.39318600 -3.90053100
 H 0.95667400 5.11555100 -4.91880900
 H -2.73207800 5.39935700 -2.72576500
 H -1.13789800 6.34502500 -4.37846500
 C 0.49244500 -0.22271500 -3.75715400

H 0.48303200 0.49447200 -4.59007400
 H 1.44377700 -0.76886000 -3.81084000
 C -0.66883500 -1.21871400 -3.93206100
 H -1.61619300 -0.66437100 -3.90161800
 H -0.68648900 -1.90130800 -3.07250100
 C -0.57703300 -2.01983200 -5.23334100
 H -0.56061500 -1.32707500 -6.08618200
 H 0.38021800 -2.55960900 -5.25846200
 C -1.73064400 -3.01248900 -5.39842600
 H -2.69752500 -2.49490800 -5.40505200
 H -1.64548800 -3.57501500 -6.33488000
 H -1.74808600 -3.73516400 -4.57355700

INT4-b

C 0.04397800 0.38055600 1.14009200
 C 0.90218200 -0.54053500 1.75490000
 C 1.15733900 1.01115400 3.58745400
 C 0.28297200 1.90933400 2.98033900
 C -0.26980400 1.59876600 1.73822700
 H -0.39676100 0.12899100 0.17774200
 H 0.04813000 2.85224200 3.46669800
 H -0.94204800 2.29272000 1.24192300
 C 1.07948200 -1.88905700 1.09411400
 H 0.58029700 -1.84064600 0.11007900
 C 0.33920000 -3.00587100 1.88417200
 H -0.71498100 -2.71673900 1.94794900
 H 0.72226100 -3.02757700 2.90622700
 C 0.48726600 -4.39194600 1.25322100
 H -0.00908100 -5.13548700 1.88749900
 H -0.01693100 -4.42025200 0.27600700
 C 1.96454200 -4.74822700 1.07458100
 H 2.08340200 -5.74339500 0.63177500
 H 2.45497500 -4.77174800 2.05608900
 C 2.66133600 -3.70779800 0.18096100
 H 2.21103200 -3.74535000 -0.82308500
 H 3.73179400 -3.90021900 0.06913400
 C 2.48852800 -2.30007700 0.70562700
 C 5.11092500 0.88924400 -0.24788500

C 6.56830000 2.13386800 1.44022300
 C 5.60488400 1.53109600 2.46348200
 C 4.28428000 2.03244500 2.68915700
 C 3.63052900 3.15489500 1.90573000
 C 3.91160000 1.59810300 -0.10005300
 H 5.09910800 0.02286700 -0.90907800
 H 6.09510300 1.05975100 3.31330500
 H 3.88381300 1.92077600 3.69558000
 H 3.03962600 1.23275000 -0.63992900
 C 6.49390000 1.42234800 0.07111100
 C 3.83384200 3.04186500 0.37669500
 H 6.36431200 3.20403500 1.32781600
 H 7.59205300 2.06268000 1.82440800
 H 6.85084000 2.09336600 -0.72586500
 H 7.17629000 0.56464600 0.08174400
 H 4.73763700 3.57824700 0.07017300
 H 3.00039800 3.54134000 -0.12965800
 H 2.55806200 3.10895800 2.12007900
 H 3.98219100 4.13513900 2.26541300
 Ir 4.16838100 0.21340700 1.64572700
 O 3.46935100 -1.55148100 0.68539100
 C 1.49504800 -0.21749800 2.99533900
 H 1.62599800 1.26836600 4.53248700
 C 3.81199000 -0.86965700 3.35027000
 C 2.51252000 -1.08627700 3.68973900
 C 2.01713200 -1.99358100 4.76310700
 C 2.49312700 -3.31499100 4.87205600
 C 1.01055700 -1.59722200 5.66227900
 C 2.02130700 -4.18212700 5.85490900
 H 3.22444700 -3.66943700 4.15328300
 C 0.53357600 -2.46372100 6.64538600
 H 0.59374700 -0.59873000 5.58561300
 C 1.04012700 -3.75939100 6.75405800
 H 2.41046700 -5.19570600 5.90854700
 H -0.23986600 -2.12321000 7.32907500
 H 0.66701900 -4.43434300 7.51912600
 C 4.97724700 -1.40938900 4.16152800

C 5.12903200 -0.63311200 5.48344900
 H 5.90387800 -1.31513700 3.58345900
 H 4.87388400 -2.47259200 4.40310000
 C 6.34972800 -1.06714500 6.29811400
 H 5.19414800 0.44248300 5.26972100
 H 4.21718700 -0.77201500 6.07809100
 C 6.48677700 -0.30166400 7.61695600
 H 6.28154600 -2.14492500 6.50277700
 H 7.25746200 -0.92727000 5.69392700
 H 7.36652400 -0.62695100 8.18425900
 H 6.58403500 0.77628200 7.43745000
 H 5.60457400 -0.45209300 8.25114200

TS3-b

C -6.38833600 -8.13413100 2.56994200
 C -5.10132100 -7.78263000 2.13729600
 C -4.40477000 -7.63492800 4.45145900
 C -5.67601100 -8.03058000 4.87319900
 C -6.67223700 -8.27450800 3.92670300
 H -7.15892900 -8.32473400 1.82950500
 H -5.88873700 -8.13426600 5.93333200
 H -7.66826300 -8.57118900 4.24323400
 C -2.84128900 -12.28749000 1.72387600
 C -3.80397100 -12.74802500 -0.58645300
 C -4.40981600 -11.36650200 -0.40974500
 C -5.36496300 -11.01631500 0.59509800
 C -5.94631200 -12.01041200 1.59958200
 C -3.67703400 -11.71086600 2.71592300
 H -1.76925300 -12.26470300 1.91559300
 H -4.44485800 -10.79127800 -1.33584200
 H -6.02516900 -10.18127400 0.36645000
 H -3.18073100 -11.27984400 3.58559900
 C -3.31301500 -13.35844300 0.74566000
 C -5.14819400 -12.01253800 2.92200800
 H -4.51118800 -13.42951600 -1.08450600
 H -2.94795600 -12.64229100 -1.26427900
 H -4.10543700 -13.95721900 1.20600200
 H -2.48976800 -14.05263100 0.54393800

H -5.28404500 -12.96589000 3.45583400
 H -5.54467400 -11.22503000 3.57275200
 H -6.98730000 -11.74188200 1.81118400
 H -5.97610000 -13.01412800 1.16296800
 Ir -3.44447300 -10.29154200 1.13132400
 C -4.10818800 -7.50157900 3.09599500
 H -3.63098900 -7.42477800 5.18560700
 C -4.79621000 -7.71383000 0.68327200
 C -3.68728100 -8.33242800 0.17078500
 C -2.75343900 -7.03075900 2.62461400
 C -2.80573500 -5.59291200 2.06478600
 H -3.12256600 -4.92038200 2.87040100
 H -3.57418200 -5.54105000 1.28757800
 C -1.47144000 -5.14320700 1.46400800
 H -1.56534100 -4.12304200 1.07294400
 H -0.70046800 -5.11268700 2.24756700
 C -1.03436900 -6.10508300 0.35412300
 H -0.07668600 -5.79000300 -0.07678200
 H -1.77028900 -6.08085100 -0.45755300
 C -0.90099600 -7.52673700 0.90303900
 H -0.08321500 -7.54139300 1.64273400
 H -0.62716500 -8.25820200 0.14446700
 C -2.09301600 -8.04051200 1.68968000
 O -1.98490000 -9.25686300 2.14198300
 H -2.07708900 -7.02247500 3.49405900
 C -5.82792400 -7.00944300 -0.13612200
 C -6.50808000 -7.66347200 -1.17552000
 C -6.19405300 -5.68910800 0.17138400
 C -7.49885000 -7.00767500 -1.90504800
 H -6.27741900 -8.70106200 -1.39440400
 C -7.16967100 -5.02540200 -0.57006200
 H -5.71219400 -5.18555400 1.00356300
 C -7.82464700 -5.68214100 -1.61365400
 H -8.01975200 -7.53546300 -2.69911100
 H -7.42732400 -3.99881900 -0.32465900
 H -8.59179500 -5.16916600 -2.18665700
 C -3.35629200 -8.20979400 -1.31128900

C -2.14242100 -9.00440600 -1.82629100
 H -3.26291300 -7.15187900 -1.59546000
 H -4.22594900 -8.56859900 -1.87178500
 C -2.30362400 -9.43921400 -3.28590500
 H -1.22581900 -8.41012500 -1.74156300
 H -2.00128400 -9.89397400 -1.19755300
 C -1.09198200 -10.21261500 -3.80997800
 H -3.20451500 -10.06289600 -3.37555600
 H -2.48117600 -8.55491500 -3.91473800
 H -1.22916700 -10.52126500 -4.85244800
 H -0.18173500 -9.60253000 -3.75832400
 H -0.91761400 -11.11603900 -3.21237500

INT5-b

C 3.62131900 3.40075900 0.98392900
 C 3.18257100 3.88326500 -0.24794100
 C 1.84943300 4.28593600 -0.43451900
 C 0.95534000 4.18407700 0.64970500
 C 1.40314600 3.70014700 1.87823600
 C 2.73227900 3.31047400 2.05570100
 H 4.65910600 3.10378600 1.10646400
 H 3.88478800 3.96853300 -1.06983100
 H 0.69962900 3.63174800 2.70482900
 H 3.06883600 2.94224700 3.02075200
 C -0.48972600 4.52035400 0.41551200
 C 1.38776100 4.89205100 -1.70447700
 C 0.21821000 5.57702800 -1.78106000
 C -0.64507400 5.73724800 -0.52388000
 C -1.21102900 3.26203100 -0.12976100
 H -0.69855900 2.93490700 -1.04356800
 H -1.09786400 2.45259100 0.60092200
 C -2.68788100 3.51827200 -0.43429400
 H -3.14760900 2.61602100 -0.85647100
 H -3.22190800 3.74007300 0.50080900
 C -2.83636400 4.70175100 -1.39386600
 H -2.39434400 4.43646200 -2.36382500
 H -3.89513400 4.92030700 -1.57951400
 C -2.14422100 5.94271100 -0.82156100

H -2.61221900 6.21140500 0.13353100
 H -2.27038600 6.80837800 -1.47793600
 C 2.11874200 9.99400800 0.03207100
 C 4.08309700 8.51867200 -0.59648300
 C 3.13975700 7.45117100 -0.04868000
 C 2.91364500 7.21393100 1.35723000
 C 3.55762600 8.00750600 2.47460500
 C 2.15857400 9.82565200 1.44725500
 H 1.35092200 10.66103000 -0.36651400
 H 3.02587200 6.58561700 -0.69200200
 H 2.65271500 6.19233200 1.63054900
 H 1.38631000 10.34210900 2.01880000
 C 3.32509500 9.83241000 -0.87816300
 C 3.43398900 9.52271800 2.22791500
 H 4.90826200 8.68302100 0.10397800
 H 4.53861900 8.14759500 -1.52100400
 H 3.99793900 10.69925900 -0.79831000
 H 2.95746600 9.82035400 -1.91149500
 H 4.30796300 9.90244100 1.68906300
 H 3.41442000 10.05593100 3.18432900
 H 3.03773600 7.74643500 3.40350200
 H 4.60701000 7.70170900 2.60777400
 Ir 1.22984900 8.11972300 0.50032800
 O -0.23016800 6.91120000 0.16446300
 H -0.95793100 4.80550500 1.36602600
 C 2.31260000 4.77856100 -2.87228200
 C 2.56284300 3.52402500 -3.44763500
 C 2.96770700 5.89896200 -3.40385000
 C 3.42872100 3.39470400 -4.53277000
 H 2.06944600 2.64823000 -3.03545900
 C 3.83701400 5.77212100 -4.48800300
 H 2.78821500 6.87484800 -2.96548100
 C 4.06958700 4.51950300 -5.05705500
 H 3.60310600 2.41534500 -4.96992400
 H 4.33242900 6.65330100 -4.88666200
 H 4.74533000 4.41928400 -5.90171300
 C -0.19561400 6.30624000 -3.03673400

C -0.01075700 7.83655600 -2.95871500
 H -1.24602300 6.09786900 -3.27222700
 H 0.38609900 5.92868200 -3.88180400
 C -0.16989500 8.52234500 -4.31694300
 H -0.72213200 8.26163400 -2.24101300
 H 0.98162000 8.06018200 -2.54843300
 C 0.03609000 10.03693800 -4.23014900
 H 0.55218400 8.09049800 -5.02423600
 H -1.16687300 8.30563200 -4.72587900
 H -0.06729400 10.51807200 -5.20931700
 H -0.69420900 10.49529100 -3.55206300
 H 1.03599300 10.27365800 -3.84434400

TS4-b

C 0.24664200 1.34551700 -0.71831200
 C -0.77970500 0.45559900 -0.40675400
 C -1.19132300 0.26569900 0.92245300
 C -0.51781700 0.95905100 1.94779900
 C 0.47847600 1.87901800 1.62206200
 C 0.86095600 2.08425100 0.29383700
 H 0.55014800 1.47683400 -1.75335700
 H -1.28362200 -0.08302500 -1.20060300
 H 0.98042500 2.41751000 2.42302500
 H 1.64314000 2.79991300 0.05643400
 C -0.74319900 0.52874300 3.37359100
 C -2.33830400 -0.59642700 1.26497600
 C -2.81794900 -0.70902100 2.52760400
 C -2.20235600 0.10486200 3.67099700
 C 0.29020700 -0.59735200 3.64749400
 H 0.14101900 -1.39596100 2.90883300
 H 1.29134000 -0.18974000 3.46755500
 C 0.17755700 -1.18078200 5.05282000
 H 0.91645000 -1.97989000 5.19121000
 H 0.40009300 -0.40484600 5.79938100
 C -1.23947000 -1.70736100 5.26198300
 H -1.41852100 -2.52981600 4.55753800
 H -1.36483200 -2.12205000 6.26991200
 C -2.26773700 -0.59468600 5.04146400

H -2.12209600 0.18872600 5.79634000
 H -3.27156200 -0.99143500 5.19109800
 H -0.52924500 1.36128200 4.05527700
 O -2.96909500 1.32574500 3.77162800
 C -3.06160400 -1.22698300 0.11856000
 C -4.03239300 -0.48772300 -0.57382900
 C -2.77461300 -2.53117900 -0.29929300
 C -4.70630600 -1.04853500 -1.65743600
 H -4.25382700 0.52381700 -0.25258900
 C -3.45271100 -3.09449400 -1.38264000
 H -2.01265200 -3.10071600 0.22567900
 C -4.41998500 -2.35420900 -2.06403700
 H -5.45105900 -0.45882800 -2.18450500
 H -3.22247400 -4.10956100 -1.69507300
 H -4.94568500 -2.79141200 -2.90860800
 C -4.12081000 -1.43316200 2.79183400
 C -4.00020600 -2.92984600 3.12369300
 H -4.76442400 -1.33495700 1.91249500
 H -4.65813500 -0.92678500 3.60388900
 C -5.37053300 -3.58351300 3.32435900
 H -3.46853600 -3.43551000 2.30773900
 H -3.39580800 -3.07524700 4.02683300
 C -5.27820000 -5.07655300 3.64753400
 H -5.90321400 -3.06311500 4.13392400
 H -5.97378300 -3.43665800 2.41799400
 H -6.27009000 -5.52067900 3.78907200
 H -4.77939000 -5.62291700 2.83781600
 H -4.70121800 -5.24650100 4.56497400
 C -4.17258400 2.75596900 -2.63993800
 C -5.35596800 2.95598500 -1.90638100
 C -5.19569900 3.16628600 -0.54379300
 C -3.93883900 3.17553800 0.05380100
 C -2.76079800 3.00863800 -0.65316700
 C -2.90902900 2.78896800 -2.03196800
 H -4.23542400 2.57340900 -3.70958700
 H -6.32541500 2.94140200 -2.39781300
 H -1.78178800 3.02598800 -0.18896900

H -2.02403300 2.63077700 -2.64177200
 C -4.50138100 3.35525700 1.45832600
 C -3.99522100 4.53175900 2.28591200
 H -4.33763900 4.39521300 3.32000000
 H -2.89822600 4.50104100 2.30964800
 C -6.63845500 4.86809200 0.77188500
 H -7.70749100 4.73927600 0.97827800
 H -6.57077600 5.29655200 -0.23512800
 C -4.50895400 5.87235300 1.75277100
 C -6.04154500 5.88493400 1.76100400
 C -5.93748600 3.48310800 0.75487500
 H -6.42102200 6.88347700 1.51221700
 H -6.38511700 5.67196700 2.78246200
 H -4.11924100 6.68884000 2.37188200
 H -4.13809100 6.04112900 0.73233400
 O -4.41054700 2.12294200 2.17050700
 H -6.60531700 2.68975900 1.10331300
 H -3.39872800 1.80025000 2.66563600
 C -5.49950500 0.55228400 5.88627000
 C -7.88183800 0.78883700 5.03777100
 C -7.18015900 1.62090800 3.96797600
 C -6.74615100 2.95927200 4.18904500
 C -6.84403400 3.70889700 5.50304000
 C -5.22158400 1.90090800 6.24836400
 H -4.70542500 -0.16466200 6.07198900
 H -7.42259400 1.34933900 2.94067800
 H -6.72198300 3.60887500 3.31764900
 H -4.22628300 2.10405000 6.64253000
 C -6.87849400 -0.07579400 5.82624200
 C -6.30718300 2.88180400 6.68907300
 H -8.43553500 1.44931200 5.71343300
 H -8.62988900 0.14459000 4.56396400
 H -7.25647000 -0.29044500 6.83733500
 H -6.77106500 -1.04480700 5.32441300
 H -7.12160400 2.33270700 7.17359000
 H -5.90044800 3.55483300 7.45117300
 H -6.24064400 4.61866100 5.39970200

H -7.87642500 4.03957700 5.69217600
Ir -5.05799300 1.68549500 4.13825500

INT6-b

C 3.35425800 1.87851200 0.15662900
C 2.61380000 2.17209500 -0.98657700
C 1.58687800 3.12898100 -0.95273900
C 1.29751900 3.77403700 0.26493800
C 2.04493300 3.47449200 1.40156900
C 3.07715200 2.53605700 1.35487800
H 4.14904200 1.13934200 0.10852300
H 2.83823100 1.66287400 -1.91730200
H 1.81217600 3.98210700 2.33511500
H 3.65636000 2.31874300 2.24799900
C 0.09137800 4.67169800 0.34080000
C 0.84484200 3.51452100 -2.16785100
C 0.03144700 4.59818500 -2.20541400
C -0.13480600 5.46940500 -0.95666400
C -1.13264500 3.80663400 0.72681600
H -1.25895200 3.01842900 -0.02739100
H -0.90993200 3.30043300 1.67274500
C -2.41872000 4.62508800 0.83324600
H -3.26227400 3.97301900 1.09130400
H -2.32269200 5.35969700 1.64558200
C -2.68134900 5.34948100 -0.48684100
H -2.87295100 4.60167500 -1.26535600
H -3.58096800 5.97366700 -0.42095100
C -1.47972600 6.22116400 -0.86939300
H -1.34100300 6.99391500 -0.10305700
H -1.67390800 6.75246000 -1.80815400
H 0.24435100 5.41941900 1.12957600
O 0.92642600 6.45521700 -0.96889900
H 0.89149100 6.90304100 -1.82937700
C 1.09968500 2.71690900 -3.40658100
C 2.18473600 3.02167900 -4.24018900
C 0.26235200 1.65031400 -3.75464300
C 2.41644800 2.28817200 -5.40346400
H 2.84343200 3.84225600 -3.96918500

C 0.49275500 0.91418600 -4.91764600
H -0.57146500 1.40014000 -3.10483200
C 1.56884900 1.23321300 -5.74650800
H 3.25880700 2.54008200 -6.04192200
H -0.16865900 0.09159400 -5.17546000
H 1.74775900 0.66184400 -6.65297200
C -0.52875400 5.09173600 -3.52655200
C -1.90433500 4.53310600 -3.93640300
H 0.17807800 4.83468000 -4.32154900
H -0.58714200 6.18903800 -3.52263700
C -2.25973500 4.87642600 -5.38536000
H -1.89556700 3.44349100 -3.81297700
H -2.68501300 4.91790200 -3.27113400
C -3.63246900 4.34278900 -5.80066300
H -2.23150300 5.96728100 -5.51898800
H -1.48681600 4.46533500 -6.04904800
H -3.86416300 4.59543800 -6.84136600
H -3.67471100 3.25110100 -5.70421300
H -4.42634400 4.76129300 -5.17001000

INT7

C -6.11118700 -0.38196500 -0.37289800
C -4.74247500 -0.36685400 -0.67200000
C -3.89703800 -1.35168600 -0.12723100
C -4.45309900 -2.30800600 0.73188600
C -5.81592600 -2.31226500 1.03206100
C -6.65340400 -1.34626600 0.47428300
H -6.75914000 0.36923700 -0.81771800
H -3.80706000 -3.05012400 1.19314900
H -6.21900700 -3.06458700 1.70535100
H -7.71722500 -1.34366600 0.69479600
Ir -1.88262900 -1.39097600 -0.71631500
C -4.18307700 0.72564700 -1.55316300
C -4.67703800 0.70396600 -2.98953600
C -4.26666200 2.13102400 -0.89933200
C -4.09540700 1.80002100 -3.88534100
C -4.00797800 3.29489800 -1.88303600
H -3.52765100 1.30310000 -4.68288100

H -4.94264000 2.29231300 -4.38076800
 C -3.24575700 2.82766500 -3.12879300
 H -4.96574300 3.72028900 -2.21247900
 H -3.46810600 4.10302200 -1.37716200
 H -3.01269800 3.67617600 -3.78229500
 H -2.28295600 2.38669400 -2.83591700
 O -5.41199900 -0.15277500 -3.44732300
 H -5.24696900 2.25074400 -0.42643400
 H -3.53003100 2.14529900 -0.08766200
 H -3.10690000 0.50918700 -1.67271600
 C -1.25695300 -4.22868100 -1.79205100
 C 0.00049900 -3.49010900 -2.28159200
 C 0.09662200 -2.10194800 -1.68090600
 C -0.35147300 -0.93335600 -2.30466300
 C -1.04120800 -0.87672100 -3.65124500
 C -2.14601200 -1.93645300 -3.82460800
 C -2.84130900 -2.27961000 -2.51342600
 C -2.43771300 -3.30343600 -1.61993100
 H -3.89236100 -2.01602900 -2.49120500
 H -2.90015300 -1.55407400 -4.51982800
 H -1.74302200 -2.84464600 -4.28486400
 H -1.48500900 0.12028500 -3.74515000
 H -0.29430800 -0.95390900 -4.45661600
 H 0.10037500 0.00637000 -2.00099500
 H 0.81133200 -2.00662000 -0.87168800
 H -3.22575100 -3.71885900 -0.99687800
 H -1.51210400 -5.05323000 -2.47560700
 H -1.04738200 -4.68531300 -0.81773100
 H 0.89292100 -4.06099600 -2.00257200
 H 0.00964100 -3.42493700 -3.37315900
 C -0.77532000 -0.11797900 0.51643600
 C -1.87673300 -0.36298400 1.12887900
 C -2.55552500 -0.19561500 2.40150400
 C -3.88428300 0.22975900 2.55353900
 C -1.78569600 -0.44115100 3.55650400
 C -4.42309000 0.40367200 3.82699500
 H -4.49194300 0.42390300 1.68129300

C -2.33301900 -0.27145100 4.82462200
 H -0.75692000 -0.76810300 3.44090100
 C -3.65704100 0.15151600 4.96543700
 H -5.45366600 0.73297500 3.92479500
 H -1.72552800 -0.47122000 5.70299400
 H -4.08660500 0.28211500 5.95469800
 C 0.39549600 0.73206100 0.65725900
 C 1.63068600 0.51391300 0.02452300
 C 0.27011700 1.85510000 1.50314000
 C 2.70054800 1.38541200 0.23142700
 H 1.77006600 -0.34367200 -0.61917700
 C 1.33696900 2.72332200 1.70240600
 H -0.67854600 2.02907800 2.00047400
 C 2.56032600 2.49327800 1.06560700
 H 3.64808200 1.19293900 -0.26397500
 H 1.21517800 3.58209500 2.35668700
 H 3.39476300 3.17090600 1.22130200

TSS

C -2.73446500 1.71140700 1.27309800
 C -1.89042200 1.01972200 0.39100500
 C -0.47040200 2.99470300 0.30573600
 C -1.31844700 3.66391900 1.17691900
 C -2.45443000 3.01407800 1.67461500
 H -3.61801500 1.21101300 1.65854500
 H -1.10116200 4.68811700 1.46736700
 H -3.12111200 3.52567300 2.36291300
 C -2.25854700 -0.37700900 -0.04512900
 H -1.54560400 -0.68928900 -0.81461500
 C -3.65871800 -0.47852100 -0.70012800
 H -3.71174300 0.25595000 -1.51210600
 H -4.43890700 -0.20803500 0.02360700
 C -3.91174700 -1.89328900 -1.23112900
 H -4.90749900 -1.95184300 -1.68708600
 H -3.18487800 -2.11337000 -2.02610000
 C -3.78460500 -2.93228200 -0.11105000
 H -3.93802900 -3.94513000 -0.50115800
 H -4.57236900 -2.75907000 0.63510300

C -2.41093600 -2.84810800 0.58303300
 H -1.62921100 -3.13717600 -0.13567000
 H -2.34230600 -3.51903400 1.44403700
 C -2.09431300 -1.43258700 1.04494400
 C 2.15342800 1.19501700 1.07830800
 C 3.94600900 -0.32046600 0.09897900
 C 2.82682300 -0.76063300 -0.83181000
 C 1.78604000 -1.64600900 -0.46507800
 C 1.60186100 -2.22850700 0.92323600
 C 1.30769700 0.20461700 1.61995700
 H 1.83709000 2.22894200 1.20829700
 H 3.06106400 -0.68146300 -1.89091800
 H 1.32743700 -2.23470800 -1.25861900
 H 0.39233700 0.54445500 2.09494800
 C 3.62788800 1.02480200 0.78719000
 C 1.75730300 -1.18560600 2.05103700
 H 4.13587000 -1.09718200 0.84557700
 H 4.87268100 -0.22053900 -0.47712800
 H 4.22687100 1.12955800 1.70536200
 H 3.93129000 1.84304500 0.12352800
 H 2.79236500 -1.15301300 2.40620500
 H 1.14614600 -1.49861500 2.90273000
 H 0.59009700 -2.64300300 0.97202300
 H 2.29093700 -3.07389800 1.07687700
 Ir 0.93925100 0.34256300 -0.55484800
 O -1.71295200 -1.18719900 2.17458900
 C -0.71267900 1.65639600 -0.06891400
 H 0.39532100 3.50505900 -0.10407200
 C 0.04439000 0.15393100 -2.36693500
 C -0.45413800 1.32066900 -2.01960600
 C -0.10246600 -0.70851100 -3.52421900
 C -1.31764100 -0.71499000 -4.23913200
 C 0.92154800 -1.57787600 -3.93788800
 C -1.49843500 -1.56504400 -5.32576400
 H -2.11333900 -0.04596100 -3.92606000
 C 0.74250100 -2.41633200 -5.03665400
 H 1.86198000 -1.58112900 -3.39899900

C -0.46817000 -2.41846000 -5.73187900
 H -2.44410900 -1.56003800 -5.86100700
 H 1.54920500 -3.07484900 -5.34688200
 H -0.60945200 -3.07965200 -6.58200200
 C -1.04637600 2.46500900 -2.71574000
 C -2.19913600 3.13841900 -2.28004200
 C -0.46506900 2.83852800 -3.94233800
 C -2.75425900 4.15493900 -3.05443600
 H -2.66401700 2.85460500 -1.34415200
 C -1.02350300 3.85687500 -4.71032900
 H 0.42583300 2.31828800 -4.27901800
 C -2.17033600 4.52042900 -4.26886200
 H -3.64954900 4.66255700 -2.70630500
 H -0.55879000 4.13592600 -5.65186600
 H -2.60446200 5.31721500 -4.86615900

INT8

C -1.98618100 2.00414200 1.30322200
 C -1.82658500 1.50000400 0.00726800
 C -0.11211000 3.17047500 -0.38087600
 C -0.29921700 3.68383700 0.89982200
 C -1.22921400 3.08687900 1.75175300
 H -2.71642900 1.56246300 1.97311600
 H 0.28569700 4.53530700 1.23659200
 H -1.37518100 3.46707200 2.75886100
 C -2.69171300 0.37997000 -0.53142400
 H -3.00986200 0.67018400 -1.54479200
 C -3.99693000 0.12772900 0.26898500
 H -4.51075100 1.08638000 0.39351000
 H -3.75075800 -0.23642500 1.27502500
 C -4.90602200 -0.88934300 -0.42620500
 H -5.82418900 -1.02789700 0.15637600
 H -5.20747800 -0.49843400 -1.40797500
 C -4.18758300 -2.22950100 -0.60410900
 H -4.81492200 -2.94475000 -1.14729500
 H -3.98374800 -2.66923900 0.38137400
 C -2.85490200 -2.04347700 -1.35403400
 H -3.06301800 -1.72631400 -2.38732800

H -2.27139100 -2.96667400 -1.39752800
 C -1.99785700 -0.95958100 -0.74289700
 C 1.27371000 -0.25473300 1.77627000
 C 3.07093300 1.48066900 1.19784200
 C 2.69742600 1.14766800 -0.24824500
 C 3.08683900 -0.05984400 -0.91522600
 C 3.87877800 -1.19499100 -0.29584900
 C 1.87650200 -1.40932900 1.25683200
 H 0.26587300 -0.34842700 2.18159700
 H 2.55914500 2.01826700 -0.88662400
 H 3.20019700 0.00107500 -1.99716800
 H 1.28774300 -2.32514900 1.25493100
 C 2.01772500 0.99118500 2.22086400
 C 3.38060600 -1.58393100 1.11420400
 H 4.05619400 1.06071300 1.42848400
 H 3.17619900 2.56672600 1.29634200
 H 2.48944400 0.83244600 3.20315700
 H 1.26870800 1.77697200 2.35610300
 H 3.89494600 -0.98970400 1.87622200
 H 3.64586800 -2.62806800 1.31514600
 H 3.77274800 -2.05965300 -0.96191700
 H 4.95274500 -0.95152600 -0.26976100
 Ir 1.05408600 -0.15391300 -0.40821100
 O -0.82542100 -1.22074900 -0.46309100
 C -0.84920900 2.06823800 -0.83762400
 H 0.62941700 3.60488000 -1.04421700
 C -0.57175900 1.48549600 -2.19584500
 C 0.42387800 0.55780200 -2.23451700
 C 0.95897700 -0.00928600 -3.48731700
 C 1.10464700 -1.40041700 -3.64099100
 C 1.39856500 0.82140600 -4.53339100
 C 1.63184200 -1.94113300 -4.81210900
 H 0.80030200 -2.04742600 -2.82289300
 C 1.94344300 0.28143900 -5.69687700
 H 1.30137700 1.89688500 -4.42147100
 C 2.05554800 -1.10267500 -5.84652200
 H 1.72345800 -3.01961000 -4.91400900

H 2.28021000 0.94326400 -6.49069100
 H 2.47841100 -1.52333800 -6.75466700
 C -1.47434900 1.90785100 -3.29487700
 C -2.07163300 3.18231300 -3.28080200
 C -1.84251100 1.02710100 -4.33276000
 C -2.96611500 3.57370000 -4.27650200
 H -1.82573100 3.87178800 -2.47919200
 C -2.73531400 1.41844300 -5.32608400
 H -1.41818200 0.02987500 -4.35501800
 C -3.30108500 2.69647100 -5.30824200
 H -3.40296500 4.56852900 -4.24355100
 H -2.99746300 0.71802700 -6.11494300
 H -3.99912300 2.99959200 -6.08358500

TS6

C 2.63565700 1.67610400 -0.55185600
 C 2.01746800 0.89179100 0.42003200
 C 0.76847500 2.84418400 1.14612800
 C 1.39186500 3.61786800 0.16890400
 C 2.32092200 3.03069800 -0.68901200
 H 3.37698700 1.23305500 -1.20809400
 H 1.15168000 4.67352000 0.07889000
 H 2.81256700 3.62472000 -1.45418200
 C 2.34165200 -0.56856300 0.63575100
 H 2.61733600 -0.70229000 1.69005600
 C 3.48672100 -1.15996100 -0.21730000
 H 4.39677300 -0.56482900 -0.07591300
 H 3.21370800 -1.09833900 -1.27757500
 C 3.73753000 -2.62457800 0.17663400
 H 4.52683700 -3.05018200 -0.45446000
 H 4.10981800 -2.65663300 1.21074400
 C 2.46490700 -3.47914500 0.07195900
 H 2.65829400 -4.49893700 0.42459900
 H 2.15296000 -3.55037500 -0.97719200
 C 1.30008200 -2.86700300 0.88948400
 H 1.54592200 -2.87086500 1.95492900
 H 0.37441000 -3.42951500 0.74710900
 C 1.13147000 -1.45689400 0.37906200

C -1.82414700 0.45911800 -2.01766200
 C -2.55828800 2.35438300 -0.50852300
 C -2.38389300 1.31541100 0.58241800
 C -3.13399800 0.10762200 0.71337600
 C -4.27003400 -0.29024900 -0.23007400
 C -2.33756900 -0.84397600 -1.80401200
 H -0.91402400 0.54037900 -2.61001600
 H -1.97866200 1.72831800 1.50528800
 H -3.23025800 -0.28405200 1.72482700
 H -1.80997700 -1.66757900 -2.28605100
 C -2.66124000 1.72550200 -1.91494000
 C -3.77184100 -1.15293900 -1.41292800
 H -3.43000300 2.99610100 -0.30589300
 H -1.67523300 3.00272400 -0.47739700
 H -3.70458600 1.50389000 -2.16145200
 H -2.31855800 2.44894300 -2.66281500
 H -4.44414600 -1.04729800 -2.27811000
 H -3.80673200 -2.20928100 -1.12183700
 H -5.02364000 -0.85348300 0.33144400
 H -4.78003600 0.60688100 -0.59725500
 Ir -1.19768400 -0.30421200 -0.07591700
 O 0.49762500 -1.30254200 -0.74351200
 C 1.04405600 1.47452400 1.26337100
 H 0.04113400 3.29392400 1.81451100
 C 0.32735800 0.63990700 2.26726100
 C -0.23497700 -0.55092800 1.87376900
 C -0.67804700 -1.59902100 2.81455100
 C -1.72080600 -2.48108200 2.47605000
 C 0.01464500 -1.84441800 4.01900700
 C -2.09086200 -3.52492600 3.32316600
 H -2.22768500 -2.34147900 1.52669100
 C -0.34939000 -2.88957400 4.86195400
 H 0.84797300 -1.20482300 4.28937900
 C -1.41213600 -3.73258700 4.52409800
 H -2.90620100 -4.18418200 3.03697200
 H 0.20205700 -3.05118700 5.78447400
 H -1.69538200 -4.54912200 5.18234200

C 0.18534400 1.23166800 3.62037200
 C -1.03407600 1.15359900 4.31571400
 C 1.25335400 1.92300100 4.21772900
 C -1.17284300 1.72837800 5.57550900
 H -1.87092100 0.63908600 3.85614900
 C 1.11859200 2.48535800 5.48579000
 H 2.19344400 2.00973600 3.68140800
 C -0.09494200 2.39008800 6.16963600
 H -2.12513400 1.66320000 6.09426800
 H 1.95997100 3.00333600 5.93779200
 H -0.20341200 2.83598700 7.15428500

INT9

C 2.78863700 -0.64328100 -0.03040600
 C 1.79249200 -1.43230800 0.86255700
 C 2.90698100 -1.27152200 -1.42445500
 H 1.94146700 -1.18625900 -1.93728200
 H 3.64089100 -0.71665100 -2.01995200
 C 3.33160600 -2.74183800 -1.34192900
 H 3.36279600 -3.17998500 -2.34723000
 H 4.35542700 -2.79640700 -0.94269200
 C 2.39386500 -3.54145200 -0.43455300
 H 1.39642200 -3.58759900 -0.88722100
 H 2.74901800 -4.57422400 -0.33113600
 C 2.27551000 -2.89781300 0.94943400
 H 3.24680500 -2.91677800 1.46250000
 H 1.57756800 -3.46419300 1.57005900
 H 3.76335000 -0.76429900 0.47265000
 O 0.50152400 -1.46596800 0.28045500
 C 2.58340200 1.64928600 -1.14782600
 C 2.35925300 3.02676700 -1.06999000
 C 2.03759400 3.60651200 0.15568500
 C 1.92829000 2.80556900 1.29124100
 C 2.14615800 1.42046100 1.22264500
 C 2.49180700 0.83722800 -0.01695300
 H 2.82936100 1.20969900 -2.10769000
 H 2.43570500 3.63800700 -1.96491800
 H 1.85868300 4.67543500 0.22925200

H 1.64857200 3.25258700 2.23826900
 C 1.91693600 0.55269400 2.39733800
 C 1.71583200 -0.78159500 2.24909500
 Ir -1.15133600 -0.55832200 -0.09896900
 C -2.74357600 1.19503400 1.78844900
 C -3.84714600 0.65383800 0.85608300
 C -3.29683900 -0.43490600 -0.06220800
 C -2.81422300 -0.18037600 -1.37977200
 C -2.75739600 1.19297700 -2.02639600
 C -2.07457400 2.22192700 -1.10587000
 C -1.06267900 1.53857100 -0.18947100
 C -1.37347900 1.09749200 1.15085500
 H -0.03089100 1.82136800 -0.37200000
 H -1.55653700 2.97615700 -1.70719900
 H -2.81282400 2.76404700 -0.50594000
 H -2.17314600 1.09722000 -2.94868000
 H -3.76023600 1.53348600 -2.32529100
 H -2.89583600 -1.00325900 -2.09486100
 H -3.69251600 -1.43321700 0.12808200
 H -0.55259300 1.11673300 1.86375800
 H -2.95033400 2.23155300 2.09606000
 H -2.71879200 0.59787300 2.70755600
 H -4.66791900 0.24550000 1.45493600
 H -4.28177500 1.46354600 0.26096100
 C 1.35749000 -1.64539300 3.40407100
 C 2.23839800 -1.79554500 4.48451900
 C 0.12965400 -2.32667600 3.43711800
 C 1.89923300 -2.59312900 5.57602200
 H 3.18779300 -1.26956700 4.46796500
 C -0.20964100 -3.12224200 4.53070600
 H -0.55624700 -2.21554800 2.60364900
 C 0.67244900 -3.25808900 5.60478700
 H 2.59406000 -2.69402600 6.40532700
 H -1.16765200 -3.63529600 4.54497400
 H 0.40588200 -3.87744900 6.45668200
 C 1.79960200 1.21653700 3.72901900
 C 0.62296900 1.13355300 4.48639200

C 2.87829600 1.95044200 4.24423900
 C 0.53067800 1.75654500 5.72983000
 H -0.21482500 0.56029400 4.10388200
 C 2.79030300 2.56858800 5.49081700
 H 3.79026100 2.03085100 3.65919500
 C 1.61489700 2.47358600 6.23850700
 H -0.38888400 1.67846000 6.30314300
 H 3.63971400 3.12460200 5.87818600
 H 1.54461200 2.95598500 7.20937100

TS7

C 2.06873700 -4.40005200 6.00750300
 C 0.87772500 -5.11422800 5.79624700
 C 0.01910900 -4.59659300 4.83659300
 C 0.32959100 -3.45348800 4.10630000
 C 1.49579100 -2.73024600 4.30759100
 C 2.36702200 -3.23365900 5.28728500
 H 2.77785600 -4.75380000 6.75143500
 H 0.65766100 -6.01174800 6.36862500
 H 1.74130400 -1.83164700 3.74880900
 H 3.29857700 -2.71260400 5.49219700
 C -0.93449600 -3.54198000 3.24798600
 C -0.65924700 -3.85409300 1.75349100
 H -0.99882900 -2.99990500 1.15832800
 H 0.42493500 -3.93206500 1.60828700
 C -1.66383100 -6.13882400 3.52397200
 H -2.74898000 -6.22196700 3.38029000
 H -1.38309500 -6.94497600 4.21427200
 C -1.30194600 -5.14793800 1.24051800
 C -0.97992100 -6.32701100 2.16490600
 C -1.33991000 -4.78856100 4.17323700
 H 0.10873700 -6.40017700 2.29740200
 H -1.31011700 -7.27143300 1.71609300
 H -2.39062500 -5.02591000 1.16846600
 H -0.94214200 -5.34481500 0.22334600
 O -1.78612800 -2.42277700 3.42113900
 H -2.15434700 -4.47796100 4.83756500
 H -1.52407000 -1.44830800 2.75012100

C -5.42560900 -0.73320700 2.40874400
 C -6.38500300 -2.49745500 3.96389900
 C -4.99289600 -3.09240200 3.77318400
 C -4.61544300 -3.80661000 2.59630200
 C -5.49489300 -4.01430900 1.37723800
 C -5.26771200 -1.48915800 1.21569700
 H -5.11307600 0.30409400 2.36822700
 H -4.47358300 -3.35855200 4.69382100
 H -3.85324300 -4.57313000 2.72010200
 H -4.84196700 -0.96888600 0.36113000
 C -6.42699800 -1.02517900 3.50911500
 C -6.13704300 -2.69942700 0.88467300
 H -7.11901200 -3.09305400 3.41050400
 H -6.67080500 -2.56690100 5.01881700
 H -7.44155900 -0.73720400 3.19510900
 H -6.17384400 -0.38107100 4.35865300
 H -7.13198500 -2.56965200 1.32439500
 H -6.28890500 -2.74975100 -0.19863100
 H -4.85335800 -4.41581400 0.58388800
 H -6.26370000 -4.77713000 1.57325700
 Ir -3.68210900 -1.92697800 2.57697400
 C -1.64571400 1.07990100 0.34647700
 C -1.61349700 0.68539600 1.84405400
 C -0.74442200 0.16326900 -0.48963500
 H -1.13948100 -0.85885000 -0.44430000
 H -0.76901200 0.47622000 -1.53926500
 C 0.70339900 0.19662300 0.01112500
 H 1.32117300 -0.49508100 -0.57455300
 H 1.11523700 1.20328600 -0.15274000
 C 0.78357700 -0.14389900 1.50023000
 H 0.51557200 -1.19672600 1.64391800
 H 1.81254300 -0.03065900 1.86417900
 C -0.14862500 0.74190800 2.33248100
 H 0.18895400 1.78569400 2.28958600
 H -0.10721600 0.44691800 3.38419200
 H -1.20958800 2.09294200 0.31602900
 C -3.47842500 0.77894300 -1.41405700

C -4.78875500 0.98508100 -1.85413000
 C -5.69922400 1.64192600 -1.02915500
 C -5.30064300 2.07474100 0.23386200
 C -3.98978700 1.86404600 0.68981200
 C -3.06335700 1.21627900 -0.15609000
 H -2.77907700 0.26689100 -2.06512400
 H -5.09071300 0.63249100 -2.83637900
 H -6.72068600 1.80825000 -1.35917100
 H -6.01881300 2.55825900 0.88596300
 C -3.59786800 2.20108700 2.07603100
 C -2.50910400 1.62845100 2.65163900
 O -2.05642100 -0.66828100 1.99024700
 C -2.16498200 1.86166000 4.07953200
 C -1.90013000 3.15899500 4.54253300
 C -2.08355500 0.79435300 4.99026400
 C -1.57819800 3.38969400 5.87866800
 H -1.96118900 3.98952800 3.84640500
 C -1.76138900 1.02703100 6.32686000
 H -2.27979800 -0.21903100 4.65721800
 C -1.50944100 2.32416000 6.77765700
 H -1.38034200 4.40321000 6.21686700
 H -1.70835600 0.18890100 7.01636700
 H -1.25964200 2.50278000 7.81981500
 C -4.51707400 3.08318100 2.85252200
 C -5.13854300 2.63243300 4.02548400
 C -4.78462800 4.38622700 2.40835100
 C -5.99682400 3.46519700 4.74091000
 H -4.93002300 1.63013000 4.38288100
 C -5.63706300 5.22341700 3.12723900
 H -4.31668300 4.73986000 1.49379100
 C -6.24717200 4.76461400 4.29630200
 H -6.46832800 3.09881300 5.64855000
 H -5.82560900 6.23344700 2.77376100
 H -6.91366500 5.41500700 4.85579400

INT10

C 14.74030600 3.66479600 -10.09579400
 C 14.40116700 4.99579400 -10.80201700

C 13.89115600 2.50579000 -10.63621300
 H 14.16500700 2.32128000 -11.68119700
 H 14.11746400 1.59288500 -10.07402600
 C 12.39246600 2.80550300 -10.53001000
 H 11.81355700 1.98004900 -10.96182200
 H 12.11039900 2.86602700 -9.46831100
 C 12.04192000 4.12547500 -11.21936000
 H 12.22212500 4.03016600 -12.29713700
 H 10.97815000 4.35905300 -11.09071500
 C 12.89126800 5.27443600 -10.66926900
 H 12.65759500 5.44666000 -9.61028700
 H 12.64648800 6.20975200 -11.18517700
 H 14.44938700 3.82973200 -9.04454500
 C 16.79651200 2.14993000 -10.26998300
 C 18.17941500 1.96088400 -10.20577000
 C 19.01721000 3.04614000 -9.96215900
 C 18.46916000 4.31542400 -9.78987300
 C 17.08285500 4.51508300 -9.85566000
 C 16.23399000 3.41300900 -10.09581300
 H 16.15804400 1.29560200 -10.46466800
 H 18.59485700 0.96720200 -10.34902500
 H 20.09394200 2.91049900 -9.91295700
 H 19.12009400 5.16505500 -9.61579900
 C 16.50032900 5.86675700 -9.74057600
 C 15.24929200 6.12366400 -10.19386400
 O 14.73990500 4.81749600 -12.19304200
 H 14.37044500 5.57308700 -12.67589400
 C 14.67708400 7.49626500 -10.15532400
 C 14.42089500 8.20216400 -11.34083000
 C 14.36902200 8.11179400 -8.93445300
 C 13.87497200 9.48443500 -11.30816900
 H 14.68345200 7.75402500 -12.29602200
 C 13.82461100 9.39419800 -8.89859500
 H 14.57319400 7.57811700 -8.01144800
 C 13.57368700 10.08492000 -10.08500000
 H 13.69340600 10.01752700 -12.23742800
 H 13.59756200 9.85571700 -7.94153800

H 13.15115600 11.08522300 -10.05699200
 C 17.35336600 6.94374500 -9.15997100
 C 17.81267100 6.83372300 -7.83945600
 C 17.71231800 8.07453200 -9.90427200
 C 18.59027100 7.84023500 -7.26965700
 H 17.55149300 5.95219500 -7.26065100
 C 18.49525200 9.07918800 -9.33800700
 H 17.36777200 8.16505200 -10.92892400
 C 18.93311000 8.96799100 -8.01774800
 H 18.92898400 7.74381100 -6.24170900
 H 18.76312100 9.95023100 -9.92962700
 H 19.54043300 9.75276300 -7.57547700

INT11

C 0.89429300 0.13017300 -0.07637300
 C 1.95733800 -0.12609700 0.99362200
 H 2.48263600 -1.05600000 0.75353800
 H 2.70229700 0.67945500 0.99098300
 C 1.27336600 -0.21998600 2.36672700
 H 2.01667800 -0.44133900 3.14117000
 H 0.59065800 -1.07564400 2.33527400
 C 0.47962600 1.07001600 2.73382900
 H -0.54242100 0.79737100 3.02495100
 H 0.92660600 1.55765200 3.60837000
 C 0.40746300 2.09031700 1.57980400
 H -0.27907800 2.90649600 1.83826300
 C -0.02374300 1.39707500 0.28630900
 C -1.59097700 -0.43224100 -2.58522500
 C -0.90377400 -0.52054000 -5.04395100
 C 0.24689400 -1.37428100 -4.51381200
 C 0.11714300 -2.72766300 -4.14434900
 C -1.17734600 -3.51721300 -4.11390800
 C -1.89411400 -1.80270800 -2.36758900
 H -1.70309100 0.22406200 -1.72687800
 H 1.24103500 -1.04261000 -4.80988500
 H 1.01118400 -3.34501500 -4.20359300
 H -2.16652600 -2.08609200 -1.35333700
 C -1.62337900 0.27021100 -3.92998800

C -2.35168800 -2.74648200 -3.47218500
 H -1.61034800 -1.16130000 -5.58160000
 H -0.50901200 0.18214800 -5.78570200
 H -2.65765700 0.49710900 -4.23147000
 H -1.11979200 1.23312400 -3.79801100
 H -2.89840500 -2.17894200 -4.23209100
 H -3.06348100 -3.46684400 -3.05569700
 H -0.98607200 -4.41913300 -3.52307100
 H -1.44765000 -3.85457800 -5.12616700
 Ir 0.25416500 -1.51593400 -2.33576300
 H 1.39162900 2.55152600 1.42954000
 O 0.13826200 -1.00826600 -0.34454100
 H -1.07998600 1.10793400 0.32835600
 C 1.18266100 -3.30763800 -1.44884000
 C 2.11919800 -2.60694500 -1.91839300
 C 0.41264800 -4.34907500 -0.83190400
 C -0.46218800 -4.03779200 0.22671000
 C 0.50442300 -5.67393200 -1.29360300
 C -1.22733800 -5.04396900 0.80779200
 H -0.51776100 -3.00333100 0.55092100
 C -0.26657800 -6.67292500 -0.70173800
 H 1.17862800 -5.90527700 -2.11259200
 C -1.13419300 -6.36144500 0.34724900
 H -1.90109400 -4.80175300 1.62511900
 H -0.19138600 -7.69515100 -1.06192500
 H -1.73537900 -7.14217200 0.80466300
 C 3.52970000 -2.35277000 -2.09626200
 C 4.03581800 -1.92421700 -3.33565400
 C 4.42212300 -2.52653200 -1.02338800
 C 5.39757500 -1.68196500 -3.49949500
 H 3.34898900 -1.78941700 -4.16580800
 C 5.78168700 -2.27314500 -1.18957600
 H 4.03345200 -2.85581900 -0.06525600
 C 6.27519400 -1.85070100 -2.42613000
 H 5.77388000 -1.35657300 -4.46530400
 H 6.45838200 -2.40604600 -0.35009600
 H 7.33561200 -1.65241000 -2.55175700

C 1.30689300 0.93759300 -1.33118900
 C 2.09257400 0.92052000 -2.47978700
 C 1.92736000 2.00686800 -3.36071400
 C 1.04340200 3.05300800 -3.07499000
 C 0.28168700 3.07519400 -1.88981700
 C 0.43450000 1.99338200 -1.03719900
 H 2.81778000 0.14332300 -2.68721200
 H 2.51177700 2.04285700 -4.27659900
 H 0.95240700 3.87426800 -3.78134300
 H -0.38704900 3.90557500 -1.67779600

TS8

C 0.70731200 0.21940100 0.10624400
 C 1.80216300 0.08407300 1.14588500
 H 2.47005600 -0.73568100 0.87846200
 H 2.39425800 1.00246600 1.17614000
 C 1.13296200 -0.15452300 2.52353200
 H 1.86991700 0.06674400 3.30443600
 H 0.87037900 -1.21229100 2.62351900
 C -0.13530800 0.71831900 2.71770200
 H -1.02726400 0.12318200 2.48343100
 H -0.22983600 1.02378000 3.76573900
 C -0.12721900 1.94787700 1.79612900
 H -0.97997700 2.60240300 2.01007800
 C -0.17834100 1.48242700 0.32435900
 C -1.41514900 0.22778100 -2.59794700
 C -0.42923500 1.26358100 -4.69875300
 C 0.79524000 0.45038300 -4.28604600
 C 0.91292500 -0.94347700 -4.48656000
 C -0.16202100 -1.83955800 -5.06996000
 C -1.43155700 -1.14815300 -2.97836900
 H -1.82835300 0.44015900 -1.61622300
 H 1.72353900 1.00948700 -4.23681900
 H 1.92155200 -1.33520000 -4.60029100
 H -1.80842000 -1.84845400 -2.23696500
 C -1.45537700 1.40176300 -3.55825800
 C -1.54353600 -1.61102000 -4.42839000
 H -0.88798800 0.79894600 -5.57853400

H -0.10013400 2.25840500 -5.01686200
 H -2.46806200 1.54977200 -3.96454000
 H -1.21648200 2.29944500 -2.97851400
 H -2.12121900 -0.87873000 -5.00314800
 H -2.11405200 -2.54468000 -4.46354300
 H 0.14415200 -2.87410500 -4.88704800
 H -0.20625500 -1.71339700 -6.16282200
 Ir 0.57504500 -0.59040900 -2.38164300
 C 2.52994500 1.92717200 -2.01697400
 C 1.42511700 1.41790100 -1.32142000
 C 0.56212200 2.32509200 -0.67289400
 C 0.69912300 3.70424800 -0.80247600
 C 1.73439700 4.19236200 -1.60720700
 C 2.65689900 3.31073200 -2.18279400
 H 3.27823600 1.26824300 -2.44049000
 H 0.04321600 4.38836400 -0.26921300
 H 1.85394400 5.26363400 -1.74654100
 H 3.48882600 3.70690900 -2.76031500
 H 0.77667200 2.54460400 1.96991500
 O 0.15401300 -0.88847300 -0.31822000
 H -1.21374700 1.25250400 0.05711400
 C 1.45124800 -2.55696300 -2.17625300
 C 2.41748200 -1.74460500 -2.05284800
 C 0.80984300 -3.84407500 -2.24794800
 C -0.29571400 -4.12535300 -1.42429000
 C 1.26106600 -4.82379000 -3.14928500
 C -0.93193900 -5.36055100 -1.50581400
 H -0.62786900 -3.36389300 -0.72639800
 C 0.61436500 -6.05601900 -3.22881700
 H 2.11533600 -4.60474300 -3.78276300
 C -0.48389300 -6.32793500 -2.41051300
 H -1.78206300 -5.57088800 -0.86257800
 H 0.96898800 -6.80522400 -3.93135400
 H -0.98708300 -7.28847000 -2.47556000
 C 3.81327900 -1.51121400 -1.76687900
 C 4.62779600 -0.80646100 -2.67047500
 C 4.39041700 -1.99985400 -0.58097800

C 5.97565600 -0.59033800 -2.39322400
 H 4.19350400 -0.44365300 -3.59765400
 C 5.73661500 -1.77291300 -0.30269100
 H 3.76984600 -2.56037300 0.11102500
 C 6.53449000 -1.06568700 -1.20476200
 H 6.59110600 -0.04831800 -3.10597900
 H 6.16513400 -2.15401400 0.62026200
 H 7.58352500 -0.88951100 -0.98528800

INT1-(*R*, *R*)

C -2.15078400 1.29906900 1.10553600
 C -0.79159100 1.20087200 0.75158300
 C 0.11456800 1.17246300 1.79914800
 C -0.30025300 1.23734800 3.14138800
 C -1.63397800 1.32368600 3.50141100
 C -2.56223900 1.34992600 2.44346100
 H -2.90312700 1.33222200 0.32181900
 H -0.49183500 1.15386500 -0.29199900
 H -1.96386400 1.38191900 4.53487900
 H -3.62390300 1.41779600 2.66589200
 C 1.14252800 1.35419500 3.65093400
 C 1.94266100 0.52529000 4.64547500
 H 1.69556100 0.77086700 5.68485500
 H 1.74454700 -0.54275200 4.49131600
 C 2.94087400 1.47514000 1.84728400
 H 2.96766600 2.56277400 1.96599500
 H 3.26155400 1.23477100 0.82614200
 C 3.43385900 0.86656500 4.36171000
 C 3.88067700 0.78148400 2.87465900
 C 1.57282700 0.92038100 2.19271700
 H 3.95608300 -0.27788500 2.59004200
 H 4.89384100 1.19426800 2.79484000
 H 3.60761900 1.88523700 4.71995800
 H 4.07851500 0.20544000 4.95406000
 Ir 1.04719900 4.52530100 3.41462600
 C -1.03341300 6.74781200 3.38134000
 C -1.37259500 5.92794800 2.11952600
 C -0.54650000 4.64445400 2.05962700

C 0.71447300 4.54609400 1.35552800
 C 1.39369900 5.69515400 0.63872500
 C 1.46397800 6.95719600 1.52088700
 C 1.53810500 6.58051500 2.99853700
 C 0.39405500 6.50845500 3.84536700
 H 2.48832000 6.81104900 3.48207800
 H 2.34439100 7.54909900 1.24917700
 H 0.59911200 7.60367600 1.34041700
 H 2.40977500 5.36788900 0.38982100
 H 0.89013100 5.90184200 -0.31833900
 H 0.94972800 3.56814700 0.93897100
 H -1.12641200 3.72792600 2.12973500
 H 0.55582400 6.71438200 4.90652300
 H -1.22098800 7.81891300 3.21322100
 H -1.69873500 6.43897000 4.19550500
 H -2.43615400 5.66787500 2.12176800
 H -1.20462800 6.51808900 1.21241700
 O 1.41843200 2.70549400 3.94393000
 H 1.68277800 -0.17459300 2.19328700

TS1-(R, R)

C 2.08455900 -0.48742100 -0.68914100
 C 3.20647100 -0.99898300 -1.55827400
 H 2.82633200 -1.78178700 -2.21961300
 H 3.65003500 -0.20439600 -2.16570800
 C 4.27852000 -1.56034700 -0.54647800
 H 5.08225400 -0.82260700 -0.43598300
 H 4.73846700 -2.45617700 -0.97657400
 C 3.70881700 -1.90793000 0.85469400
 H 2.95523200 -2.69129100 0.73125700
 H 4.51377900 -2.32936600 1.46679000
 C 3.04694000 -0.69630900 1.59113900
 H 2.17765300 -1.03684400 2.16090500
 C 2.63659700 0.30883500 0.51152300
 C -1.41856000 -1.66835800 1.08513600
 C -2.81260700 0.35580200 1.76189200
 C -2.04095400 1.01953800 0.62281200
 C -2.34890400 0.80151000 -0.75027200

C -3.42806600 -0.13376300 -1.26864600
 C -1.94725900 -1.91211400 -0.21796700
 H -0.61381500 -2.32647700 1.41443500
 H -1.56827500 1.96801700 0.87338500
 H -2.11879200 1.61816600 -1.43301400
 H -1.50582200 -2.73785500 -0.77521900
 C -2.15560700 -0.96981700 2.21160900
 C -3.36985200 -1.53280800 -0.61765800
 H -3.84906400 0.18235300 1.45376200
 H -2.86130600 1.04112000 2.61500700
 H -2.90443300 -1.63772200 2.66423200
 H -1.41818700 -0.75385200 2.99305000
 H -4.02300500 -1.57533100 0.26059500
 H -3.76068700 -2.27711600 -1.31987700
 H -3.26794700 -0.24187400 -2.34805500
 H -4.42846800 0.30958100 -1.14606900
 Ir -0.57591600 -0.26465900 -0.25126800
 C 0.39683500 2.42459800 -1.32391600
 C 0.98328400 1.28730300 -0.73721200
 C 1.64532900 1.43593900 0.51370700
 C 1.58198800 2.62088700 1.24566700
 C 0.88900700 3.69943500 0.68776000
 C 0.33710500 3.61822300 -0.60054900
 H -0.06051800 2.36707500 -2.30849700
 H 2.09171700 2.72717300 2.19997800
 H 0.81574700 4.63347200 1.23908900
 H -0.15320800 4.48910300 -1.02830700
 H 3.74723900 -0.23323000 2.29601900
 O 1.13441500 -1.35737400 -0.45930400
 H 3.56344900 0.78227600 0.15552900

INT1-(S, S)

C 2.15099900 1.29850500 1.10564300
 C 0.79177600 1.20091200 0.75164200
 C -0.11439800 1.17252600 1.79920000
 C 0.30041600 1.23695100 3.14145500
 C 1.63417000 1.32271600 3.50151800
 C 2.56245400 1.34887900 2.44358600

H	2.90337000	1.33156100	0.32194700
H	0.49200600	1.15428500	-0.29195200
H	1.96406600	1.38060200	4.53500400
H	3.62414000	1.41630800	2.66604600
C	-1.14232100	1.35417900	3.65101200
C	-1.94262900	0.52517500	4.64537800
H	-1.69553800	0.77052900	5.68481500
H	-1.74460600	-0.54283600	4.49098700
C	-2.94064900	1.47594300	1.84745100
H	-2.96726800	2.56355400	1.96655400
H	-3.26132800	1.23599400	0.82622000
C	-3.43379400	0.86663700	4.36163600
C	-3.88056800	0.78204800	2.87455000
C	-1.57272800	0.92078200	2.19271600
H	-3.95607900	-0.27722300	2.58959700
H	-4.89367600	1.19499100	2.79482600
H	-3.60746000	1.88522200	4.72016800
H	-4.07856600	0.20541500	4.95375600
Ir	-1.04697400	4.52518600	3.41467700
C	1.03309300	6.74831300	3.38115900
C	1.37251400	5.92833000	2.11948200
C	0.54662600	4.64469800	2.05963100
C	-0.71436800	4.54600500	1.35557200
C	-1.39404800	5.69482100	0.63881900
C	-1.46435100	6.95694800	1.52083400
C	-1.53836200	6.58039700	2.99850100
C	-0.39428200	6.50863600	3.84529600
H	-2.48867500	6.81057000	3.48201400
H	-2.34481700	7.54877300	1.24910700
H	-0.59954500	7.60345700	1.34022900
H	-2.41014300	5.36728600	0.39031600
H	-0.89087100	5.90151600	-0.31844700
H	-0.94935500	3.56799600	0.93899700
H	1.12676900	3.72830200	2.12966600
H	-0.55603400	6.71446400	4.90646600
H	1.22036600	7.81943700	3.21282000
H	1.69853500	6.43981700	4.19535500

H	2.43611000	5.66841000	2.12191400
H	1.20459800	6.51832100	1.21227200
O	-1.41797800	2.70546300	3.94425500
H	-1.68297600	-0.17417100	2.19308800

TS1-(S,S)

C	-2.08456100	-0.48741600	-0.68914200
C	-3.20647800	-0.99897100	-1.55827200
H	-2.82634500	-1.78176800	-2.21962200
H	-3.65004600	-0.20437700	-2.16569400
C	-4.27852100	-1.56034400	-0.54647400
H	-5.08226200	-0.82261200	-0.43597900
H	-4.73845900	-2.45617900	-0.97656800
C	-3.70881600	-1.90792200	0.85470000
H	-2.95523300	-2.69128600	0.73126300
H	-4.51377800	-2.32935500	1.46679700
C	-3.04693400	-0.69630200	1.59114200
H	-2.17764600	-1.03683900	2.16090400
C	-2.63659400	0.30884100	0.51152500
C	1.41855100	-1.66835400	1.08514200
C	2.81259800	0.35581000	1.76189300
C	2.04095200	1.01953800	0.62280400
C	2.34890500	0.80150000	-0.75027800
C	3.42806500	-0.13377900	-1.26864500
C	1.94725400	-1.91211900	-0.21795800
H	0.61380400	-2.32646800	1.41444400
H	1.56827400	1.96802100	0.87336700
H	2.11879700	1.61815300	-1.43302500
H	1.50581900	-2.73786200	-0.77520900
C	2.15560200	-0.96981100	2.21161200
C	3.36985000	-1.53281600	-0.61764200
H	3.84905900	0.18236700	1.45377400
H	2.86128300	1.04113200	2.61500500
H	2.90443400	-1.63771600	2.66422800
H	1.41818700	-0.75385000	2.99305800
H	4.02299700	-1.57532700	0.26061700
H	3.76069200	-2.27713200	-1.31985000
H	3.26794400	-0.24190100	-2.34805200

H 4.42846800 0.30956500 -1.14607500
 Ir 0.57591400 -0.26466200 -0.25127200
 C -0.39682700 2.42459700 -1.32391800
 C -0.98328100 1.28730500 -0.73721400
 C -1.64532200 1.43594200 0.51370700
 C -1.58197400 2.62089000 1.24566800
 C -0.88898900 3.69943500 0.68776200
 C -0.33708900 3.61822100 -0.60054900
 H 0.06052400 2.36707400 -2.30849900
 H -2.09170000 2.72717700 2.19998000
 H -0.81572200 4.63347000 1.23909100
 H 0.15322800 4.48909900 -1.02830600
 H -3.74722900 -0.23322300 2.29602600
 O -1.13442100 -1.35737200 -0.45930600
 H -3.56344600 0.78228500 0.15553500

BCB-INT1

C -1.90817100 -0.59781500 2.14130500
 C -0.58123500 -0.42023200 1.71748500
 C 0.13930500 0.57139300 2.36844800
 C -0.41126000 1.32710500 3.40392200
 C -1.72029600 1.16529900 3.83231300
 C -2.46596600 0.17852300 3.16815800
 H -2.52446300 -1.35306200 1.66028900
 H -0.16622300 -1.02681400 0.91675200
 H -2.15829000 1.75696400 4.63147800
 H -3.49971300 0.00506700 3.45570200
 C 0.89019500 2.08175200 3.66606200
 C 1.48664900 1.27469200 2.42880900
 O 0.82988500 3.46749900 3.56394400
 H 1.70129600 1.93710400 1.58386600
 H 1.36814400 1.78114300 4.61327500
 H 2.36525400 0.65068600 2.63538100
 Ir 2.24115200 4.80109900 3.59594600
 C 3.35657000 6.56194800 4.15096300
 C 3.50650000 6.29831800 2.75861200
 C 3.99321200 3.67984200 3.51334600
 C 3.59712400 3.91542200 4.89048200

C 4.45623100 6.28506600 5.17422300
 H 2.66072100 7.35641800 4.42435900
 C 4.74231400 5.67255600 2.13036100
 H 2.93239200 6.92992200 2.07605000
 C 5.18153700 4.38123400 2.85634700
 H 3.77426100 2.68997400 3.11407000
 C 4.28168100 4.89467700 5.82393900
 H 3.11552600 3.07968100 5.40216400
 H 4.43495600 7.05530000 5.95209000
 H 5.43876500 6.36662700 4.69770500
 H 4.49243200 5.42658400 1.09223000
 H 5.57338500 6.39216900 2.08961500
 H 5.65170800 3.69907300 2.14077000
 H 5.94155500 4.59939400 3.61415700
 H 5.24717400 4.49036500 6.16470100
 H 3.65125100 4.98761400 6.71515800

BCB-TS1

C 1.57430900 -1.83398900 -0.72412200
 C 2.34419600 -1.93648400 0.62021200
 C -2.10742800 -1.08228400 0.71744000
 C -1.93116500 1.11964800 1.98819100
 C -0.77313600 1.35436500 1.01923200
 C -0.95720400 1.72664100 -0.34436700
 C -2.30203000 1.89533200 -1.02828800
 C -2.49192700 -0.59573300 -0.56310000
 H -1.96631900 -2.15962100 0.80890300
 H 0.16122900 1.66675400 1.48484400
 H -0.16465800 2.32648100 -0.79068900
 H -2.60668500 -1.33768400 -1.35256000
 C -2.35580400 -0.36639600 2.03088900
 C -3.25554600 0.70771300 -0.76655100
 H -2.78040100 1.75279000 1.71082900
 H -1.63408500 1.43844400 2.99307000
 H -3.41071900 -0.45945500 2.33083800
 H -1.76824300 -0.88424500 2.79748600
 H -3.88482000 0.90712300 0.10720700
 H -3.94073000 0.59717000 -1.61384100

H	-2.11151700	1.96357900	-2.10606700
H	-2.77933700	2.84359000	-0.73681100
Ir	-0.38337800	-0.31680100	-0.24530400
C	2.19788300	1.22214700	-1.06669200
C	1.87124100	0.00558400	-0.44031400
C	2.69425400	-0.47303100	0.60155100
C	3.74408500	0.27896200	1.11929000
C	3.96495800	1.54792500	0.57515500
C	3.21823700	2.00280900	-0.52303300
H	1.64608200	1.57474700	-1.93271500
H	4.39382900	-0.11078900	1.89858800
H	4.76031800	2.17281400	0.97271700
H	3.44712600	2.97208500	-0.95816600
O	0.30812100	-2.17695700	-0.79925900
H	1.68749100	-2.26560700	1.43082600
H	2.18511400	-2.02277600	-1.61731500
H	3.21195400	-2.60532400	0.56240200

BCB-INT3

C	4.77800700	0.19663800	0.88903200
C	3.41802600	-0.02553800	1.14466600
C	2.96227100	2.22996900	0.43190500
C	4.31758600	2.44098700	0.17091800
C	5.23739100	1.42138400	0.41128600
H	5.48635700	-0.61071100	1.06521700
H	4.65039800	3.39913700	-0.22091800
H	6.29585900	1.57199600	0.21828100
C	2.99991600	-1.39408400	1.62546100
H	1.96493000	-1.62029400	1.33512500
C	3.07704900	-1.64130600	3.11708000
C	-1.13201800	-0.18421900	2.71501000
C	0.43764400	0.56356000	4.58723500
C	1.19467600	1.25590200	3.46304000
C	0.77005100	2.43178400	2.79721400
C	-0.50841200	3.19629400	3.06015900
C	-1.65839600	1.05645200	2.33787300
H	-1.47462500	-1.05664200	2.16286800
H	2.26211100	1.06880300	3.46523400

H	1.56118900	3.04630800	2.37503000
H	-2.33275300	1.07151500	1.48686100
C	-0.51578600	-0.52179200	4.05561200
C	-1.72951300	2.27516300	3.23943800
H	-0.10638100	1.29903200	5.18850300
H	1.16649600	0.09661900	5.25616200
H	-1.30884200	-0.74433100	4.78656400
H	0.05025600	-1.45082000	3.92261500
H	-1.82308200	1.95972700	4.28245200
H	-2.64282600	2.83394000	3.00809400
H	-0.68338700	3.85563500	2.20188100
H	-0.38727300	3.85148600	3.93663800
Ir	0.45719500	0.77153100	1.44129200
O	3.45911700	-0.86094300	3.96056200
C	2.48368000	1.01214400	0.94025400
H	2.25904000	3.03342800	0.22743500
C	-0.56495100	-0.14281800	-0.13994400
C	0.61140400	0.05065200	-0.54974400
H	-1.57220200	-0.50142700	-0.26315600
H	1.42498000	0.01592900	-1.24842800
H	3.61596600	-2.18200000	1.16224500
H	2.74241400	-2.66367700	3.41293900

BCB-TS2

C	-3.71831900	0.30238200	0.51011600
C	-2.53275600	0.36305600	-0.23983200
C	-1.99561900	-1.87064000	0.55971200
C	-3.18225800	-1.92263600	1.27472500
C	-4.04669300	-0.82004400	1.26156600
H	-4.39326100	1.15365600	0.49077300
H	-3.43593600	-2.81121000	1.84641500
H	-4.97758500	-0.84588500	1.82067800
C	-2.25326900	1.61422200	-1.04421500
H	-1.90113400	1.35230300	-2.04678100
C	-1.20497300	2.49880600	-0.37561300
C	2.32999200	0.91827600	-0.54069300
C	1.45111700	1.70348000	1.73241300
C	0.55608800	0.48471100	1.61449700

C 1.01504000 -0.84973900 1.59148800
 C 2.48413300 -1.22768600 1.71859100
 C 2.61389400 -0.45611800 -0.71408300
 H 2.29627900 1.52348800 -1.44463700
 H -0.46696400 0.65145200 1.94512800
 H 0.30437600 -1.61977900 1.88445600
 H 2.77662700 -0.80222800 -1.73400300
 C 2.63816900 1.68329000 0.74444300
 C 3.17120100 -1.38353100 0.34350200
 H 1.81892400 1.80563100 2.76525400
 H 0.83028700 2.58214700 1.53871500
 H 3.52741000 1.25208000 1.21670100
 H 2.90742300 2.71289200 0.48506200
 H 4.25908200 -1.24182600 0.43969100
 H 3.02187500 -2.40833500 -0.01514300
 H 2.56899700 -2.17306300 2.26545400
 H 3.00851500 -0.48121900 2.32401300
 O -1.39859100 3.09165300 0.66528200
 C -1.62474200 -0.72374300 -0.17725800
 H -1.32491500 -2.72516000 0.56510200
 C -0.89133100 -1.16104300 -1.95733300
 C 0.03501400 -0.39404100 -2.44480900
 H 0.48379100 -0.23846600 -3.41710200
 H -1.56783600 -1.96748100 -2.19450600
 Ir 0.46483700 -0.23089700 -0.45670600
 H -0.23354700 2.57058700 -0.90563500
 H -3.17422000 2.20227700 -1.12882700

BCB-INT4

C 2.55189300 -0.89216500 1.68284600
 C 1.55479800 -0.91901400 0.70038900
 C 1.16903800 1.43408400 1.08119800
 C 2.16417100 1.45506200 2.05543900
 C 2.85038000 0.28102700 2.37280000
 H 3.10958100 -1.80070800 1.90037600
 H 2.39885600 2.38168100 2.57225200
 H 3.62403700 0.28279600 3.13518600
 C 1.35465700 -2.19241700 -0.08775000

H 1.12731000 -1.95790500 -1.14046200
 C 0.26966200 -3.15669200 0.30269400
 C -0.86911900 -1.61558900 3.78484500
 C -1.37182400 0.88518300 4.03081900
 C -1.95848500 0.74003000 2.62664900
 C -3.20630800 0.10423700 2.33804400
 C -4.12489700 -0.54577200 3.35495100
 C -2.17319400 -2.12851700 3.73950800
 H -0.04917400 -2.32380700 3.65637000
 H -1.63773500 1.50513600 1.92260000
 H -3.72859100 0.45463200 1.44675300
 H -2.28744600 -3.19216400 3.53770000
 C -0.45825700 -0.30032100 4.42081900
 C -3.37202100 -1.43617200 4.36778300
 H -2.18097700 1.00681500 4.75939500
 H -0.78400000 1.80845900 4.07334400
 H -0.40811200 -0.39609800 5.51666900
 H 0.55849300 -0.08375000 4.07762900
 H -3.04791300 -0.84167500 5.22792900
 H -4.06084900 -2.19025600 4.76486700
 H -4.83604300 -1.16689500 2.79719700
 H -4.72249000 0.21545900 3.88130300
 Ir -1.62148700 -1.16200100 1.77621800

O -0.73453900 -2.94413300 0.97302200
 C 0.81948100 0.25072200 0.41245500
 H 0.61691800 2.34049300 0.84944700
 C -0.35495600 0.23028300 -0.50727100
 C -1.50321600 -0.34002500 -0.09252800
 H -2.35840100 -0.29130600 -0.77590600
 H -0.26058600 0.75241100 -1.46349900
 H 2.28556300 -2.77510100 -0.11293600
 H 0.38419000 -4.17561700 -0.10514800

BCB-TS3

C -2.79398700 1.40167600 1.29885400
 C -2.44866400 0.08632100 0.97059600
 C -3.34899300 0.42521600 -1.25243100
 C -3.64694600 1.75429700 -0.93308800

C	-3.38136400	2.23787500	0.34782300
H	-2.56311600	1.78142100	2.29083300
H	-4.10246600	2.40054600	-1.67785200
H	-3.62587600	3.26428600	0.60618900
C	2.33709200	0.09872100	-1.29941800
C	3.38376500	0.41137200	0.99447100
C	1.94279300	0.31669400	1.46368200
C	0.91312600	1.24767400	1.13088400
C	1.13426500	2.49987600	0.28596600
C	1.15651000	0.81281600	-1.62358100
H	2.58605000	-0.74777600	-1.93784500
H	1.82322200	-0.22173100	2.40542900
H	0.08163200	1.31779900	1.82884700
H	0.58953500	0.45906900	-2.48491700
C	3.49917000	0.70077200	-0.51908000
C	0.84226000	2.23649400	-1.20830200
H	3.93666000	1.16675000	1.57417400
H	3.86087100	-0.55248800	1.20866800
H	3.54906200	1.77919700	-0.70063700
H	4.44079900	0.28762700	-0.89653100
H	1.38433800	2.95551200	-1.84164400
H	-0.22590400	2.39707900	-1.39348200
H	0.47217100	3.29595900	0.64322500
H	2.15555200	2.87086500	0.42126000
Ir	0.69449700	-0.52878000	-0.02070000
C	-2.76538600	-0.41578200	-0.30919100
H	-3.58303600	0.03809100	-2.24069100
C	-1.69235100	-0.77593300	1.89417700
C	-0.60186300	-1.44682500	1.45595400
H	-0.10672500	-2.14902400	2.13025900
H	-2.01613900	-0.82147300	2.93611100
C	-2.49184900	-1.87850400	-0.58222800
C	-1.04249100	-2.29153400	-0.38110600
O	-0.16782500	-1.92979900	-1.27739000
H	-3.11872900	-2.49462900	0.07504100
H	-0.89546200	-3.27630600	0.08300300
H	-2.74663700	-2.12369200	-1.62032500