

DFT study on the Au(I)-catalyzed cyclization of indole-allenoate: Effects of counterion and solvent

Binfang Yuan,^{a,b} Rongxing He,^b Xiaogang Guo,^a Wei Shen,^b Fengying Zhang,^b Yanyan Xu^b and Ming Li^{*b}

^a School of Chemistry and Chemical Engineering, Yangtze Normal University, Chongqing 408100, China

^bKey Laboratory of Luminescence and Real-Time Analytical chemistry (Southwest University), Ministry of Education, College of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, China

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Table S1. Exploring the effects of different functionals on energies by comparing the activation free energy barrier of tsal (see path **a** of Figure 1) at B3LYP (B3P86, B3PW91, M06 and PBE0)/6-311++G**//B3LYP (B3P86, B3PW91, M06 and PBE0)/6-31G* levels, respectively.

Species	Activation Free Energy Barriers (kJ/mol)				
	B3LYP	B3P86	B3PW91	M06	PBE0
tsal	46.2	43.7	42.4	42.1	39.1

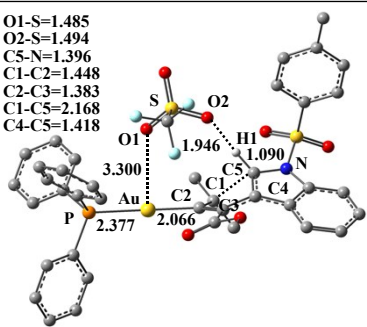
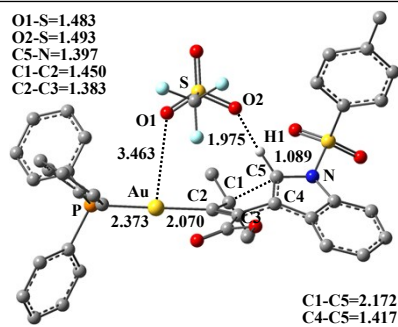
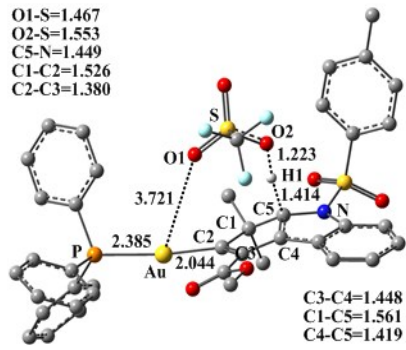
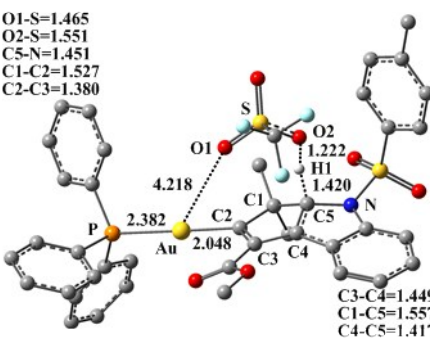
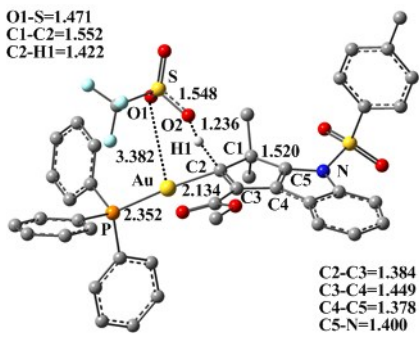
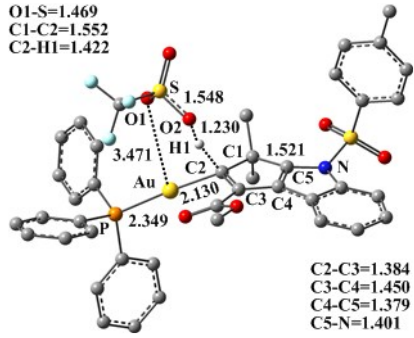
Table S1 shows that the effects of DFT functionals B3LYP, B3P86, B3PW91, M06, and PBE0 on the activation free energy barrier of tsal is very small.

Table S2. Exploring the effects of polarization and diffusion on energies by comparing the activation free energy barriers of tsa1, tsa2 and tsa3 (see path **a** of Figure 1) at PCM//B3LYP/6-311++G**//B3LYP/6-31G* (6-31G** and 6-31+G*) levels.

Species	Activation Free Energy Barriers (kJ/mol)		
	6-31G*	6-31G**	6-31+G*
tsa1	46.2	46.0	50.1
tsa2	39.4	42.8	33.3
tsa3	17.7	17.5	14.9

Table S2 shows that the effects of polarization and diffusion on energies are quite small for the present calculation.

Table S3. Exploring the effects of diffusion on structures by comparing the optimized geometries of tsa1, tsa2 and tsa3 (see path **a** of Figure 1) at B3LYP/6-31G* (6-31+G*) levels.

Species	Optimized Geometries	
	6-31G*	6-31+G*
tsa1	O1-S=1.485 O2-S=1.494 C5-N=1.396 C1-C2=1.448 C2-C3=1.383 C1-C5=2.168 C4-C5=1.418 	O1-S=1.483 O2-S=1.493 C5-N=1.397 C1-C2=1.450 C1-C3=1.383  C1-C5=2.172 C4-C5=1.417
tsa2	O1-S=1.467 O2-S=1.553 C5-N=1.449 C1-C2=1.526 C2-C3=1.380 	O1-S=1.465 O2-S=1.551 C5-N=1.451 C1-C2=1.527 C2-C3=1.380  C3-C4=1.449 C1-C5=1.557 C4-C5=1.417
tsa3	O1-S=1.471 C1-C2=1.552 C2-H1=1.422 	O1-S=1.469 C1-C2=1.552 C2-H1=1.422  C2-C3=1.384 C3-C4=1.450 C4-C5=1.379 C5-N=1.401

In Table S3, the optimized structures of tsa1 (tsa2 or tsa3) at B3LYP/6-31G* and B3LYP/6-

31+G* levels are nearly the same.

Table S4. Exploring the effects of basis sets (double-zeta vs. triple-zeta) on energies by comparing the activation free energy barrier of tsal (see path **a** of Figure 1) at PCM//B3LYP/6-311++G**//B3LYP/6-31G* (6-311G* and cc-pVTZ) levels.

Species	Activation Free Energy Barriers (kJ/mol)		
	6-31G*(double-zeta)	6-311G*(triple-zeta)	cc-pVTZ (triple-zeta)
tsal	46.2	46.6	49.4

Table S4 shows that double-zeta basis set (6-31G*) and triple-zeta basis set (6-311G* and cc-pVTZ) have extremely approximate calculation results in our present calculation.

Table S5. Exploring effects of basis set LanL2DZ ($\zeta=1.05$) for Au by comparing the activation free energy barriers of tsa1, tsa2 and tsa3 (see path a of Figure 1) at PCM//B3LYP/LanL2DZ (LanL2DZ ($\zeta=1.05$))/B3LYP/ LanL2DZ (LanL2DZ ($\zeta=1.05$)) levels.

Species	Activation Free Energy Barriers (kJ/mol)	
	LanL2DZ	LanL2DZ ($\zeta=1.05$)
tsa1	46.2	45.4
tsa2	39.4	39.1
tsa3	17.7	19.7

Obviously, the application of large basis set LanL2DZ ($\zeta=1.05$) does not give a better result than that of LanL2DZ. In order to save computational cost, LanL2DZ is selected as the economical basis set used in our present system.

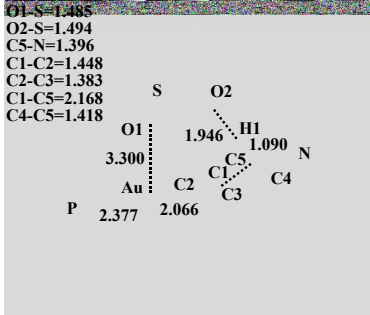
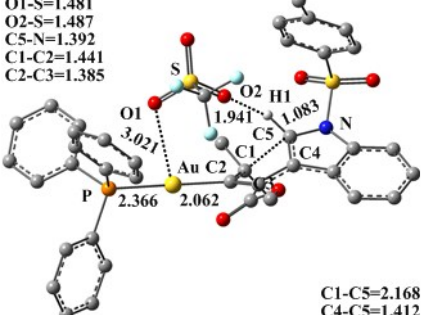
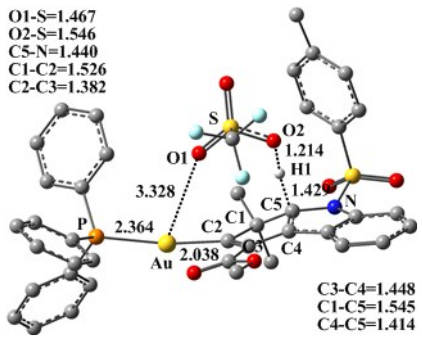
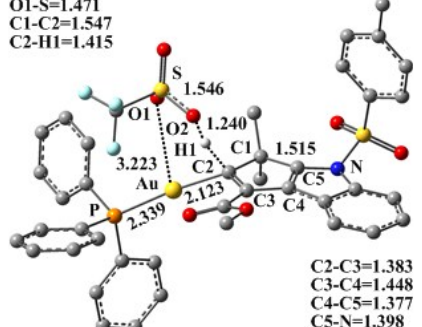
Table S6. Exploring the effects of temperatures (298.15 vs. 403.15 K) by comparing the activation free energy barriers of tsa1, tsa2 and tsa3 (see path **a** of Figure 1) at PCM//B3LYP/6-311++G**//B3LYP/6-31G*level.

Species	Activation Free Energy Barriers (kJ/mol)	
	298.15 K	403.15 K
tsa1	46.2	50.5
tsa2	39.4	39.8
tsa3	17.7	19.3

Table S7. Exploring the dispersion effects on energies by comparing the activation free energy barriers of tsa1, tsa2 and tsa3 (see path **a** of Figure 1) at B3LYP/6-311++G**//B3LYP/6-31G* and B3LYP-D3 (adding dispersion function on the basis of B3LYP)/6-311++G**//B3LYP-D3/6-31G* levels, respectively.

Species	Activation Free Energy Barriers (kJ/mol)	
	B3LYP	B3LYP-D3
tsa1	46.2	51.3
tsa2	39.4	43.7
tsa3	17.7	15.0

Table S8. Exploring the dispersion effects on structures by comparing the optimized geometries of tsa1, tsa2 and tsa3 (see path **a** of Figure 1) at B3LYP/6-311++G**//B3LYP/6-31G* and B3LYP-D3 (adding dispersion function on the basis of B3LYP/6-311++G**//B3LYP-D3/6-31G* levels, respectively.

Species	Optimized Geometries	
	B3LYP	B3LYP-D3
tsa1		
tsa2		
tsa3		

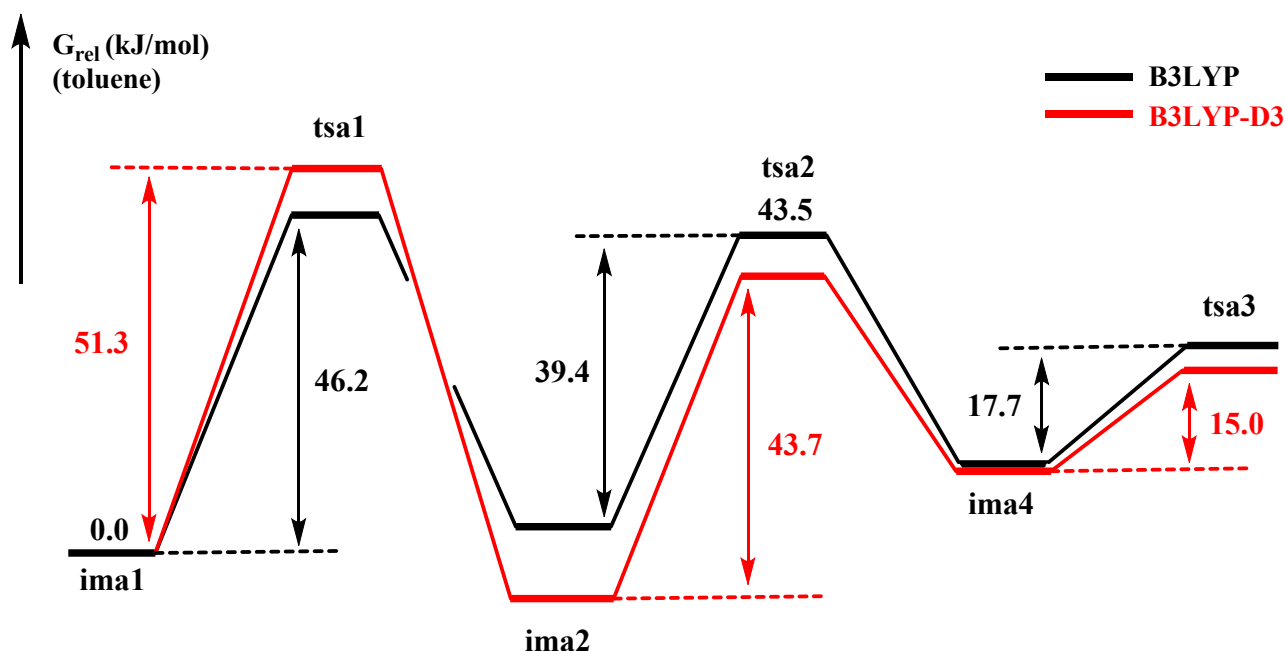


Figure S1. Exploring the dispersion effects by comparing the reaction profiles (at B3LYP and B3LYP-D3 levels).

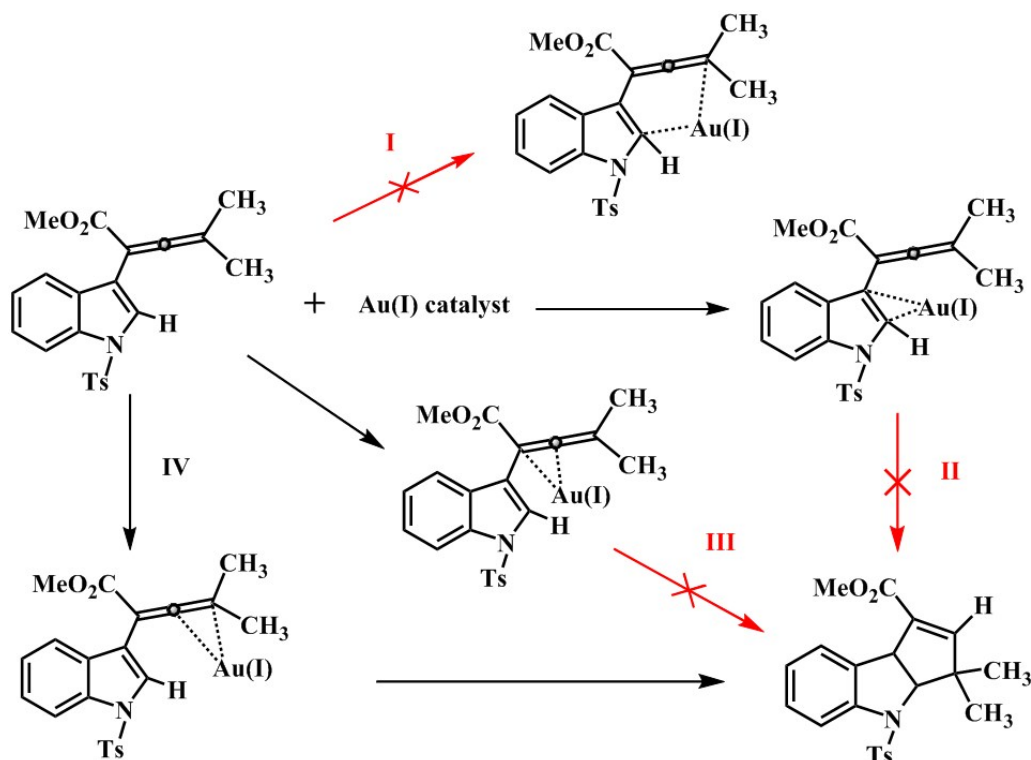
The geometric structures of ima1, ima2, ima4, tsa1, tsa2 and tsa3 are re-optimized using B3LYP-D3 (adding dispersion function on the basis of B3LYP) method, and the optimal structures of transition states tsa1, tsa2 and tsa3 are described in Table S8. The activation free energy barriers of tsa1, tsa2 and tsa3 are calculated at B3LYP-D3/6-311++G**//B3LYP-D3/6-31G* level (see Table S7). Tables S7 and S8 show that the effects of dispersion on energies and structures are very small. More importantly, the introduction of dispersion function does not change the reaction profile, and the rate-determining step is still the intramolecular cyclization process (see Figure S1). In order to save computational cost, B3LYP is selected as the economical calculation method.

Table S9. Exploring the solvent (toluene) effects on the geometry optimization by comparing the activation free energy barriers of tsa1, tsa2 and tsa3 (see path **a** of Figure 1) at B3LYP/6-311++G**(PCM, single point calculations)//B3LYP/6-31G*(geometry optimization in gas or in toluene) level.

Species	Activation Free Energy Barriers (kJ/mol)	
	In gas	In toluene
tsa1	46.2	40.5
tsa2	39.4	44.2
tsa3	17.7	19.7

Table S9 shows that the calculation results in toluene are very close to those in gas at B3LYP/6-311++G**(PCM, single point calculations)//B3LYP/6-31G*(geometry optimization in gas or in toluene) level

Scheme S1. Different coordination modes of indole-allenoate (**R**) with Au(I) catalyst.



Theoretically, there are four possible coordination modes of **R** with Au(I) catalyst, which are schematically illustrated in Scheme S1. The coordination of Au(I) catalyst to C1 and C5 of **R** simultaneously fails to be found in the present calculations through our various attempts (in mode I of Scheme S1). As reported in the previous literatures (Y. Liu, D. Zhang and S. Bi, *J. Phys. Chem. A* 2010, **114**, 12893-12899; Q. Zhang, X. Qu, H. Wang, F. Xu, X. Shi and W. Wang, *Environ. Sci. Technol.* 2009, **43**, 4105-4112; R.-X. Zhu, D.-J. Zhang, J.-X. Guo, J.-L. Mu, C.-G. Duan and C.-B. Liu, *J. Phys. Chem. A* 2010, **114**, 4689-4696), the coordination of Au(I) catalyst to the C3-C5 double bond of **R** cannot carry out the desired transformation, leading to a “dead path” (in mode II of Scheme S1). In mode III of Scheme S1, the coordination of Au(I) catalyst to the C2-C3 double bond of **R** is inappropriate because it is unfavorable to both the proton-shift and the intramolecular cyclization between C1 and C5 in the subsequent reactions. Thus, the catalytic reaction of **R** is believed to start from the coordination of Au(I) catalyst with the C1-C2 double bond of **R** (in mode

IV of Scheme S1). This coordination mode has also been proposed by Ma and co-workers in the original literature.

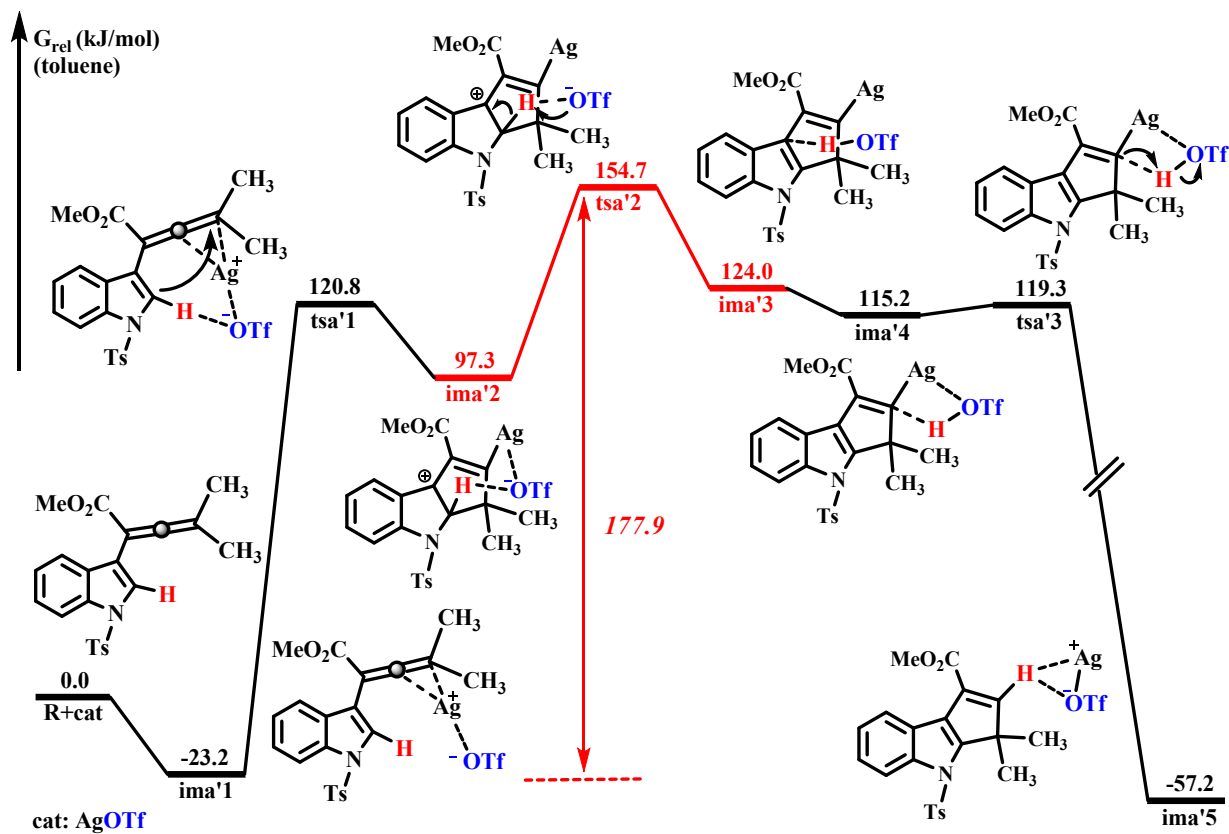


Figure S2. Energy profile for the AgOTf-catalyzed cyclization reaction of indole-allenoate in toluene at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

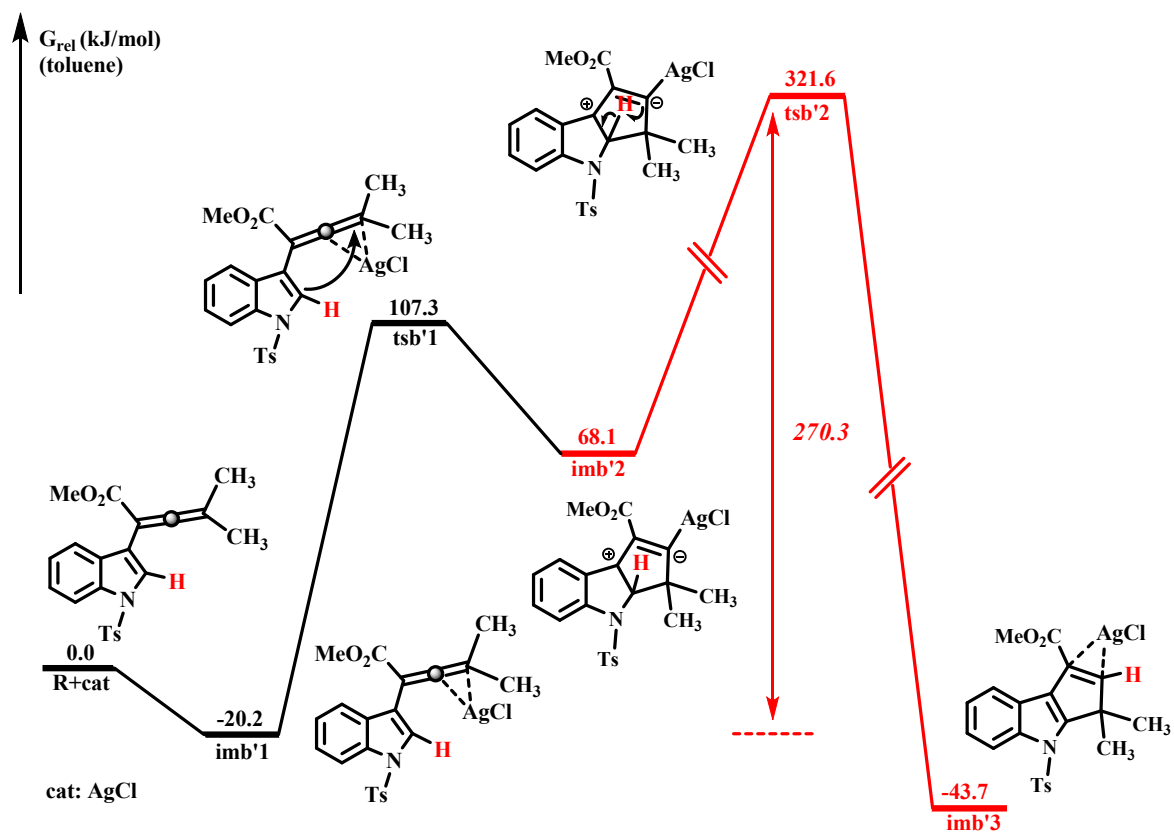


Figure S3. Energy profile for the AgCl-catalyzed cyclization reaction of indole-allenoate in toluene at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

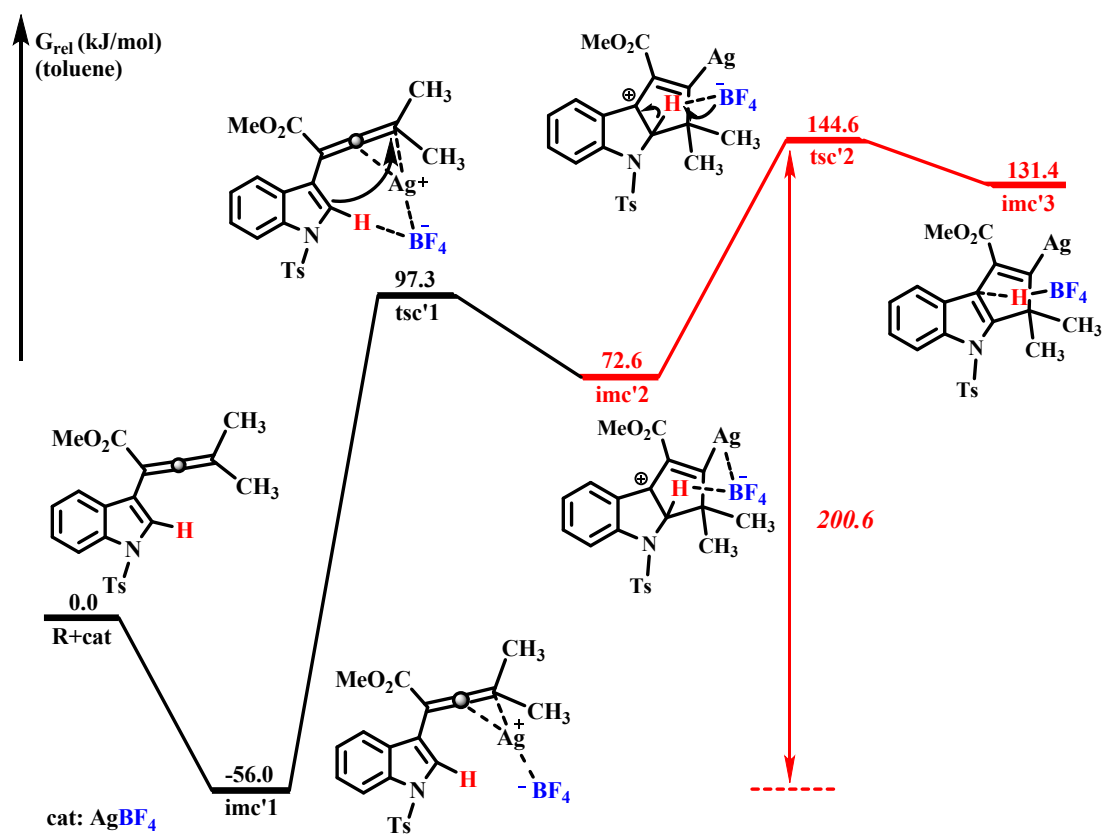


Figure S4. Energy profile for the AgBF_4 -catalyzed cyclization reaction of indole-allenoate in toluene at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

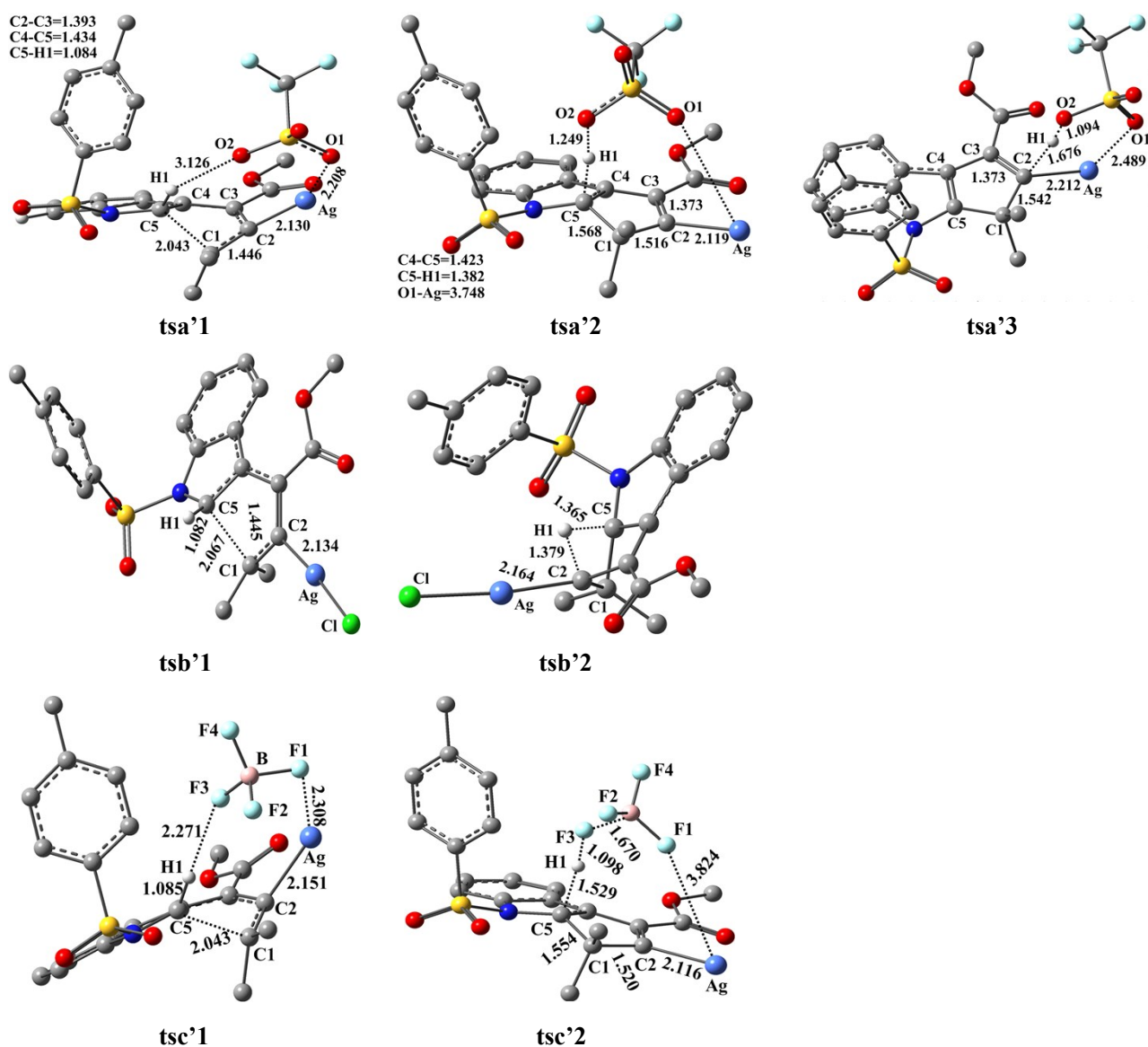


Figure S5. Optimized geometries involved in the AgCl- AgOTf- and AgBF₄-catalyzed cyclization reactions of indole-allenoate at B3LYP/6-31G* level. The hydrogen atoms not participating in the reaction have been omitted for clarity. Bond distances are given in Å.

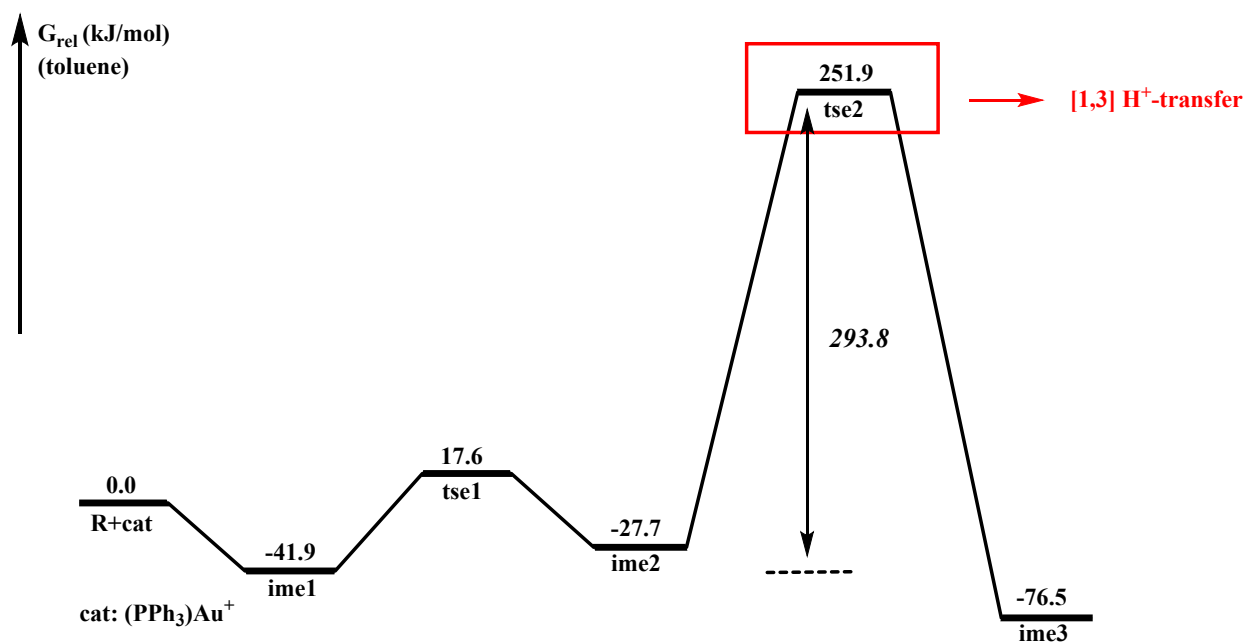


Figure S6. Energy profile for the $(\text{PPh}_3)\text{Au}^+$ -catalyzed cyclization reaction of indole-allenoate in toluene at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

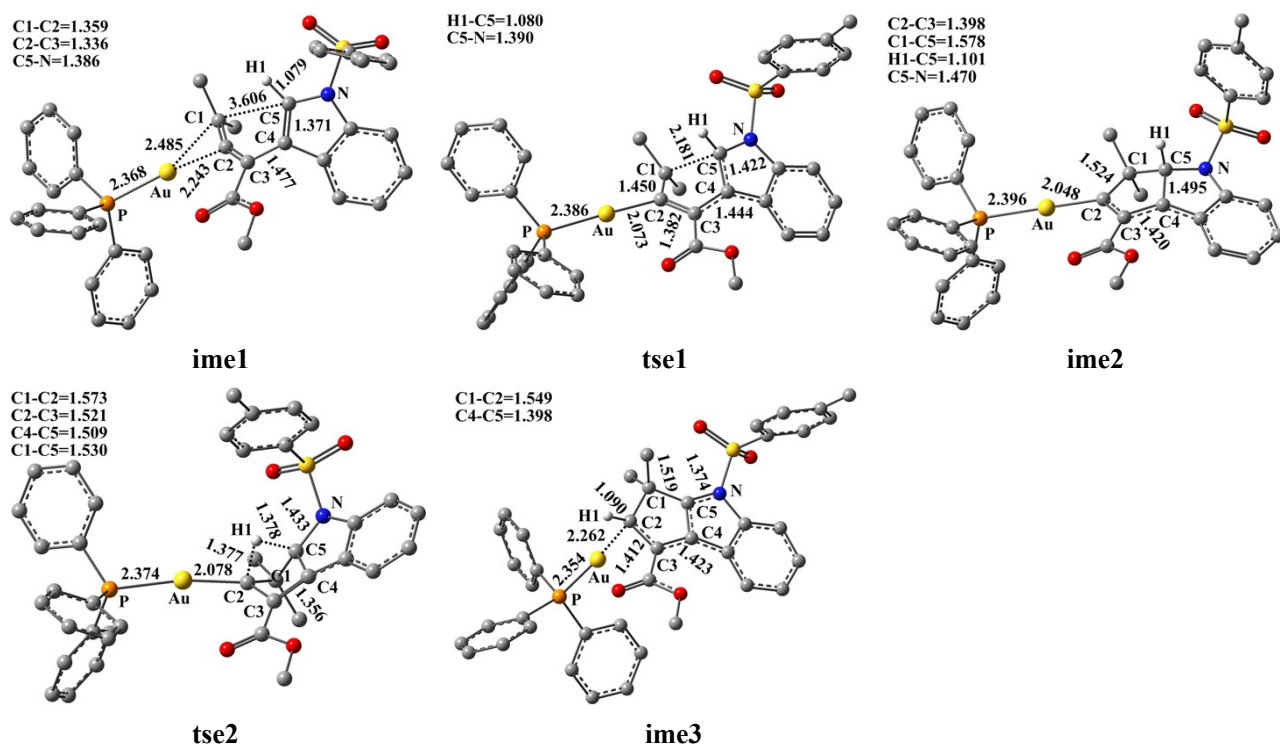
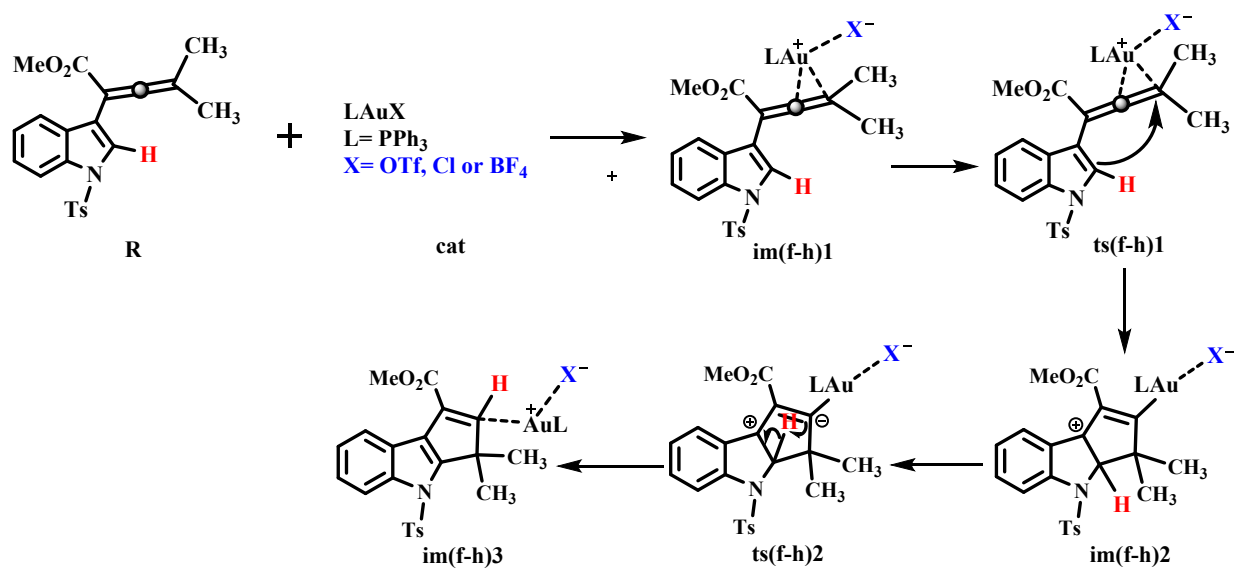


Figure S7. Optimized geometries involved in the $(\text{PPh}_3)\text{Au}^+$ -catalyzed cyclization reaction of indole-allenoate at B3LYP/6-31G* level. The hydrogen atoms not participating in the reaction have been omitted for clarity. Bond distances are given in Å.

Scheme S2. The mechanism of Au(I)-catalyzed cyclization reaction of indole-allenoate to form dihydrocyclopenta-[b]indole derivatives without OTf, Cl⁻ and BF₄⁻ as assisted catalysts.



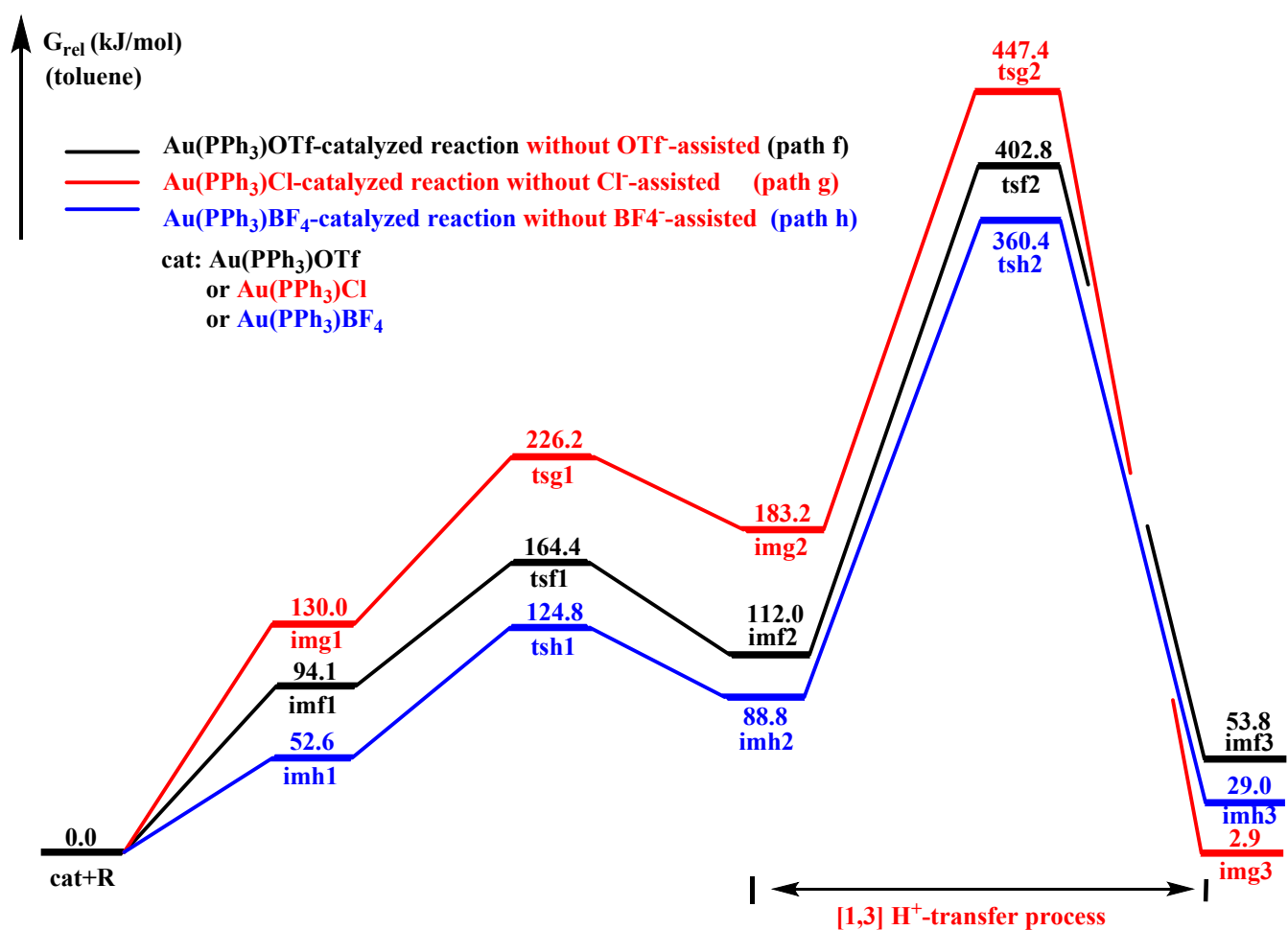


Figure S8. Energy profiles for the $(\text{PPh}_3)\text{AuOTf}$ -, $(\text{PPh}_3)\text{AuCl}$ -, and $(\text{PPh}_3)\text{AuBF}_4$ -catalyzed cyclization reactions of indole-allenoate without OTf⁻, Cl⁻ and BF₄⁻ as assisted catalysts in toluene at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

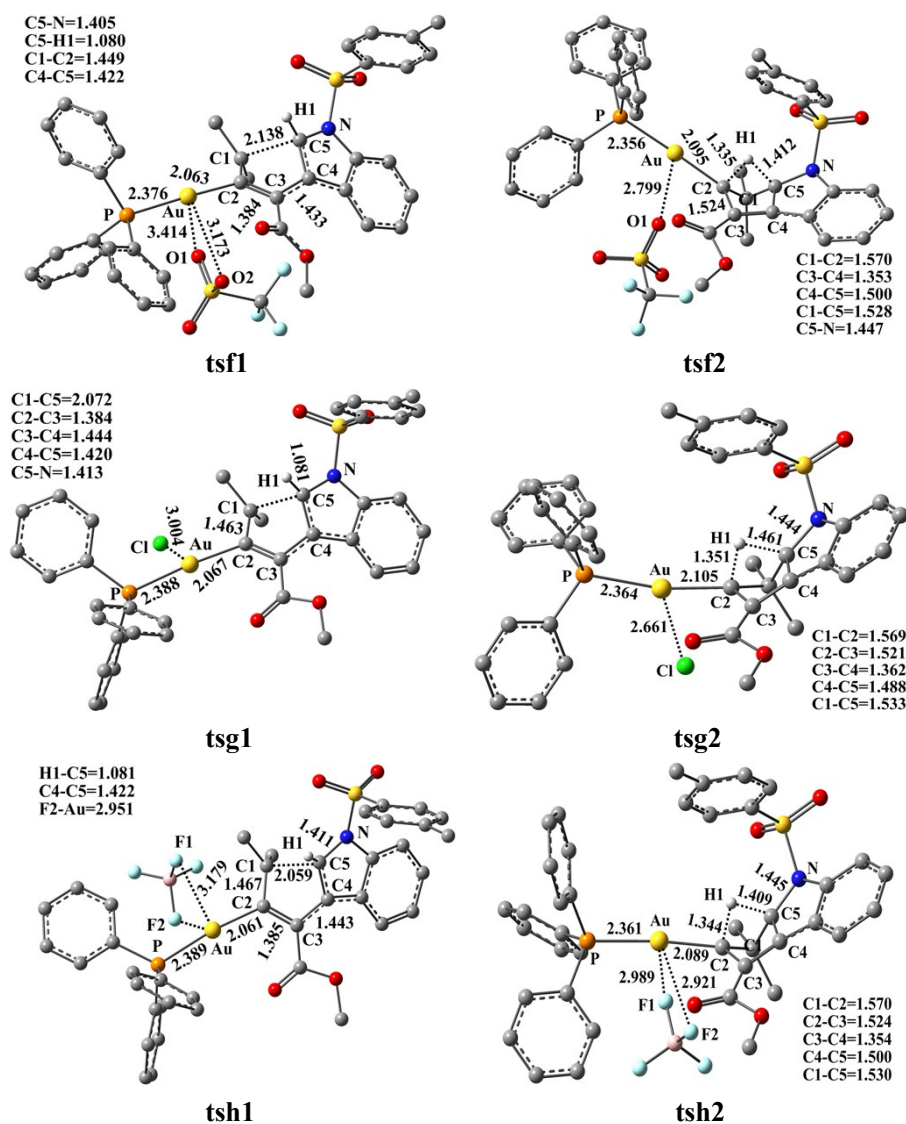
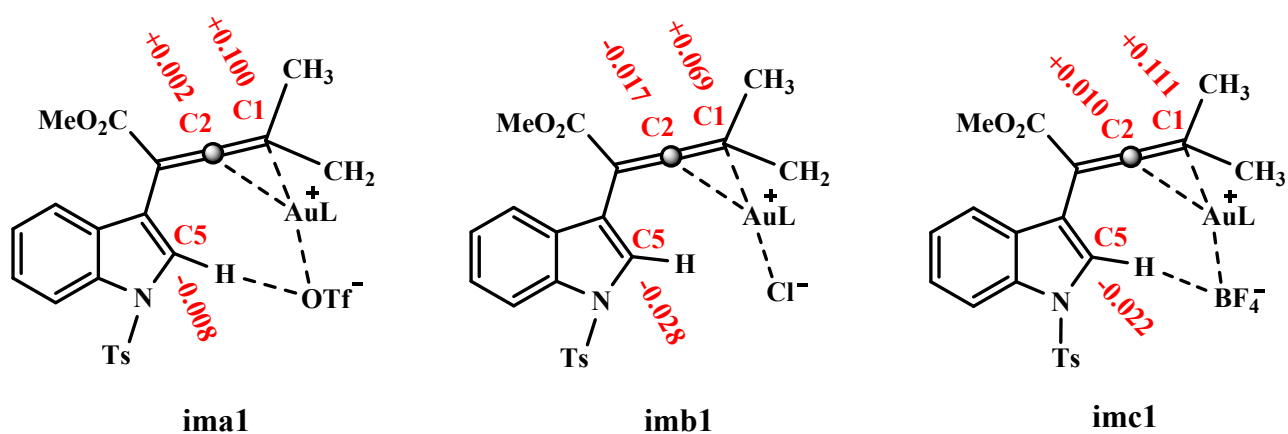


Figure S9. Optimized geometries involved in the $(\text{PPh}_3)\text{AuOTf}^-$, $(\text{PPh}_3)\text{AuCl}^-$, and $(\text{PPh}_3)\text{AuBF}_4^-$ -catalyzed cyclization reactions of indole-allenoate without OTf^- , Cl^- and BF_4^- as assisted catalysts at B3LYP/6-31G* level. The hydrogen atoms not participating in the reaction have been omitted for clarity. Bond distances are given in Å.

Scheme S3. The Mulliken charges of C1, C2 and C5 atoms in ima1, imb1 and imc1.



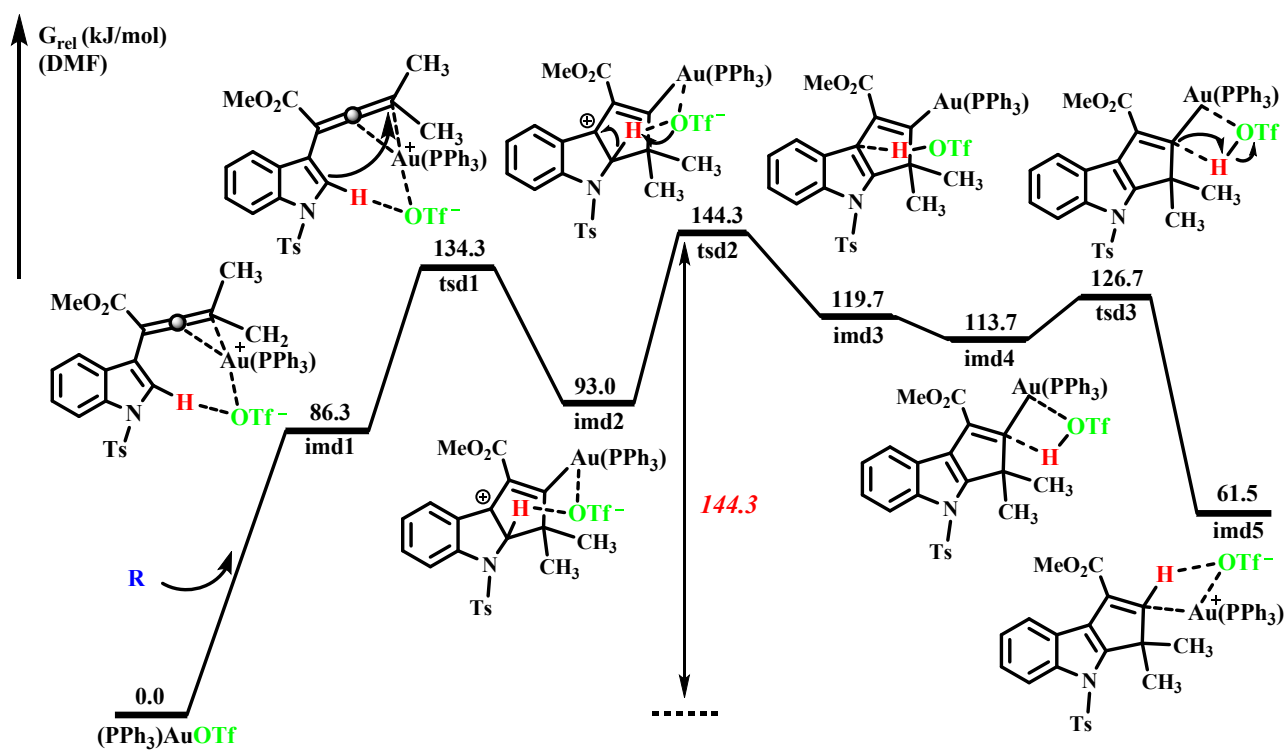


Figure S10. Energy profiles for the $(\text{PPh}_3)\text{AuOTf}$ -catalyzed cyclization reaction of indoles in DMF at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

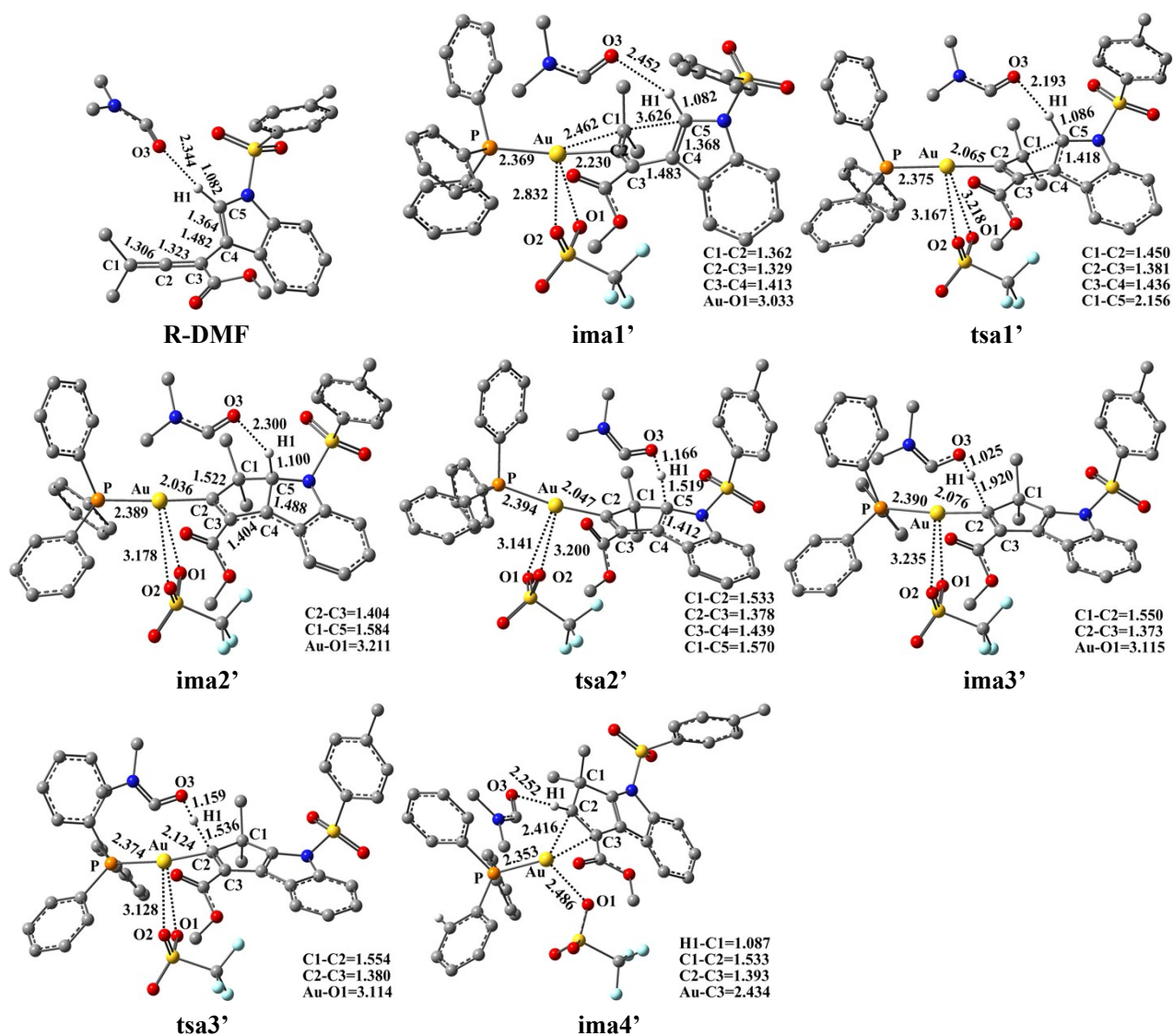
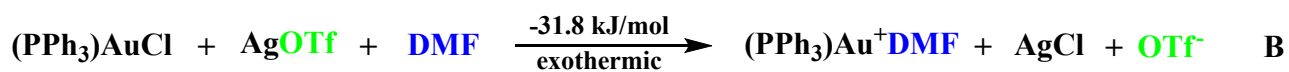
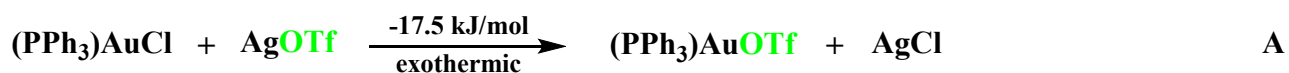


Figure S11. Optimized geometries involved in the $(\text{PPh}_3)\text{AuOTf}$ -catalyzed cyclization reaction of indole-allenoate with the assistance of DMF in DMF solvent at B3LYP/6-31G* level. The hydrogen atoms not participating in the reaction have been omitted for clarity. Bond distances are given in Å.

Scheme S4. The formation of (PPh₃)AuOTf and (PPh₃)Au⁺DMF in DMF solution.



Equation A indicates that (PPh₃)AuOTf is formed accompanied by 17.5 kJ/mol energy released. This conversion from (PPh₃)AuCl and AgOTf to (PPh₃)AuOTf and AgCl is easy. Furthermore, DMF has the strong coordination ability with the Au compared with OTf, and the formation of (PPh₃)Au⁺DMF releases energy of 31.8 kJ/mol, as described in Equation B of Scheme S4, indicating that the main mode of coordination is (PPh₃)Au⁺DMF in DMF solvent.

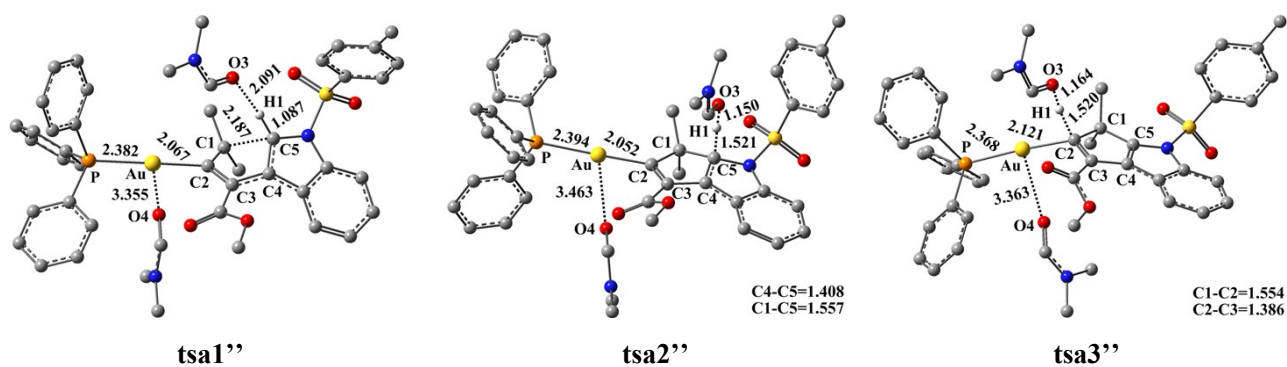


Figure S12. Optimized geometries involved in the $(\text{PPh}_3)\text{Au}^+\text{DMF}$ -catalyzed cyclization reaction of indole-allenoate with the assistance of DMF in DMF solvent at B3LYP/6-31G* level. The hydrogen atoms not participating in the reaction have been omitted for clarity. Bond distances are given in Å.

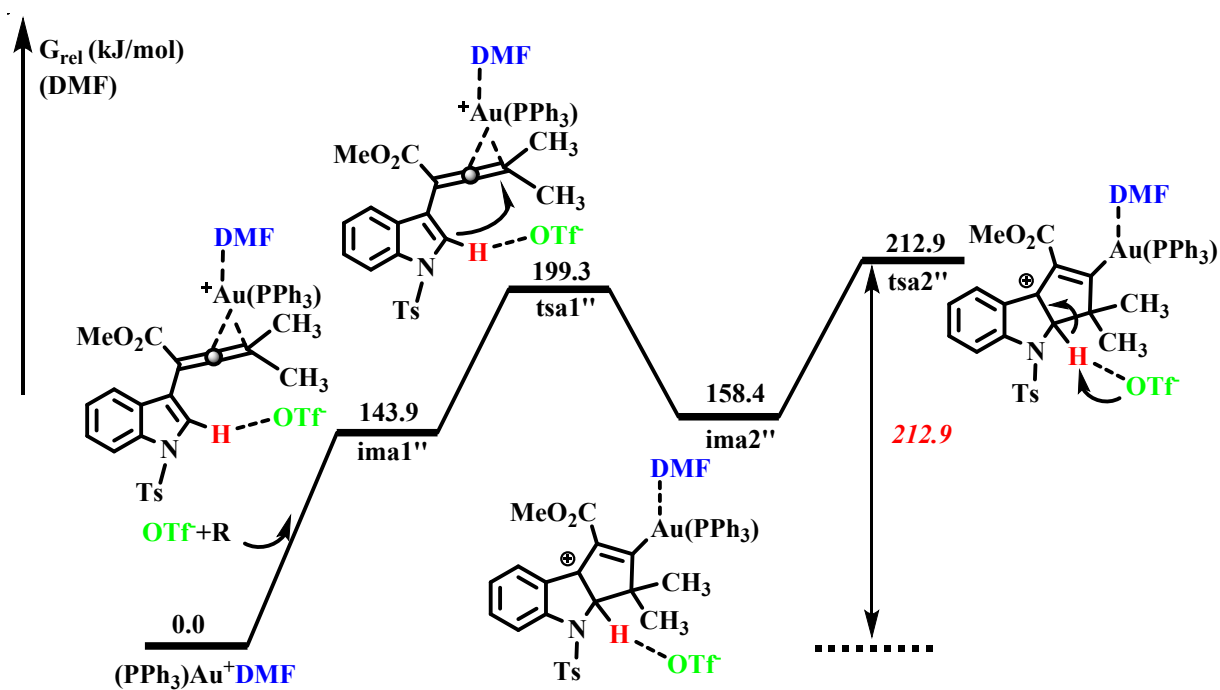


Figure S13. Energy profile for the $(\text{PPh}_3)\text{Au}^+\text{DMF}$ -catalyzed cyclization reaction of indole-allenoate with OTf as the proton-shuttle at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

Effects of solvent DMSO on the Au(I)-catalyzed cyclization reaction of indole-allenoate.

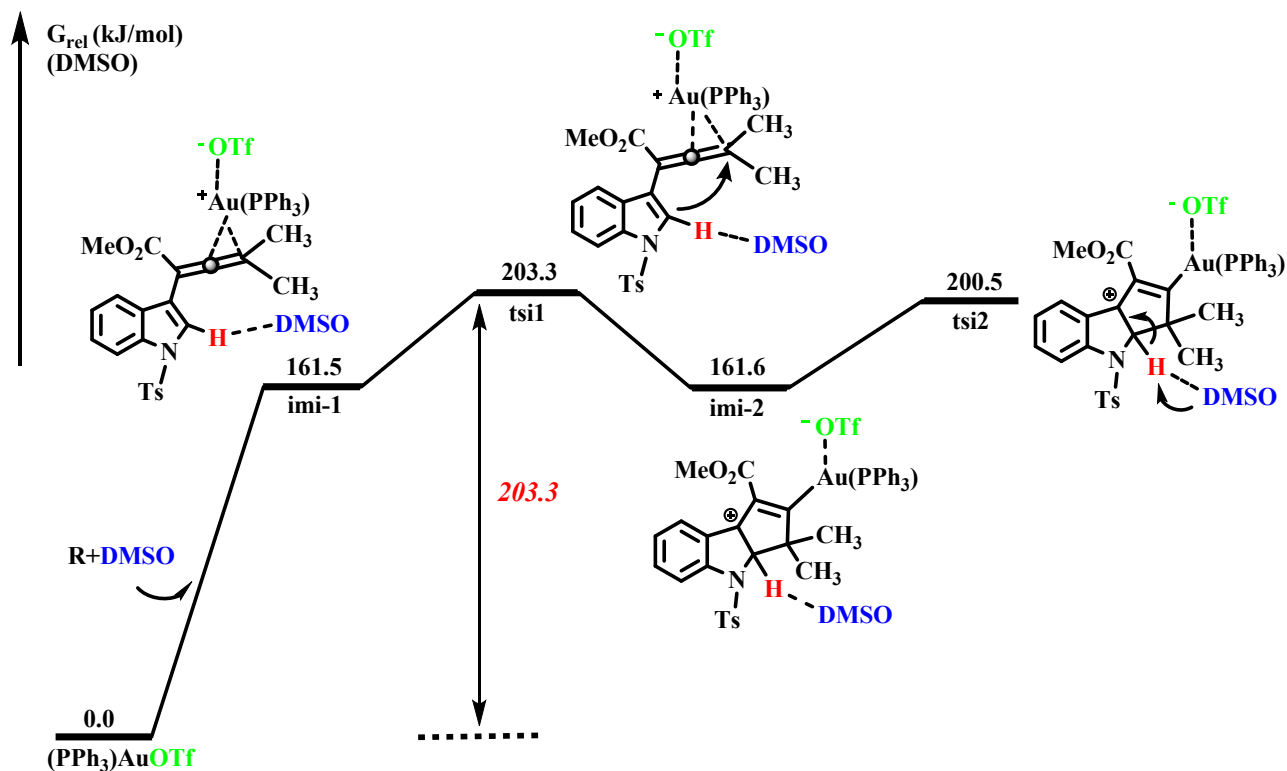


Figure S14. Energy profile for the $(\text{PPh}_3)\text{AuOTf}$ -catalyzed cyclization reaction of indole-allenoate with DMSO as the proton-shuttle at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

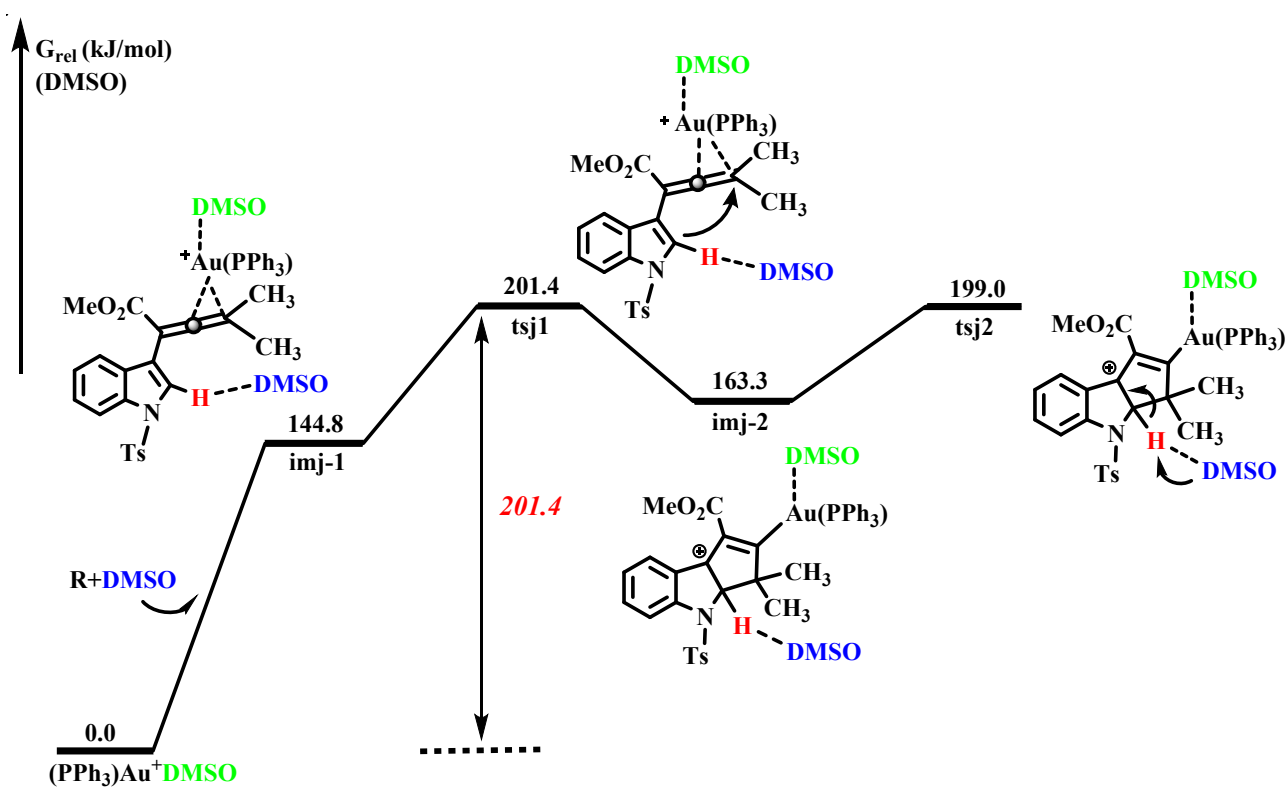


Figure S15. Energy profile for the $(\text{PPh}_3)\text{Au}^+\text{DMSO}$ -catalyzed cyclization reaction of indole-allenoate with DMSO as the proton-shuttle at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

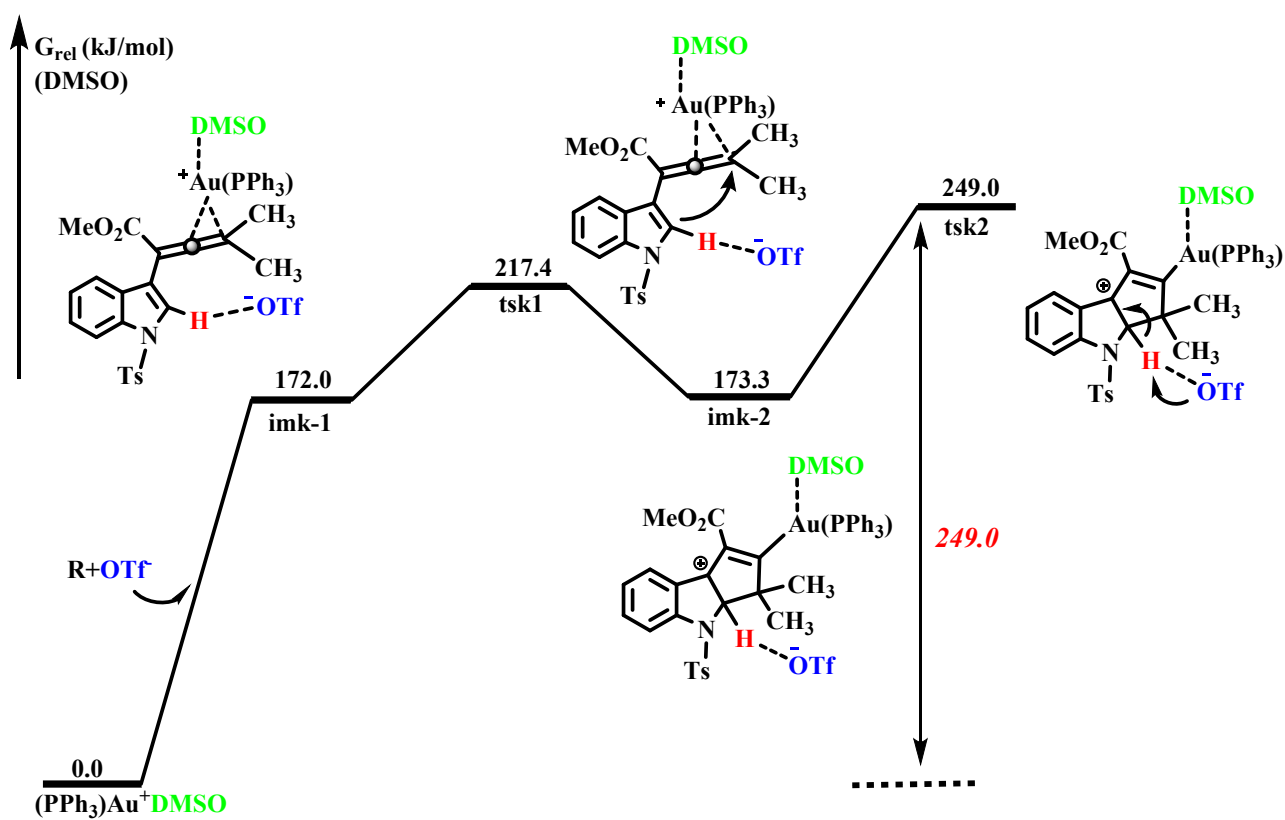


Figure S16. Energy profile for the $(\text{PPh}_3)\text{Au}^+$ DMSO-catalyzed cyclization reaction of indole-allenoate with OTf as the proton-shuttle at PCM//B3LYP/6-311++G**//B3LYP/6-31G* level.

Intrinsic Reaction Coordinates.

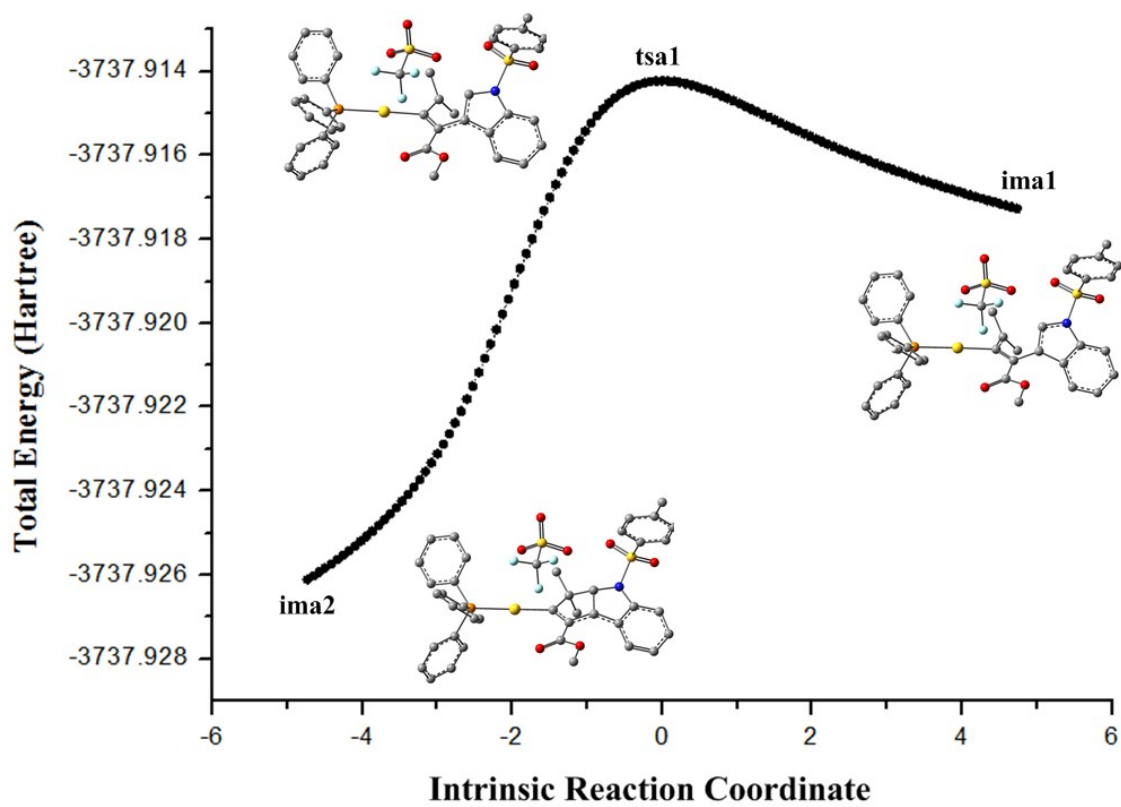


Figure S17. IRC results for tsal1.

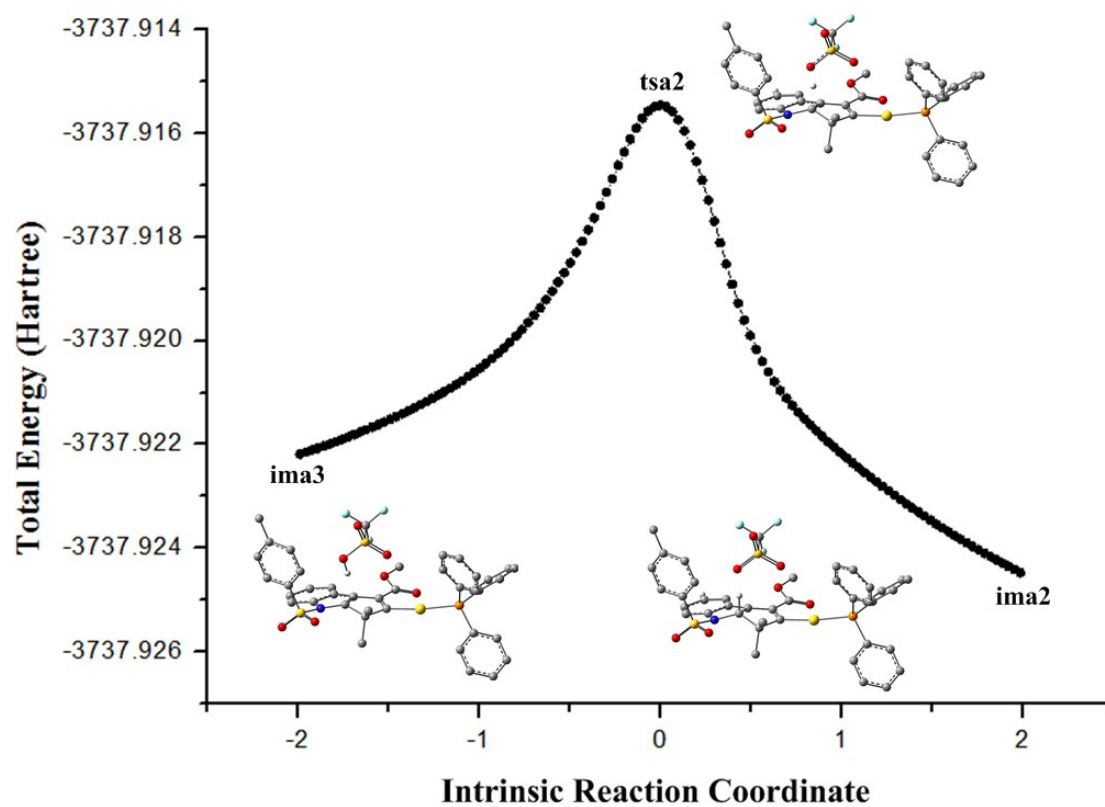


Figure S18. IRC results for tsa2.

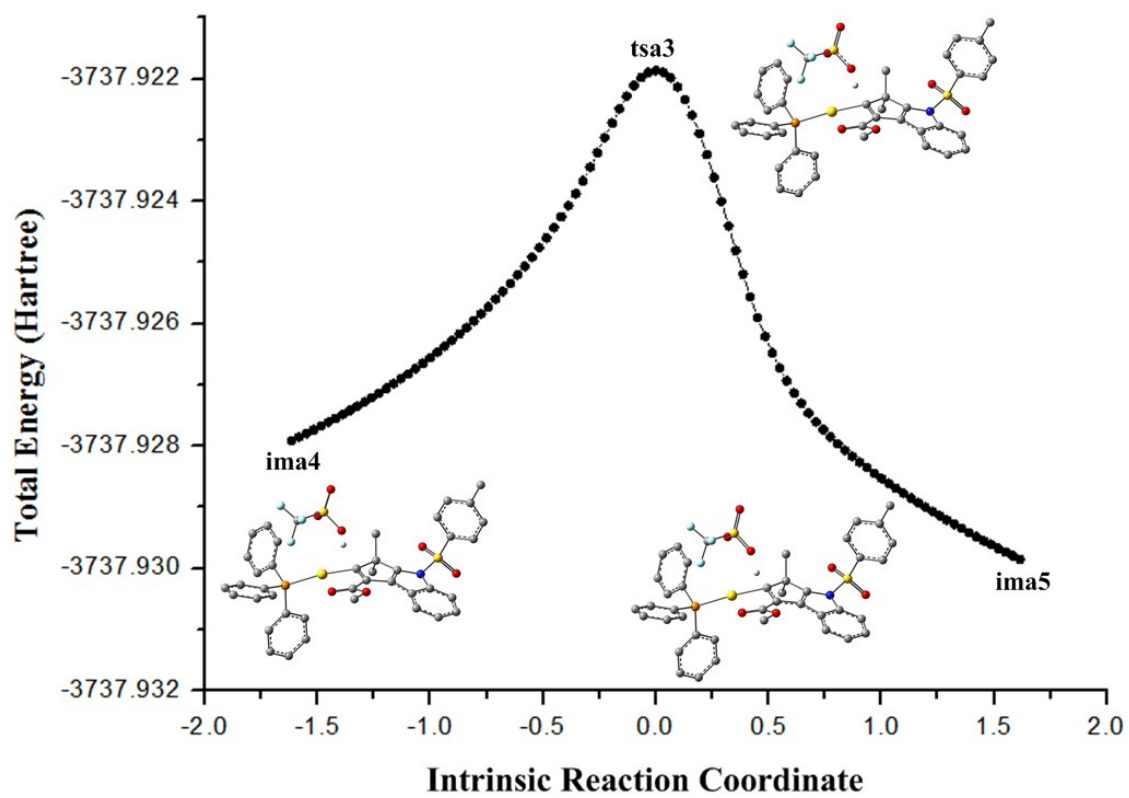


Figure S19. IRC results for tsa3.

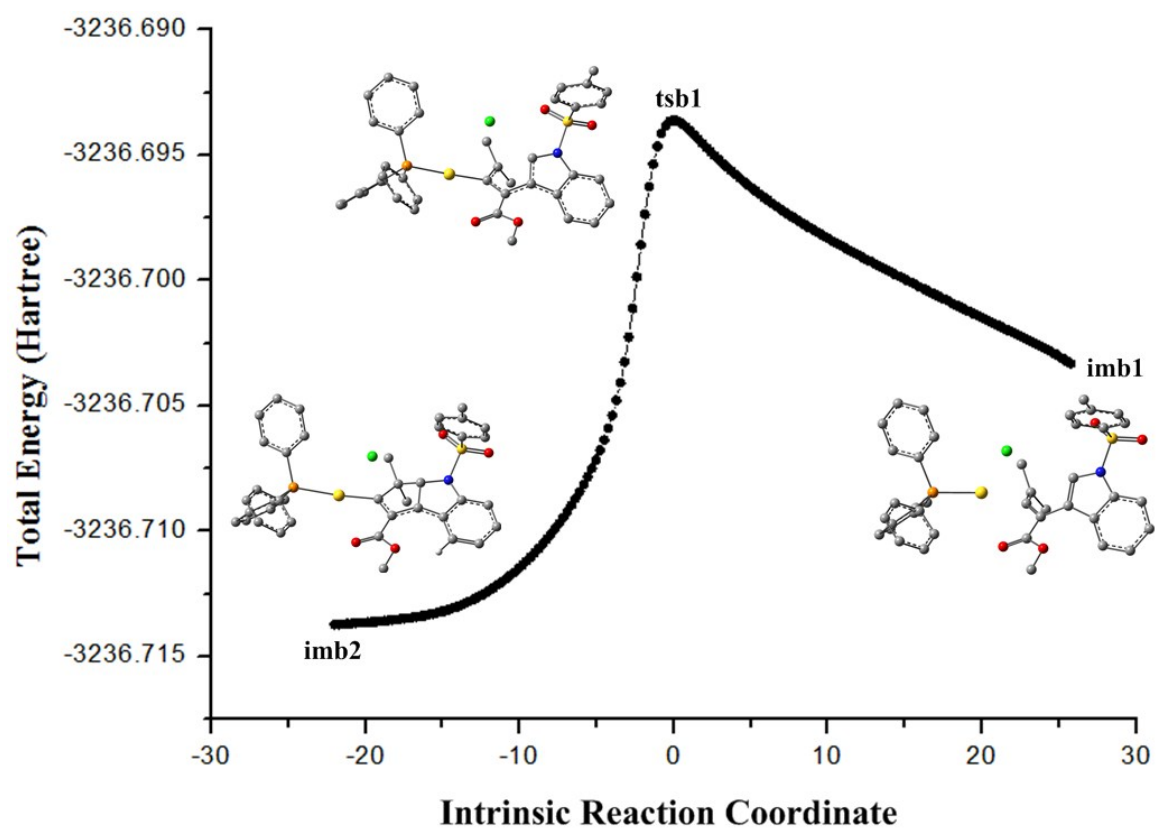


Figure S20. IRC results for tsb1.

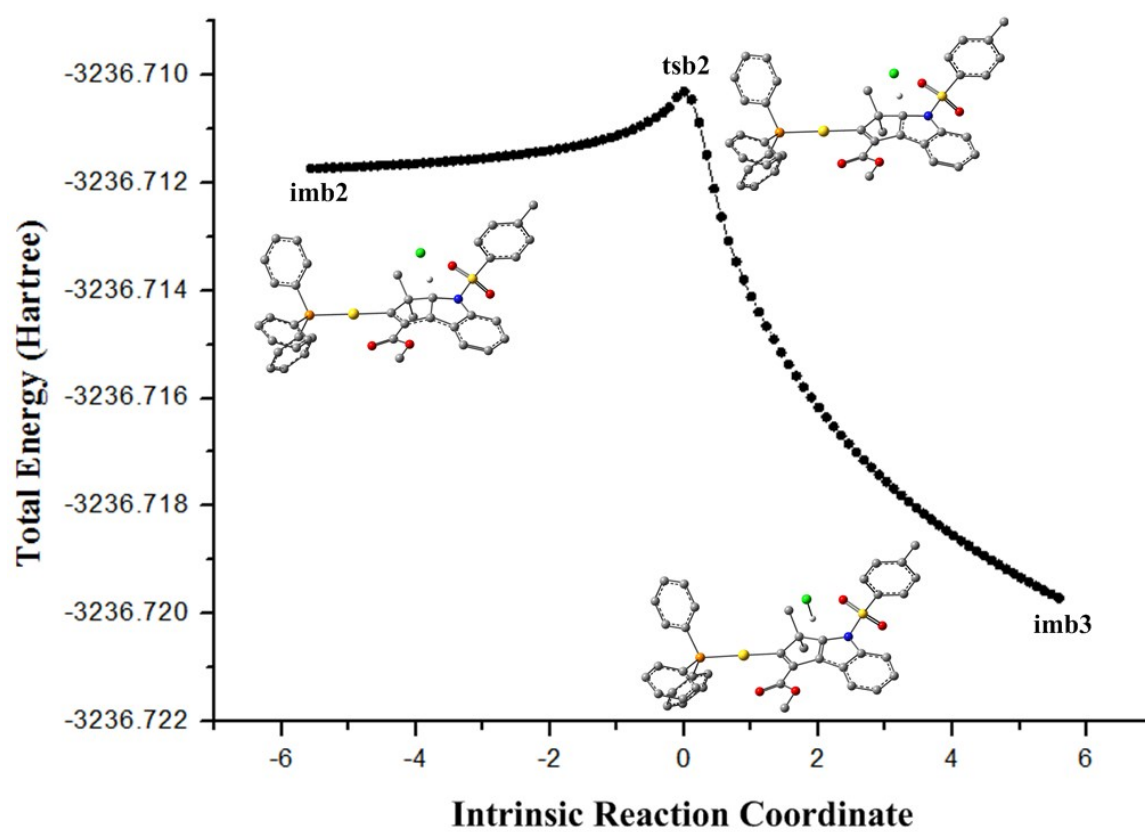


Figure S21. IRC results for **tsb2**.

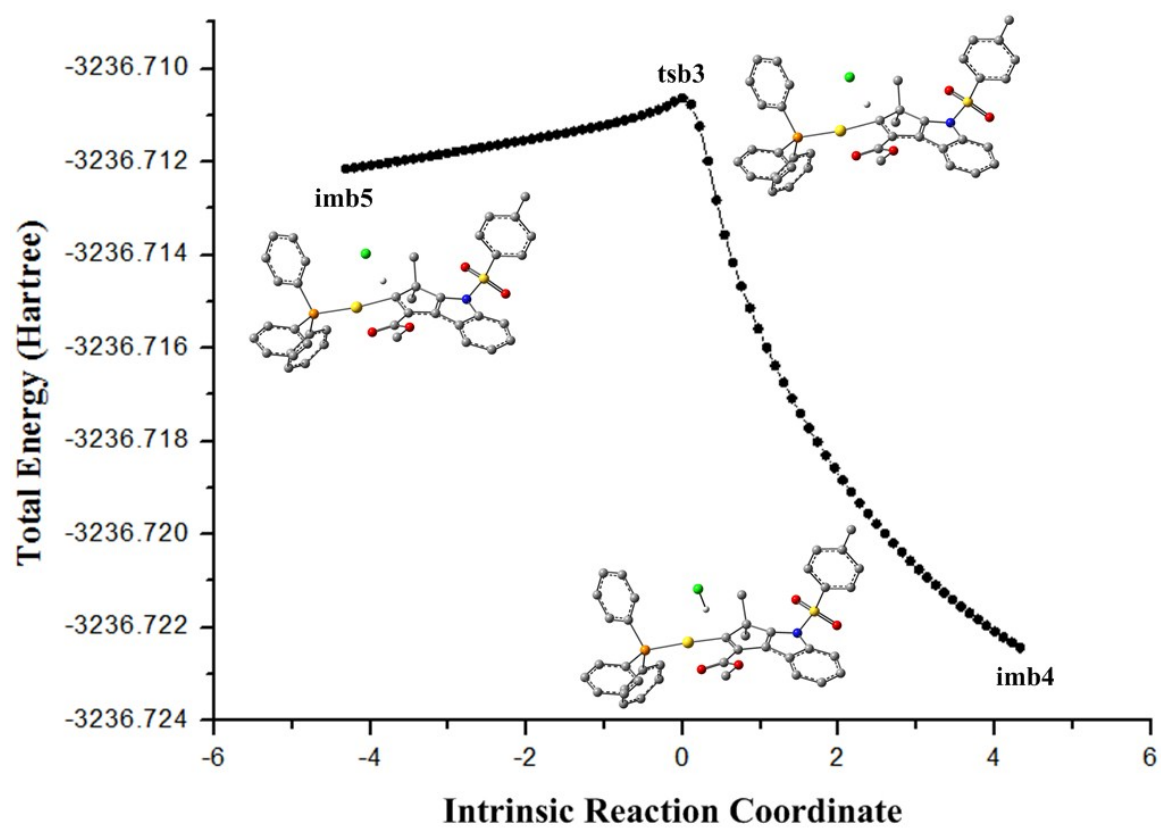


Figure S22. IRC results for **tsb3**.

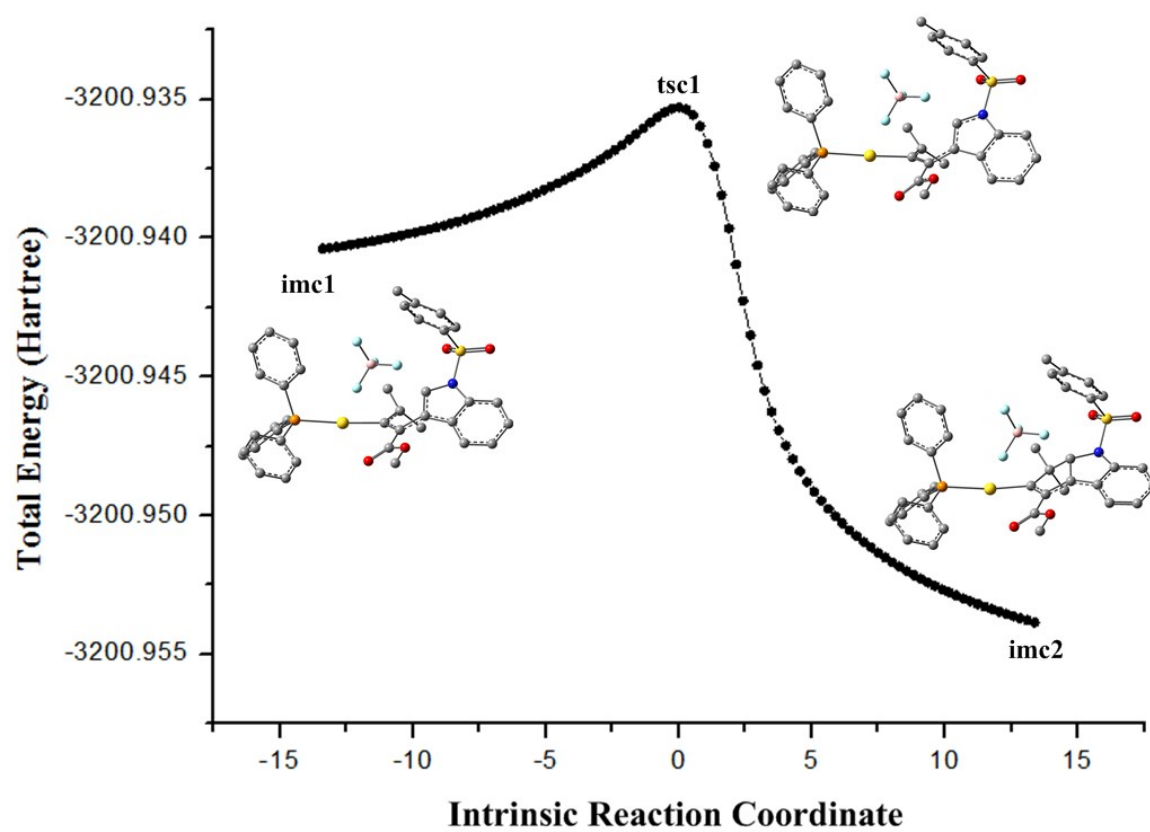


Figure S23. IRC results for tsc1.

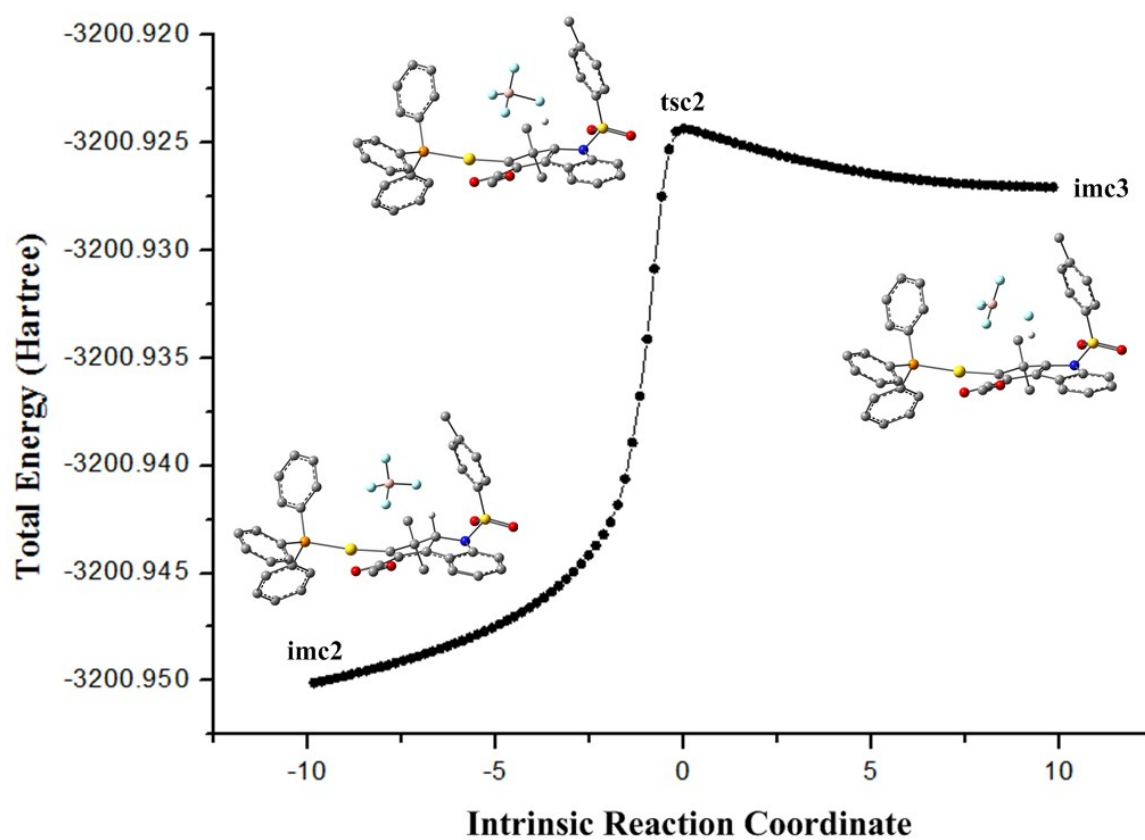


Figure S24. IRC results for tsc2.

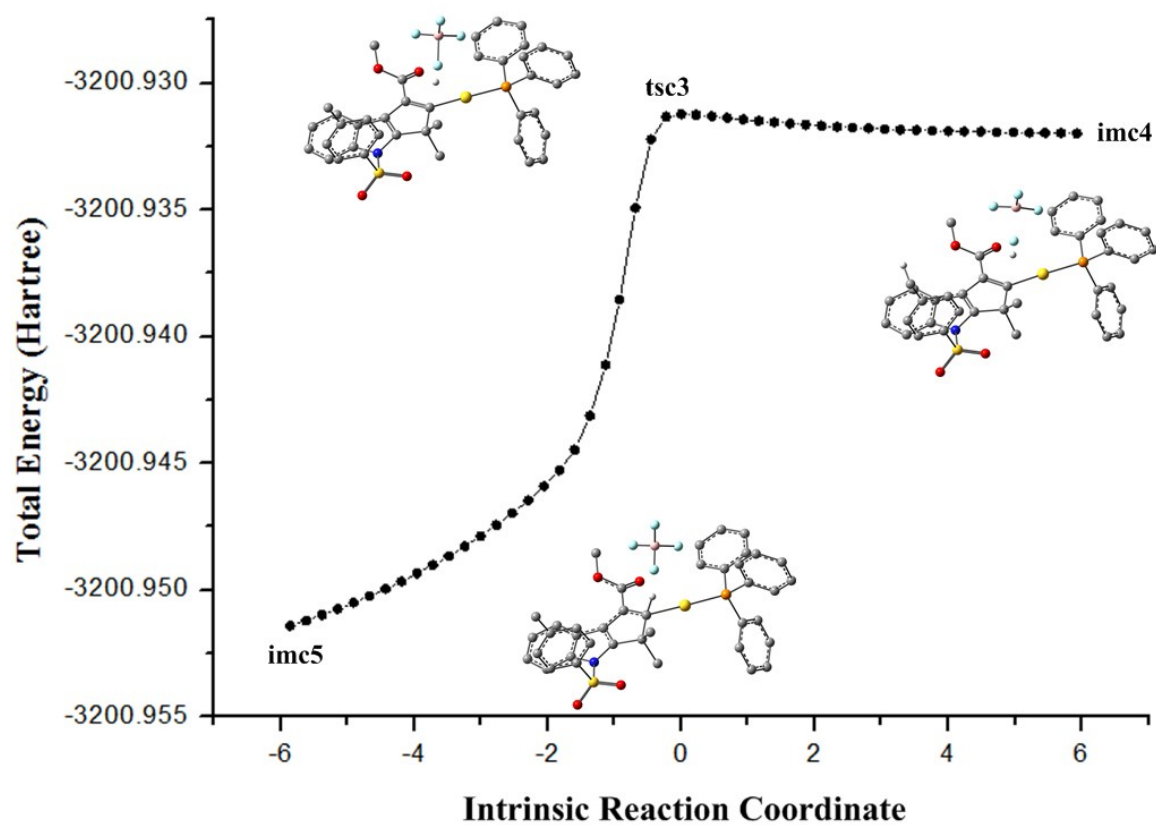


Figure S25. IRC results for tsc3.

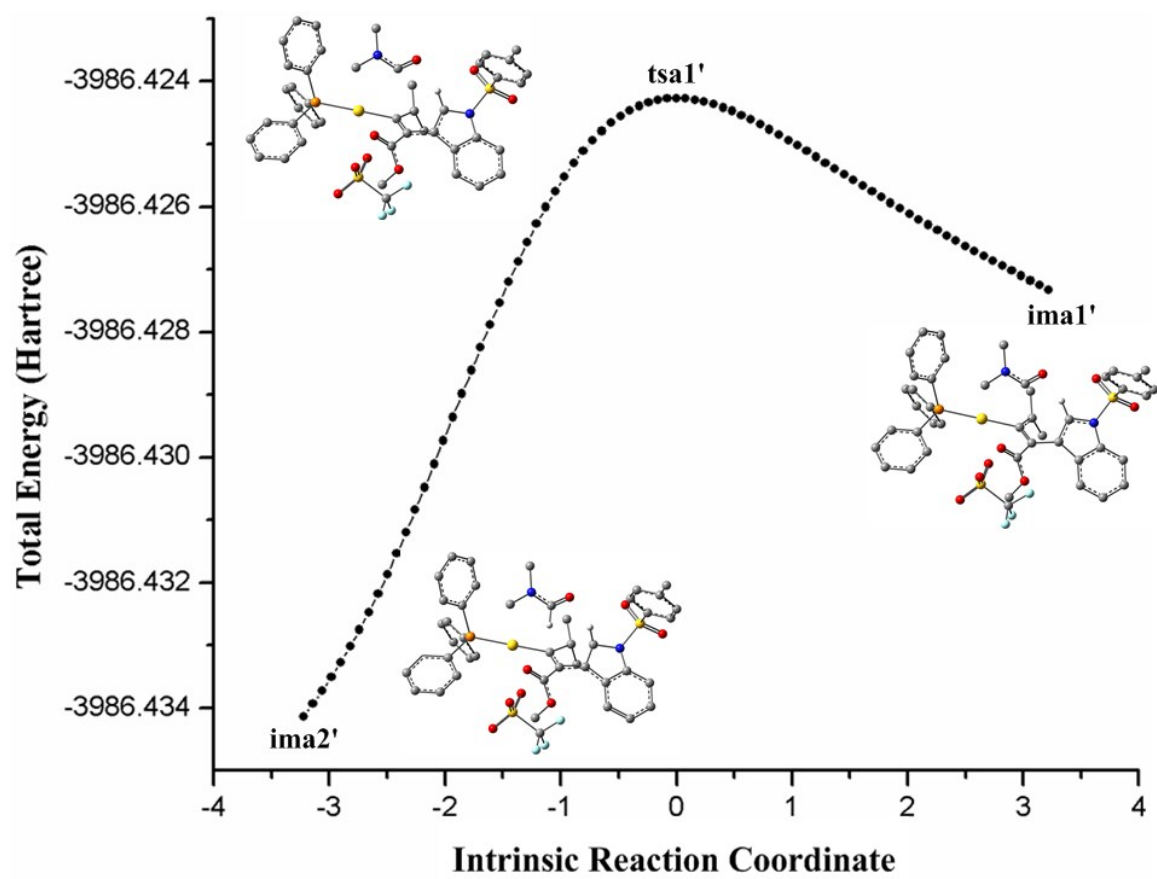


Figure S26. IRC results for tsal'.

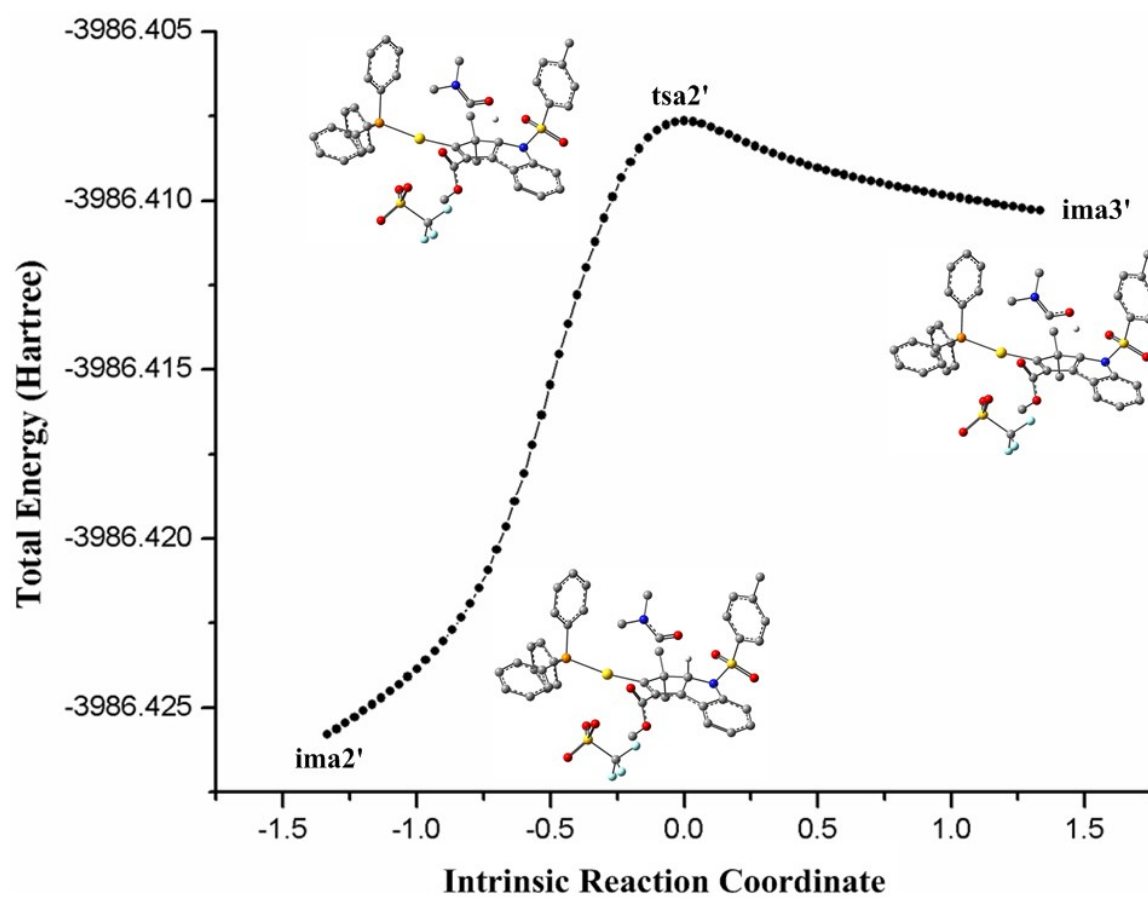


Figure S27. IRC results for tsa2'.

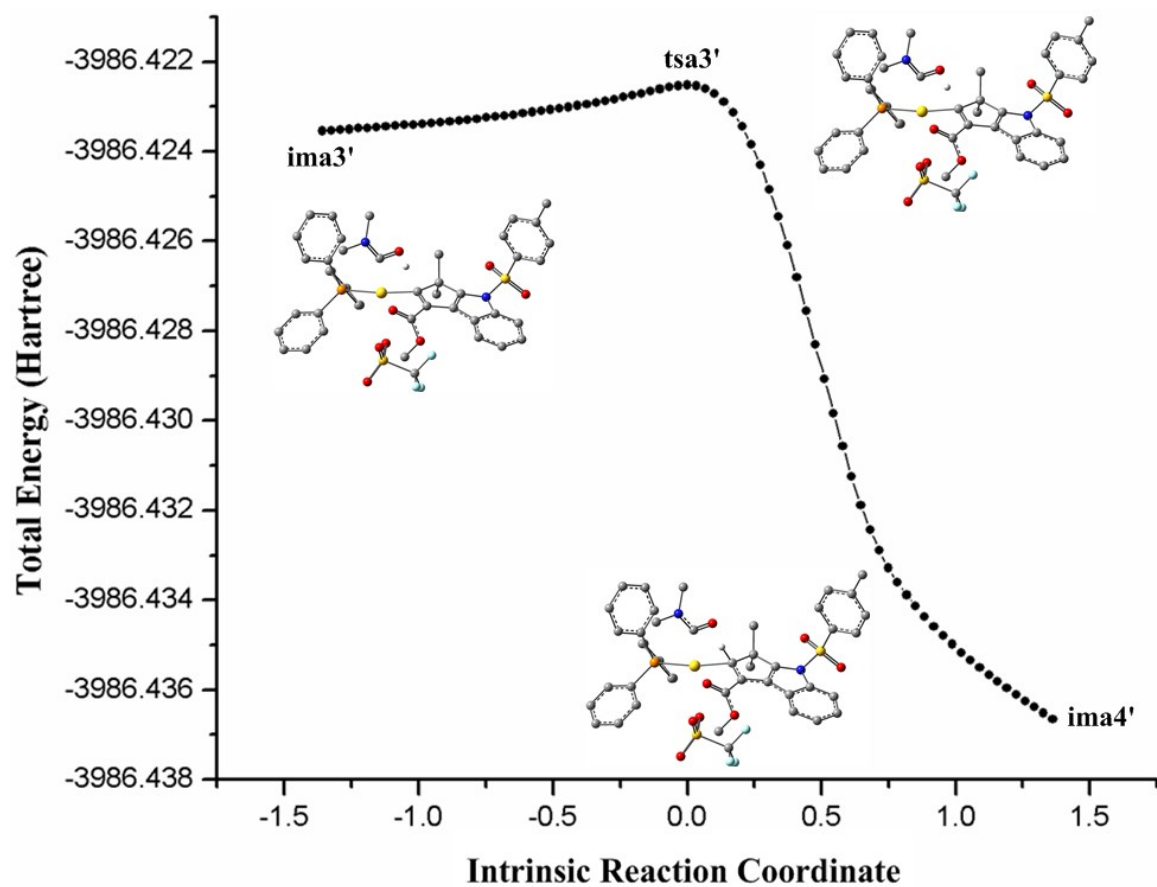


Figure S28. IRC results for tsa3'.

Cartesian coordinates of the optimized stationary points on the optimal reaction channels

Table S10. The cartesian coordinates of the optimized stationary points on the optimal reaction channels (paths a, b and c) in Figure 1.

Species	Cartesian coordinates			
R	C	-0.54939600	1.78764800	3.50598000
	C	0.62216600	1.05941600	3.77985700
	C	1.05559100	0.04057800	2.93609500
	C	0.28868700	-0.21720300	1.79726400
	C	-0.89148700	0.50706300	1.49805700
	C	-1.44419800	-0.04193600	0.27114400
	C	-0.60820400	-1.04431500	-0.12573300
	N	0.43889900	-1.19383900	0.79243900
	C	-2.71708900	0.30957500	-0.40415900
	C	-3.60806600	-0.61697300	-0.71845300
	C	-4.49306100	-1.52824800	-1.02415300
	C	-5.62997200	-1.87231900	-0.08338200
	C	-4.43939200	-2.28343100	-2.33656000
	C	-3.03161100	1.72229400	-0.80138300
	O	-4.08451600	2.10293600	-1.26909800
	O	-1.97653200	2.54378300	-0.58415900
	C	-2.18982500	3.91650200	-0.94264400
	S	1.87986600	-2.03464300	0.39197900
	O	2.51314000	-2.38220500	1.66111200
	O	1.46318300	-3.04221300	-0.58056000
	C	2.90117700	-0.82713600	-0.44404700
	C	2.74855900	-0.64232500	-1.82034100
	C	3.83159000	-0.08467100	0.28511800
	C	3.53516300	0.30792300	-2.46502500
	C	4.60905900	0.86119100	-0.37964000
	C	4.47051400	1.07806800	-1.75761600
	C	5.29567600	2.12741200	-2.46253000
	H	-2.22043100	2.07452300	2.17469700
	H	-0.86579500	2.56783200	4.19287600
	H	1.19505600	1.28367100	4.67536400
	H	1.93554900	-0.54841900	3.16418500
	H	-0.67250800	-1.70734400	-0.97490200
	H	-6.59488200	-1.68323200	-0.57139200
	H	-5.59969400	-2.93798500	0.17844200
	H	-5.58805000	-1.28643800	0.83772300
	H	-5.36650200	-2.12518700	-2.90237000
	H	-3.59834200	-1.96520800	-2.95755100
	H	-4.34951200	-3.36231300	-2.15398000

	H	-1.26553100	4.43289300	-0.68153100
	H	-2.39273400	4.00669900	-2.01340800
	H	-3.03483300	4.33405200	-0.38844100
	H	2.04135100	-1.24898700	-2.37550300
	H	3.95676100	-0.26116800	1.34738500
	H	3.42661500	0.44910200	-3.53741500
	H	5.34096500	1.43624100	0.18181300
	H	4.76272600	3.08691200	-2.49492000
	H	6.24764200	2.30029500	-1.95069200
	H	5.51082700	1.84035000	-3.49694100
imal	C	3.34211200	-3.30306600	2.22152200
	C	4.48241900	-3.92650300	2.71543300
	C	5.70677000	-3.84526500	2.02704400
	C	5.82156300	-3.14466900	0.82899300
	C	4.67429200	-2.51112200	0.34577300
	C	3.43140800	-2.57549600	1.02591300
	C	2.47337500	-1.82527300	0.23827800
	C	3.13544800	-1.34370200	-0.85753500
	N	4.46198800	-1.76561500	-0.83094300
	C	1.04921700	-1.55873100	0.50725300
	C	0.13593000	-1.77174800	-0.43598100
	C	-0.33736400	-2.15236000	-1.64739300
	C	-0.86188900	-3.55942100	-1.85901200
	C	-0.14651000	-1.29774900	-2.88356400
	C	0.61579600	-0.91662200	1.79071400
	O	-0.52948200	-0.93097100	2.21618800
	O	1.63438400	-0.32506200	2.41543300
	C	1.29194500	0.47446500	3.56043600
	S	5.65829300	-1.00708000	-1.81780400
	O	6.80181600	-1.91728300	-1.83404600
	O	4.94342700	-0.63555600	-3.03425300
	C	6.09776200	0.46562900	-0.90856300
	C	5.17905700	1.51734700	-0.80643700
	C	7.35836900	0.53896800	-0.31567600
	C	5.54239300	2.65073000	-0.08590100
	C	7.70334500	1.69048300	0.39170300
	C	6.80546700	2.75756100	0.51912500
	C	7.18132300	4.00544600	1.28191100
	H	2.39728500	-3.37692800	2.75298600
	H	4.42768500	-4.49007700	3.64284200
	H	6.58131900	-4.34754000	2.43104600
	H	6.75637500	-3.10018600	0.28405900
	H	2.77912100	-0.68476200	-1.63514000
	H	-1.78458900	-3.55458200	-2.44839800
	H	-0.10825300	-4.11686100	-2.43233000
	H	-1.03927700	-4.07964700	-0.91571700

	H	-1.06577500	-1.24366300	-3.47650700
	H	0.20679200	-0.29384400	-2.64021900
	H	0.61664100	-1.79133000	-3.50366500
	H	2.24080800	0.85190000	3.94031000
	H	0.64674600	1.29858300	3.24794400
	H	0.78415600	-0.13156600	4.31500100
	H	4.19849700	1.46118000	-1.26964200
	H	8.05412700	-0.28639700	-0.41748300
	H	4.82628000	3.46069700	0.00845600
	H	8.68584900	1.75747000	0.85197300
	H	6.42108600	4.25628000	2.03090000
	H	8.13994000	3.88915000	1.79682300
	H	7.26523200	4.86826500	0.60909100
	P	-4.09675200	0.01698000	0.04275200
	C	-5.43262600	-1.22047600	-0.20790000
	C	-6.52232600	-1.33756900	0.66534500
	C	-7.51450200	-2.29226200	0.42637300
	C	-7.43022500	-3.13111100	-0.68465500
	C	-6.34600900	-3.01920100	-1.56004600
	C	-5.34962100	-2.07524700	-1.32001400
	C	-4.36695800	0.76016700	1.69445200
	C	-3.58042900	0.34821600	2.78051600
	C	-3.80296200	0.89501800	4.04598200
	C	-4.79869700	1.85444700	4.23392900
	C	-5.57356500	2.27842100	3.15107700
	C	-5.35789000	1.73792400	1.88403000
	C	-4.39024100	1.34645700	-1.17984700
	C	-5.63065000	1.52680200	-1.81188500
	C	-5.79785700	2.57337800	-2.72071000
	C	-4.73503500	3.43581700	-3.00350000
	C	-3.49972900	3.25551400	-2.37687600
	C	-3.32387200	2.21344700	-1.46685500
	Au	-1.95150900	-0.92561700	-0.22174900
	S	0.52135200	2.22469300	-0.81138100
	O	1.48444000	1.38754200	-1.57057100
	O	-0.17329500	3.27101700	-1.58296300
	O	-0.35277300	1.45327900	0.12309700
	C	1.61038700	3.16865800	0.36522000
	F	2.45563800	3.97359400	-0.30829300
	F	0.88277100	3.92813500	1.19669200
	F	2.35200700	2.32731700	1.11192500
	H	-6.59726800	-0.69047300	1.53291800
	H	-8.35213800	-2.37802500	1.11299200
	H	-8.20254200	-3.87310900	-0.86734500
	H	-6.27274100	-3.67256400	-2.42500700
	H	-4.50100200	-2.00088000	-1.99551600

	H	-2.77829800	-0.36898600	2.63835200
	H	-3.18594200	0.57663100	4.88140200
	H	-4.96382700	2.28185800	5.21925700
	H	-6.33882900	3.03700300	3.29004600
	H	-5.94847400	2.08575400	1.04152600
	H	-6.45697800	0.85280100	-1.60588100
	H	-6.75774200	2.70963000	-3.21180100
	H	-4.87010100	4.24403100	-3.71749300
	H	-2.65530200	3.90392000	-2.58877900
	H	-2.35501300	2.08388200	-0.99455800
tsa1	C	3.79237800	-3.65911800	1.57885100
	C	5.01569000	-4.30984500	1.57103200
	C	6.02845900	-3.93218900	0.66618200
	C	5.84471900	-2.90475000	-0.25198700
	C	4.61746100	-2.23333200	-0.22699700
	C	3.58261800	-2.59143600	0.68472200
	C	2.44375400	-1.77223400	0.35946800
	C	2.83737900	-0.88089200	-0.67006800
	N	4.14367400	-1.19552700	-1.04777000
	C	1.02391900	-1.81848300	0.60274400
	C	0.27955800	-1.41035800	-0.48949300
	C	1.01509000	-1.37387100	-1.73671300
	C	1.45067700	-2.68799300	-2.36059100
	C	0.75998800	-0.26718800	-2.72719300
	C	0.40484800	-2.14361900	1.91899600
	O	-0.78685200	-2.23554000	2.13848700
	O	1.33934400	-2.32116300	2.88068900
	C	0.82580300	-2.58627600	4.19660900
	S	5.09359900	-0.14298500	-2.06615700
	O	6.16457000	-0.98858200	-2.58944400
	O	4.09777800	0.47637700	-2.93283400
	H	3.00949500	-3.94547900	2.26962700
	H	5.19672600	-5.12580500	2.26443800
	H	6.97541500	-4.46467500	0.67610700
	H	6.61158500	-2.63814900	-0.96753000
	H	2.48073400	0.14693600	-0.74135200
	H	0.61671400	-3.05524600	-2.97490700
	H	2.30694400	-2.54208200	-3.02642100
	H	1.68654500	-3.45275100	-1.61807700
	H	-0.06819300	-0.57173300	-3.38375300
	H	0.48457800	0.66777400	-2.23515400
	H	1.64230600	-0.11052000	-3.35575200
	H	1.70341300	-2.70725200	4.83202100
	H	0.21673800	-1.74607600	4.53920700
	H	0.21650300	-3.49398600	4.19775500
	Au	-1.67591900	-0.74697800	-0.41318400

	S	0. 65801900	2. 75794500	0. 04310800
	O	1. 86096700	1. 89104000	-0. 14025300
	O	0. 93109500	4. 20057700	0. 07312100
	O	-0. 51124800	2. 32142100	-0. 76141200
	C	0. 14358800	2. 35657900	1. 78632100
	F	1. 09802600	2. 70565100	2. 66302700
	F	-0. 98687500	2. 99860900	2. 11384100
	F	-0. 08112300	1. 02935100	1. 93688400
	P	-3. 92546300	0. 00218600	-0. 24726600
	C	-5. 13399100	-1. 38077500	-0. 33799600
	C	-6. 32460400	-1. 38438500	0. 40367800
	C	-7. 22390900	-2. 44608900	0. 28562100
	C	-6. 94436300	-3. 51091800	-0. 57270800
	C	-5. 75925100	-3. 51590900	-1. 31204800
	C	-4. 85586800	-2. 46011600	-1. 19193400
	C	-4. 24094100	0. 83402300	1. 35753700
	C	-3. 53883100	0. 39479400	2. 49192800
	C	-3. 76909700	0. 99544300	3. 72970600
	C	-4. 68881500	2. 03989600	3. 84516500
	C	-5. 38184000	2. 48615100	2. 71835300
	C	-5. 15942200	1. 88785700	1. 47719700
	C	-4. 43107400	1. 19459500	-1. 54658400
	C	-5. 69002600	1. 14026700	-2. 16422400
	C	-6. 03154400	2. 08056000	-3. 13825400
	C	-5. 12296200	3. 07757200	-3. 49870800
	C	-3. 86923100	3. 13312300	-2. 88523600
	C	-3. 51451800	2. 19491800	-1. 91481900
	H	-6. 54665200	-0. 56291000	1. 07785100
	H	-8. 14125800	-2. 44087100	0. 86806500
	H	-7. 64425900	-4. 33751200	-0. 66054300
	H	-5. 53272900	-4. 34615100	-1. 97535000
	H	-3. 92659600	-2. 47448600	-1. 75561500
	H	-2. 80774100	-0. 40497900	2. 40669700
	H	-3. 21829800	0. 65491700	4. 60204300
	H	-4. 85710800	2. 51267100	4. 80902500
	H	-6. 08934900	3. 30664000	2. 80125100
	H	-5. 68951800	2. 24941200	0. 60124100
	H	-6. 40092200	0. 36593100	-1. 89264500
	H	-7. 00664100	2. 03019000	-3. 61559800
	H	-5. 39045400	3. 80703100	-4. 25875000
	H	-3. 15563400	3. 90394800	-3. 16197700
	H	-2. 53079300	2. 24772900	-1. 45374400
	C	5. 78369100	1. 07030100	-0. 96120500
	C	7. 12761400	0. 96150200	-0. 59540100
	C	4. 97322600	2. 11021400	-0. 49110500
	C	7. 66558700	1. 91789400	0. 26381200

	H	7.73833300	0.15680300	-0.98913800
	C	5.53508500	3.04628700	0.37179700
	H	3.92556700	2.19199900	-0.76471500
	C	6.88213800	2.96926900	0.76044300
	H	8.71162800	1.84664800	0.55033800
	H	4.90609000	3.84927700	0.74693000
	C	7.46952700	4.00787300	1.68528700
	H	8.48793800	3.74766400	1.98940100
	H	7.50502000	4.99071700	1.19881000
	H	6.86126700	4.12059400	2.59020500
ima2	C	4.00266100	-2.61148400	2.61052300
	C	5.24708200	-3.18749900	2.77145700
	C	6.13278900	-3.28754000	1.67473200
	C	5.80676600	-2.82582500	0.40684200
	C	4.54969900	-2.22331200	0.23503300
	C	3.64502900	-2.10890900	1.33943200
	C	2.44546100	-1.55798500	0.82318700
	C	2.67155900	-1.13321400	-0.57505400
	N	3.96658900	-1.73244700	-0.93824200
	C	1.06726100	-1.44961500	1.11545100
	C	0.35332300	-1.28403700	-0.07675300
	C	1.28211800	-1.42975000	-1.27216800
	C	1.25257600	-2.90075000	-1.75704100
	C	0.91520900	-0.47980300	-2.42108100
	C	0.43038500	-1.44233500	2.45739000
	O	-0.75982400	-1.55269000	2.67352200
	O	1.33907500	-1.25982500	3.44241300
	C	0.78635900	-1.08449800	4.75896000
	S	4.91468400	-1.02643600	-2.22817900
	O	6.06772700	-1.91178700	-2.38764800
	O	3.94880700	-0.82316300	-3.30212800
	C	5.45797500	0.54871200	-1.59932100
	C	4.57080500	1.63021500	-1.60005100
	C	6.74239300	0.66301300	-1.05758300
	C	4.96740900	2.83181500	-1.02092700
	C	7.12906200	1.88357500	-0.50932400
	C	6.24994300	2.97743200	-0.47171900
	C	6.67145300	4.29232700	0.13773100
	H	3.30337600	-2.52298000	3.43176600
	H	5.54941400	-3.57222500	3.74042700
	H	7.10265100	-3.75485400	1.82346100
	H	6.48661700	-2.93422000	-0.42718900
	H	2.74696000	-0.03098000	-0.53381700
	H	0.24671900	-3.16101000	-2.10116400
	H	1.95110700	-3.01204700	-2.59238600
	H	1.53635000	-3.60107100	-0.96455300

	H	-0.05983600	-0.76556200	-2.83118400
	H	0.83873500	0.55222800	-2.06967200
	H	1.65835700	-0.54370900	-3.21867100
	H	1.64346600	-0.94489000	5.41815100
	H	0.14371600	-0.20093100	4.77368700
	H	0.20607800	-1.96200400	5.05556800
	H	3.57903600	1.53932100	-2.02505200
	H	7.42295500	-0.18071200	-1.08140700
	H	4.24968900	3.64588200	-0.96843900
	H	8.12830500	1.98557100	-0.09348100
	H	5.86392000	4.72318900	0.73897400
	H	7.55421600	4.17735100	0.77464100
	H	6.91819300	5.02397300	-0.64276400
	P	-3.90644800	-0.11580700	-0.35678500
	C	-4.18992400	1.26305500	-1.53008000
	C	-5.37833900	1.38052200	-2.26902600
	C	-5.56035700	2.46326100	-3.13028900
	C	-4.56078500	3.43099300	-3.26015900
	C	-3.37595900	3.31314400	-2.53105800
	C	-3.18252800	2.23196500	-1.66931700
	C	-4.99782900	-1.48332600	-0.92404800
	C	-4.55478600	-2.28282500	-1.99108800
	C	-5.35024200	-3.32193200	-2.47119800
	C	-6.59127500	-3.58283800	-1.88393300
	C	-7.03381400	-2.79891200	-0.81784700
	C	-6.24272200	-1.75185200	-0.33845600
	C	-4.57691400	0.43237000	1.26125300
	C	-5.62233900	1.36493000	1.35109600
	C	-6.11861800	1.74444200	2.59869600
	C	-5.57433100	1.20047700	3.76428400
	C	-4.52723900	0.28089100	3.68085600
	C	-4.02320500	-0.10101300	2.43656300
	Au	-1.61834500	-0.78595300	-0.21264900
	S	1.05335600	2.75043700	0.14587200
	O	2.00797100	1.60752900	0.22660400
	O	1.68883700	4.07050000	-0.01224400
	O	-0.12954300	2.48564900	-0.70741200
	C	0.33861900	2.77463100	1.86365600
	F	1.28479000	3.01923200	2.78362800
	F	-0.61384500	3.71087300	1.97721000
	F	-0.22262300	1.57874600	2.16400100
	H	-6.15471300	0.62603200	-2.18110900
	H	-6.48040600	2.54704100	-3.70270500
	H	-4.70386500	4.27095200	-3.93491100
	H	-2.58728900	4.05298500	-2.63130700
	H	-2.24364300	2.15347500	-1.12690300

	H	-3.58417600	-2.09131500	-2.44185100
	H	-4.99761500	-3.93271000	-3.29770800
	H	-7.20763600	-4.39777200	-2.25363900
	H	-7.99559100	-3.00090500	-0.35419400
	H	-6.59340300	-1.14967800	0.49371500
	H	-6.03811200	1.80512200	0.44969700
	H	-6.92415600	2.47117200	2.65919000
	H	-5.95827800	1.50221000	4.73512000
	H	-4.08957400	-0.13291200	4.58500300
	H	-3.18800700	-0.79396500	2.38425800
tsa2	C	-3.61017400	3.76717400	0.24375700
	C	-4.88230300	4.28093700	0.06499800
	C	-5.82657000	3.59375800	-0.72511700
	C	-5.52899900	2.38993700	-1.34866100
	C	-4.24047700	1.86168200	-1.16809700
	C	-3.27676900	2.54022200	-0.36374900
	C	-2.07759400	1.76289000	-0.43269100
	C	-2.34499300	0.54881000	-1.11649800
	N	-3.66488200	0.69835900	-1.69566700
	C	-0.64996900	1.87477900	-0.21799300
	C	-0.00180900	0.88793800	-0.93319900
	C	-1.00190100	0.09966400	-1.77380200
	C	-0.95024600	0.65167000	-3.22585400
	C	-0.70136700	-1.40959100	-1.78348400
	C	0.05176200	2.82747600	0.66885100
	O	1.25796200	2.98782900	0.73342100
	O	-0.80415400	3.53025700	1.45216700
	C	-0.18579700	4.43633600	2.37755000
	S	-4.58084800	-0.54733200	-2.48045700
	O	-5.52066000	0.16368600	-3.34580500
	O	-3.57876400	-1.45846100	-3.02502300
	H	-2.87088000	4.28168200	0.84246400
	H	-5.15736900	5.22304800	0.52991500
	H	-6.81508000	4.02331400	-0.86430600
	H	-6.25039000	1.90158700	-1.98885100
	H	-2.47747800	-0.26578100	0.03152500
	H	0.04567400	0.48454400	-3.64860000
	H	-1.68747300	0.12627600	-3.83934800
	H	-1.16148500	1.72529100	-3.25394400
	H	0.27075300	-1.58113500	-2.25815300
	H	-0.64919700	-1.81043500	-0.76934400
	H	-1.46359700	-1.94618200	-2.35079200
	H	-1.00724800	4.90784000	2.91846400
	H	0.46291300	3.89135000	3.06806100
	H	0.40734800	5.18626000	1.84718000
	Au	1.96471000	0.38103200	-0.70554100

	S	-1.78629800	-1.45056500	2.05428700
	O	-2.78389500	-1.01702600	0.94632100
	O	-2.21705100	-2.70731500	2.66144300
	O	-0.38582900	-1.27992000	1.65248400
	C	-2.08772000	-0.12917500	3.32866900
	F	-3.34544600	-0.18212500	3.77459800
	F	-1.25203900	-0.30279000	4.35779100
	F	-1.86950700	1.08183000	2.79445900
	P	4.17652300	-0.35245200	-0.19760900
	C	4.16803500	-2.07012300	0.45301900
	C	5.24070500	-2.95303000	0.25218000
	C	5.19695800	-4.24220300	0.78543200
	C	4.08419700	-4.65996900	1.51892300
	C	3.01085600	-3.78846100	1.71555800
	C	3.04629700	-2.49916600	1.18258400
	C	5.32250400	-0.37719100	-1.63570800
	C	4.83191300	-0.88431600	-2.85117900
	C	5.65161500	-0.93369000	-3.97728700
	C	6.96617600	-0.46437400	-3.90796000
	C	7.45668700	0.05151100	-2.70810100
	C	6.64080400	0.09541300	-1.57456400
	C	4.98440800	0.67113600	1.09439500
	C	6.04800300	0.18270900	1.87158900
	C	6.64929000	0.99692400	2.83110600
	C	6.19078800	2.30219900	3.02839300
	C	5.12440000	2.78755400	2.27044100
	C	4.51702600	1.97763700	1.30833700
	H	6.10313200	-2.64009300	-0.32949200
	H	6.02978800	-4.92094500	0.62184000
	H	4.05027400	-5.66600700	1.92843800
	H	2.13559500	-4.10948600	2.27283300
	H	2.19360700	-1.84031900	1.32576900
	H	3.80447600	-1.23381100	-2.91419400
	H	5.26084400	-1.32867600	-4.91095800
	H	7.60217400	-0.49500500	-4.78844300
	H	8.47563800	0.42464200	-2.65041500
	H	7.03087900	0.50378800	-0.64776100
	H	6.39750000	-0.83698300	1.73770600
	H	7.46970700	0.60955600	3.42915900
	H	6.65733400	2.93357200	3.77991700
	H	4.75200500	3.79521700	2.43207100
	H	3.66547800	2.35350300	0.74871800
	C	-5.51317700	-1.40587800	-1.22283800
	C	-6.83822900	-1.03749400	-0.97631600
	C	-4.91418100	-2.45898600	-0.52549200
	C	-7.55891600	-1.72565500	-0.00206900

	H	-7.30325600	-0.24758600	-1.55418300
	C	-5.64966300	-3.12808400	0.44678200
	H	-3.89203800	-2.74595400	-0.73523500
	C	-6.97724800	-2.77114500	0.72817200
	H	-8.59178300	-1.44740000	0.19052500
	H	-5.17693700	-3.93273400	1.00324600
	C	-7.75272400	-3.50020600	1.79883600
	H	-7.74148400	-4.58339100	1.62946900
	H	-7.31195500	-3.32536100	2.78816100
	H	-8.79645100	-3.17347300	1.83363400
ima3	C	-3.80225000	0.06495700	-3.49593000
	C	-5.04916900	-0.22365800	-4.03878400
	C	-5.88657400	-1.18571100	-3.45123800
	C	-5.49854600	-1.88536300	-2.31056400
	C	-4.24579400	-1.59156100	-1.76617600
	C	-3.38793300	-0.61572000	-2.34126900
	C	-2.19121900	-0.59796300	-1.52010100
	C	-2.34386000	-1.51678000	-0.50665400
	N	-3.58135600	-2.17242800	-0.64766800
	C	-0.77787800	-0.16496300	-1.53435600
	C	-0.07630800	-0.84676500	-0.57770700
	C	-1.00707400	-1.82403200	0.16173400
	C	-0.59925500	-3.28434800	-0.16104100
	C	-0.92754700	-1.57524600	1.68502100
	C	-0.20508500	0.91159800	-2.36245100
	O	0.97779200	1.16129900	-2.52457700
	O	-1.17893500	1.67381100	-2.93120900
	C	-0.71994400	2.81010000	-3.67464200
	S	-4.46485100	-2.90889100	0.64923400
	O	-5.44613500	-3.79030900	0.02115800
	O	-3.45468200	-3.43081800	1.56550600
	C	-5.32064900	-1.54200400	1.41763700
	C	-4.61619500	-0.68229500	2.26734000
	C	-6.66574500	-1.31900300	1.11902100
	C	-5.27112100	0.42205700	2.80196600
	C	-7.30361600	-0.20731600	1.66962900
	C	-6.61815900	0.68517900	2.50356300
	C	-7.29073800	1.91470000	3.06304600
	H	-3.15075600	0.80221800	-3.94774900
	H	-5.37771300	0.29684200	-4.93426500
	H	-6.85167500	-1.40401400	-3.90002900
	H	-6.12921900	-2.65371300	-1.88298900
	H	-2.92705700	1.06278100	-0.42374700
	H	0.41077100	-3.47459400	0.21707700
	H	-1.29463600	-3.97912100	0.31868400
	H	-0.60278900	-3.46583900	-1.24077600

	H	0.09935700	-1.75065700	2.02218700
	H	-1.18836500	-0.54115600	1.92958100
	H	-1.59089700	-2.25673000	2.22095200
	H	-1.61560200	3.26031000	-4.10464000
	H	-0.22186000	3.52084100	-3.00935900
	H	-0.02399100	2.50618600	-4.46064300
	H	-3.57621300	-0.86977500	2.50720000
	H	-7.20106300	-2.00619700	0.47405900
	H	-4.72071400	1.10025900	3.44772500
	H	-8.34980000	-0.02673600	1.43691200
	H	-6.75827700	2.81956400	2.74629300
	H	-8.32919000	1.99395800	2.72779500
	H	-7.28883100	1.90468900	4.15996900
	P	4.23600600	-0.24949200	0.26521300
	C	4.70887700	-0.34813400	2.03894200
	C	5.93406000	-0.88052600	2.46766100
	C	6.24744800	-0.91611000	3.82802700
	C	5.34315300	-0.42222500	4.76986500
	C	4.11937700	0.10505800	4.35049400
	C	3.79998800	0.13733500	2.99324500
	C	5.29348400	-1.48716500	-0.58920200
	C	4.82940300	-2.81111300	-0.66208400
	C	5.59745500	-3.79458700	-1.28440900
	C	6.83086900	-3.46518200	-1.85158000
	C	7.29371300	-2.14956200	-1.79349100
	C	6.53040100	-1.16279000	-1.16571300
	C	4.81577900	1.39619200	-0.30831700
	C	5.90645600	2.05358800	0.28305400
	C	6.32442000	3.29454200	-0.19923700
	C	5.65642400	3.89002600	-1.27174400
	C	4.56487600	3.24532300	-1.85657800
	C	4.13765400	2.00541100	-1.37755500
	Au	1.90622600	-0.58685100	-0.14831500
	S	-2.83858400	2.70353000	1.01794600
	O	-3.37194500	1.94177200	-0.28850400
	O	-3.88161500	3.61871600	1.44395000
	O	-2.19206500	1.77408400	1.93663900
	C	-1.48226100	3.74332100	0.26641300
	F	-1.95461500	4.44090000	-0.76558900
	F	-1.02761100	4.57823600	1.20028400
	F	-0.48669900	2.95707200	-0.14863900
	H	6.63956400	-1.27551600	1.74283400
	H	7.19713100	-1.33447500	4.15035600
	H	5.58762100	-0.45469000	5.82810700
	H	3.40791900	0.48206000	5.07988400
	H	2.83968900	0.53194900	2.67145500

	H	3. 86098400	-3. 06699800	-0. 23998400
	H	5. 22703400	-4. 81461000	-1. 33591500
	H	7. 42499900	-4. 22995400	-2. 34432800
	H	8. 24823400	-1. 88658600	-2. 24128900
	H	6. 89414300	-0. 14041800	-1. 13478200
	H	6. 42216900	1. 60383900	1. 12649700
	H	7. 16743300	3. 79755900	0. 26684100
	H	5. 98082600	4. 85834400	-1. 64351900
	H	4. 03312300	3. 70980000	-2. 68227400
	H	3. 26966100	1. 52706600	-1. 82384900
ima4	F	-0. 06289000	4. 77266100	-0. 72313800
	C	-4. 20568300	0. 23472400	-3. 53563600
	C	-5. 48510300	0. 04421800	-4. 04611800
	C	-6. 41606000	-0. 76577200	-3. 37642200
	C	-6. 09058600	-1. 40473500	-2. 18156400
	C	-4. 80834700	-1. 20231000	-1. 66665500
	C	-3. 85180200	-0. 38322200	-2. 32666500
	C	-2. 65394300	-0. 43888800	-1. 51988900
	C	-2. 89531300	-1. 22455100	-0. 42428500
	N	-4. 20370000	-1. 74540400	-0. 49629000
	C	-1. 22261200	-0. 10068300	-1. 52520800
	C	-0. 59416300	-0. 70128900	-0. 46399600
	C	-1. 61914700	-1. 51515800	0. 35141000
	C	-1. 27312300	-3. 02344600	0. 27977200
	C	-1. 60996100	-1. 03701600	1. 82241100
	C	-0. 52273100	0. 79011400	-2. 47731300
	O	0. 68641000	0. 89881400	-2. 60496600
	O	-1. 38447000	1. 54303500	-3. 20271900
	C	-0. 77325000	2. 50363000	-4. 07620600
	S	-5. 14062100	-2. 32902300	0. 82498700
	O	-6. 14927800	-3. 21674400	0. 25100200
	O	-4. 17787000	-2. 81491000	1. 81096400
	C	-5. 96909400	-0. 88405800	1. 48044900
	C	-7. 32263300	-0. 68721600	1. 20374800
	C	-5. 25237500	0. 02944300	2. 25964900
	C	-7. 95855800	0. 44586100	1. 71042300
	C	-5. 90431600	1. 15592500	2. 75089600
	C	-7. 26436300	1. 38343300	2. 48567000
	C	-7. 96142400	2. 59957300	3. 04682600
	H	-3. 48324300	0. 85128900	-4. 05525600
	H	-5. 76570800	0. 52136500	-4. 98137900
	H	-7. 40529900	-0. 91322600	-3. 80102100
	H	-6. 79579900	-2. 06164700	-1. 68926800
	H	-0. 34546400	1. 36040400	0. 37858100
	H	-0. 30728700	-3. 20664200	0. 76305100
	H	-2. 04198000	-3. 60653800	0. 79411200

	H	-1.20675300	-3.35965700	-0.76021300
	H	-0.60215700	-1.15031800	2.23583200
	H	-1.88398200	0.02149800	1.89501200
	H	-2.30285600	-1.62838600	2.42347900
	H	-1.59902000	3.01444200	-4.57269900
	H	-0.17625000	3.21334200	-3.49693600
	H	-0.12947500	2.00868700	-4.80828900
	H	-7.86738000	-1.41551800	0.61428300
	H	-4.20560900	-0.14056500	2.48318500
	H	-9.01305900	0.60224100	1.49800600
	H	-5.34830400	1.87075600	3.35224000
	H	-8.18138300	2.46853400	4.11447600
	H	-7.33751200	3.49527500	2.95346300
	H	-8.91000600	2.79028600	2.53557700
	P	3.79560700	-0.75369600	0.22717400
	C	4.35455300	-0.79282300	1.97681700
	C	5.40736800	-1.61138700	2.41185000
	C	5.79773400	-1.59901600	3.75273500
	C	5.14325500	-0.77098900	4.66598800
	C	4.09408800	0.04608500	4.23737500
	C	3.69415200	0.03413700	2.90117200
	C	4.53667700	-2.24396300	-0.55534100
	C	3.84013100	-3.45998300	-0.45682800
	C	4.36659800	-4.62238500	-1.01899100
	C	5.58783400	-4.58146800	-1.69617700
	C	6.28135800	-3.37520500	-1.80678900
	C	5.76086900	-2.21019300	-1.23889200
	C	4.63867600	0.68691500	-0.53671300
	C	5.84312000	1.19891600	-0.02953000
	C	6.46065500	2.28504800	-0.65132000
	C	5.88110300	2.86773700	-1.78060800
	C	4.67920200	2.36634700	-2.28439500
	C	4.05297100	1.28316600	-1.66573300
	Au	1.42465400	-0.68750200	-0.07928100
	S	0.36826300	3.19763200	1.34656200
	O	-0.72721500	2.23299500	0.67380900
	O	-0.34401300	4.15290500	2.17251500
	O	1.50292900	2.42729800	1.84055800
	C	0.95439400	4.11363600	-0.16962500
	H	5.91875700	-2.26209700	1.70934300
	H	6.61147400	-2.23982100	4.08153300
	H	5.44667000	-0.76517400	5.70945700
	H	3.57880300	0.69057100	4.94403800
	H	2.87536600	0.67019500	2.57803200
	H	2.88154800	-3.49328400	0.05463200
	H	3.81778800	-5.55643100	-0.93714600

	H	5.99339800	-5.48559000	-2.14198400
	H	7.22800000	-3.33677400	-2.33890400
	H	6.30451300	-1.27554500	-1.33553500
	H	6.29256800	0.75773100	0.85524600
	H	7.39062800	2.67827600	-0.24965700
	H	6.36126600	3.71619500	-2.26086300
	H	4.21790900	2.82406900	-3.15502500
	H	3.10499600	0.91757700	-2.05119100
	F	1.45156800	3.24759300	-1.05357900
	F	1.90175200	4.97714900	0.19444900
tsa3	F	-1.43947200	4.20362800	2.22804400
	C	4.00045900	-2.13116700	3.07509200
	C	5.18642900	-2.81112900	3.33010000
	C	6.09254500	-3.09183000	2.29542500
	C	5.83806300	-2.69865700	0.98279900
	C	4.65226100	-2.00478400	0.73358700
	C	3.72115900	-1.71420500	1.76587900
	C	2.61989100	-1.03368200	1.12392500
	C	2.89527400	-0.90523800	-0.22060800
	N	4.12803300	-1.50737000	-0.49733400
	C	1.27519300	-0.54167400	1.34652800
	C	0.70113500	-0.10856100	0.16399800
	C	1.70752800	-0.35188900	-0.99173900
	C	1.17309300	-1.42853400	-1.97425000
	C	1.95939300	0.96892200	-1.75670300
	C	0.59537300	-0.38975600	2.66417800
	O	-0.60613000	-0.29094800	2.83321800
	O	1.47969200	-0.33903400	3.68232500
	C	0.91079600	-0.12228700	4.98449700
	S	5.12042000	-1.27160500	-1.89797000
	O	5.92483200	-2.48319000	-2.02892700
	O	4.21368400	-0.84224400	-2.95765300
	C	6.19797400	0.08497600	-1.45582300
	C	7.52094700	-0.18141400	-1.10097400
	C	5.70704500	1.39441300	-1.48635300
	C	8.35535700	0.88262400	-0.75913600
	C	6.55534400	2.44001400	-1.13807200
	C	7.88845000	2.20310200	-0.76420700
	C	8.78766000	3.35037800	-0.37159600
	H	3.29608500	-1.91982900	3.87003000
	H	5.41094000	-3.13732100	4.34195600
	H	7.00586300	-3.63817600	2.51372000
	H	6.51963000	-2.95481200	0.18269800
	H	0.35948900	1.25588500	0.37027000
	H	0.28539400	-1.04906200	-2.49010600
	H	1.93815600	-1.66122300	-2.71948500

	H	0.90000700	-2.34585900	-1.44169800
	H	1.00420500	1.36108000	-2.11815000
	H	2.39873500	1.72689700	-1.10050000
	H	2.61562800	0.80009300	-2.61200200
	H	1.75600400	-0.11241400	5.67298600
	H	0.38136600	0.83341200	5.01213100
	H	0.21409100	-0.92600300	5.23748600
	H	7.89306400	-1.19920000	-1.11228000
	H	4.68555500	1.59407500	-1.78843100
	H	9.38813500	0.68066600	-0.48753900
	H	6.17730000	3.45888000	-1.16157500
	H	9.83224200	3.03424400	-0.29425200
	H	8.73172700	4.16733600	-1.09994200
	H	8.49156300	3.76480800	0.60056200
	P	-3.70336000	-0.70788300	-0.41648300
	C	-4.40831500	0.05972300	-1.92610600
	C	-5.47260300	-0.52967900	-2.62721100
	C	-5.99865000	0.09691200	-3.75776700
	C	-5.46559200	1.31075800	-4.19748300
	C	-4.40241300	1.89641100	-3.50728700
	C	-3.86807900	1.27552700	-2.37699900
	C	-4.06644900	-2.50456300	-0.56591600
	C	-3.19827700	-3.29677200	-1.33536500
	C	-3.44272600	-4.66003100	-1.49456100
	C	-4.54962000	-5.24994800	-0.87857800
	C	-5.41153100	-4.47122300	-0.10547900
	C	-5.17379400	-3.10359700	0.05163200
	C	-4.70958700	-0.10897800	0.99615100
	C	-6.03668000	0.31807000	0.83354900
	C	-6.77829200	0.73922000	1.93827600
	C	-6.20188100	0.73958700	3.21021000
	C	-4.87881600	0.32490800	3.37539100
	C	-4.12914200	-0.09337000	2.27527800
	Au	-1.40679700	-0.29942200	-0.11201100
	S	-0.45304300	3.46133500	-0.11307500
	O	0.40198300	2.44934100	0.68826600
	O	0.21298500	4.75368300	-0.23161400
	O	-1.05777800	2.84635100	-1.30495500
	C	-1.87422000	3.73118500	1.05730400
	H	-5.88355500	-1.47978300	-2.29868300
	H	-6.81996100	-0.36705500	-4.29728600
	H	-5.87328500	1.79442400	-5.08113400
	H	-3.97577100	2.83473600	-3.84982800
	H	-3.02888700	1.73440700	-1.86136400
	H	-2.32768300	-2.84550400	-1.80405500
	H	-2.76377900	-5.26254800	-2.09150900

	H	-4.73488400	-6.31411400	-0.99632200
	H	-6.26986500	-4.92627400	0.38127600
	H	-5.84638100	-2.50771000	0.66056300
	H	-6.48788800	0.33314100	-0.15394000
	H	-7.80343300	1.07288800	1.80242800
	H	-6.77938800	1.07280500	4.06832700
	H	-4.42059000	0.33878300	4.36028000
	H	-3.09110200	-0.38479700	2.41076500
	F	-2.52627900	2.57725200	1.27321400
	F	-2.73069300	4.60883300	0.52251700
ima5	F	1.99927000	5.34964400	1.08573900
	C	-2.52250300	-3.02468700	-1.29540100
	C	-3.28710900	-4.09325200	-0.83761200
	C	-4.14030100	-3.94962600	0.26880700
	C	-4.25421600	-2.73550900	0.94321600
	C	-3.49495500	-1.66172300	0.47399700
	C	-2.62506000	-1.78747300	-0.64197600
	C	-2.00456800	-0.49443000	-0.80116800
	C	-2.49524200	0.36108200	0.15810700
	N	-3.39748400	-0.33079900	0.97472600
	C	-0.94163400	0.19795600	-1.52878800
	C	-0.72318600	1.43445800	-0.91961000
	C	-1.73522300	1.67937000	0.21320200
	C	-1.07995500	1.92010800	1.59442500
	C	-2.56203800	2.92532800	-0.20422300
	S	-4.64862500	0.37215600	1.95195700
	O	-4.90947600	-0.58876200	3.01911100
	O	-4.20683000	1.73398600	2.23339800
	C	-6.07415200	0.43024900	0.87356200
	C	-7.10984600	-0.48612900	1.05943800
	C	-6.14457100	1.40867100	-0.12341000
	C	-8.22409800	-0.42436700	0.22299700
	C	-7.26303400	1.44960200	-0.94916400
	C	-8.31683400	0.53369000	-0.79470900
	C	-9.51277500	0.58016200	-1.71461100
	H	-1.85439800	-3.13215500	-2.14069200
	H	-3.22050000	-5.05446100	-1.34022300
	H	-4.71491700	-4.80259900	0.61851700
	H	-4.88071800	-2.64010700	1.82044600
	H	-0.21293000	2.25630400	-1.41335300
	H	-0.36539300	2.74239800	1.52463500
	H	-1.84982900	2.15743800	2.33174900
	H	-0.53285900	1.03363100	1.93332000
	H	-1.89736800	3.79077100	-0.27436000
	H	-3.03715800	2.77781800	-1.18091400
	H	-3.32766200	3.13573000	0.54500900

	H	-7.05149000	-1.21825700	1.85660800
	H	-5.34685100	2.13330100	-0.24151300
	H	-9.03650100	-1.13136900	0.36872900
	H	-7.32405900	2.21110500	-1.72251900
	H	-9.85065200	1.60932800	-1.87854400
	H	-9.26580800	0.16043900	-2.69847000
	H	-10.35217600	0.00572700	-1.31156400
	P	2.90758400	-1.23960100	0.34217500
	C	3.02353000	-1.36578400	2.16925700
	C	3.15495500	-2.59634200	2.82880800
	C	3.26013900	-2.63448500	4.22100000
	C	3.23628500	-1.44966100	4.95810600
	C	3.10545000	-0.22249000	4.30265100
	C	2.99473400	-0.17247800	2.91307800
	C	2.59894600	-2.94869400	-0.26302200
	C	1.29137800	-3.45632800	-0.18366400
	C	1.01084100	-4.75420000	-0.60735700
	C	2.02961500	-5.55552200	-1.13025200
	C	3.32838900	-5.05401700	-1.22403900
	C	3.61601100	-3.75725400	-0.79037100
	C	4.57495000	-0.75641000	-0.23315600
	C	5.72750700	-1.26500500	0.39110600
	C	6.99047200	-0.89508500	-0.06783800
	C	7.11344600	-0.00624300	-1.13988100
	C	5.97265100	0.51582600	-1.74886400
	C	4.70353300	0.14409700	-1.30072600
	Au	1.17891100	0.24932100	-0.29622100
	S	2.76564100	3.16551800	-0.21498400
	O	2.17098100	2.37060200	0.91662600
	O	4.17329400	3.54231500	-0.04340200
	O	2.36846900	2.62645600	-1.54331400
	C	1.82333300	4.76658300	-0.10564800
	H	3.17010800	-3.52242800	2.26251900
	H	3.35819800	-3.59139500	4.72659000
	H	3.31555400	-1.48210800	6.04144800
	H	3.08323200	0.70197400	4.87278400
	H	2.88318000	0.78570000	2.40990200
	H	0.48983300	-2.83274300	0.20275700
	H	-0.00611700	-5.12988400	-0.53781400
	H	1.81010600	-6.56487200	-1.46790500
	H	4.12327600	-5.66995600	-1.63578000
	H	4.62925100	-3.37694600	-0.86879700
	H	5.63834200	-1.93420700	1.24226300
	H	7.87773800	-1.28858100	0.42067600
	H	8.09939600	0.29242800	-1.48550600
	H	6.06110600	1.23361400	-2.55850000

	H	3.82464300	0.59360300	-1.75271500
	F	0.49567000	4.53873200	-0.26295500
	F	2.20959100	5.61594400	-1.06289000
	C	-0.41223000	-0.12676100	-2.89514600
	O	0.04448700	0.69267000	-3.65985100
	O	-0.53412900	-1.44001000	-3.18516000
	C	-0.04612100	-1.82227000	-4.48443800
	H	-0.58657800	-1.28576500	-5.26824700
	H	1.02050800	-1.60021900	-4.56753900
	H	-0.22234300	-2.89547300	-4.55722300
imbl	C	2.76246800	0.45088100	3.04334700
	C	3.67916800	0.50956000	4.08627300
	C	4.96879200	-0.03610800	3.94747300
	C	5.37250800	-0.65350400	2.76666300
	C	4.44864400	-0.69690300	1.71868100
	C	3.14582700	-0.15282400	1.83658100
	C	2.45032100	-0.40393700	0.58645400
	C	3.32415200	-1.06312600	-0.22899400
	N	4.53759600	-1.27568000	0.43794500
	C	1.03079800	-0.10286800	0.25389400
	C	0.17113000	-1.10859900	0.06770800
	C	-0.00194500	-2.47122400	-0.05432300
	C	-0.23614100	-3.35645000	1.15634000
	C	0.39995700	-3.18432200	-1.33111100
	C	0.60143900	1.31921200	0.08140200
	O	-0.36257500	1.69660100	-0.55728900
	O	1.44788700	2.17112200	0.69624800
	C	1.13751900	3.56596400	0.55202100
	S	5.97155700	-1.70958200	-0.39895300
	O	6.86532000	-2.28371900	0.60266200
	O	5.50803800	-2.45868900	-1.56416200
	C	6.65937900	-0.15736200	-0.95810700
	C	6.27150800	0.35167900	-2.19981900
	C	7.56585700	0.52918300	-0.14691700
	C	6.79750000	1.56967600	-2.62385600
	C	8.07897400	1.74625300	-0.58961700
	C	7.70567500	2.28530300	-1.82952800
	C	8.29398600	3.58945000	-2.31222100
	H	1.76740000	0.87071600	3.14989400
	H	3.39582800	0.97586600	5.02591200
	H	5.66253100	0.01174100	4.78220900
	H	6.35120000	-1.10749200	2.67085500
	H	3.19454500	-1.44037500	-1.23185400
	H	-0.99207900	-4.11608000	0.93492400
	H	0.70781900	-3.86593600	1.39766000
	H	-0.55111400	-2.78411000	2.03253900

	H	-0.37723600	-3.89690600	-1.62503200
	H	0.55987200	-2.48398900	-2.15478400
	H	1.33408600	-3.73452600	-1.14783300
	H	1.93219800	4.09413600	1.07986900
	H	1.12365500	3.84743100	-0.50446200
	H	0.16336600	3.78938000	0.99445100
	H	5.58372700	-0.20599600	-2.82621200
	H	7.87221800	0.11001400	0.80471300
	H	6.50149500	1.96909500	-3.59052900
	H	8.78524600	2.28450400	0.03736900
	H	7.61753200	4.10337800	-3.00257300
	H	8.50972400	4.26493400	-1.47796800
	H	9.23827500	3.41882500	-2.84607300
	P	-3.63361700	0.47492700	-0.06060000
	C	-5.24649900	-0.06987700	0.64134400
	C	-6.00360100	0.76119800	1.48427600
	C	-7.23697100	0.32939800	1.97397000
	C	-7.72590200	-0.93225100	1.62800700
	C	-6.97634000	-1.76203600	0.79238300
	C	-5.73975100	-1.33997600	0.30044200
	C	-3.10887100	1.83190900	1.06958000
	C	-2.48191800	1.48700500	2.27728100
	C	-2.09726900	2.47548800	3.18223300
	C	-2.32504800	3.82317700	2.88677300
	C	-2.94089700	4.17402200	1.68409500
	C	-3.33297500	3.18385100	0.77909900
	C	-4.04149000	1.28506600	-1.65916800
	C	-5.36163500	1.56940700	-2.03757300
	C	-5.62428300	2.16623200	-3.27264000
	C	-4.57502500	2.48401100	-4.13587900
	C	-3.25817000	2.20266500	-3.76293500
	C	-2.98812800	1.60071200	-2.53443300
	Au	-1.97212200	-1.30773800	-0.33652400
	H	-5.63197900	1.74231300	1.76222100
	H	-7.81281400	0.97904700	2.62791600
	H	-8.68524000	-1.26804300	2.01317400
	H	-7.34568800	-2.74822900	0.52516500
	H	-5.15478200	-2.00284400	-0.33221400
	H	-2.28969000	0.44176700	2.50694200
	H	-1.61775500	2.19498500	4.11629100
	H	-2.02454800	4.59393600	3.59162100
	H	-3.12032600	5.21952200	1.44737000
	H	-3.80837500	3.46640000	-0.15485700
	H	-6.18444700	1.31962300	-1.37570100
	H	-6.65103900	2.37693700	-3.55949000
	H	-4.78237100	2.94394900	-5.09848500

	H	-2.43799400	2.44391000	-4.43377100
	H	-1.96505600	1.38688000	-2.24200900
	Cl	-3.23060300	-3.32508200	-1.24824100
tsb1	C	4.04588700	-3.62230800	0.77043000
	C	5.35300300	-4.08017800	0.68996100
	C	6.33801300	-3.33630200	0.01315900
	C	6.04237000	-2.12488900	-0.60388600
	C	4.72903600	-1.65705000	-0.50353700
	C	3.71774200	-2.38562200	0.18527100
	C	2.48232900	-1.66028700	-0.00428000
	C	2.79253600	-0.47312900	-0.71507700
	N	4.14061000	-0.50008400	-1.05325100
	C	1.07465700	-1.91604300	0.12574000
	C	0.32129000	-1.25206400	-0.83703400
	C	1.05257100	-0.88076400	-2.02118000
	C	1.65572100	-1.97082600	-2.88981000
	C	0.73114600	0.38958600	-2.76143600
	C	0.44554500	-2.66316200	1.24974800
	O	-0.74576500	-2.86705600	1.38741000
	O	1.36343000	-3.10742300	2.13952600
	C	0.83188300	-3.81101100	3.27306500
	S	4.96064100	0.91160500	-1.66744100
	O	6.19895300	0.40673700	-2.25872800
	O	3.94075800	1.58482800	-2.46218000
	H	3.28464000	-4.19269400	1.28676700
	H	5.62024800	-5.02769800	1.14881700
	H	7.35294700	-3.72029300	-0.04094100
	H	6.79184100	-1.56737200	-1.15034400
	H	2.26585400	0.47932200	-0.54832100
	H	0.90821400	-2.24395400	-3.64802400
	H	2.53757800	-1.60365600	-3.42475500
	H	1.91320400	-2.87059000	-2.32842300
	H	-0.13202100	0.20677400	-3.41807400
	H	0.48639400	1.19764300	-2.06647300
	H	1.57461500	0.68841200	-3.39137200
	H	1.69808500	-4.09626200	3.87076000
	H	0.16873100	-3.15840700	3.84656300
	H	0.27377600	-4.69479700	2.95226500
	Au	-1.58728900	-0.54508400	-0.48979000
	P	-3.72073900	0.35004600	0.03285800
	C	-3.83541900	2.15487500	-0.26591800
	C	-5.04042800	2.77347500	-0.63765100
	C	-5.08600400	4.15465000	-0.83078300
	C	-3.93228400	4.92386900	-0.65782700
	C	-2.73207600	4.31010600	-0.29463500
	C	-2.67419800	2.92854300	-0.10067200

	C	-5.09468700	-0.40120000	-0.93319800
	C	-4.88318700	-0.64517700	-2.30033500
	C	-5.89527000	-1.19774500	-3.08367000
	C	-7.12596100	-1.52584800	-2.50884000
	C	-7.34031800	-1.29642000	-1.14931200
	C	-6.33106300	-0.73550200	-0.36270200
	C	-4.15011100	0.08976700	1.80011200
	C	-4.99461000	0.96976800	2.49489300
	C	-5.31438900	0.72808700	3.83161100
	C	-4.79228800	-0.38995600	4.48564900
	C	-3.94319300	-1.26264000	3.80246900
	C	-3.61599000	-1.02531700	2.46646200
	H	-5.93739700	2.17888600	-0.78587400
	H	-6.02038800	4.62727300	-1.12212800
	H	-3.96934000	5.99892300	-0.81429700
	H	-1.82616500	4.89603900	-0.16945300
	H	-1.71995200	2.47190300	0.16286500
	H	-3.92079200	-0.40811500	-2.74669000
	H	-5.71955300	-1.38148900	-4.14006800
	H	-7.91163700	-1.96476700	-3.11783700
	H	-8.29300700	-1.55597700	-0.69551500
	H	-6.50592900	-0.56559500	0.69503200
	H	-5.39105000	1.84965200	1.99704100
	H	-5.96482100	1.41769200	4.36286700
	H	-5.03840800	-0.57374100	5.52815200
	H	-3.52301100	-2.12595700	4.31109400
	H	-2.93163400	-1.69484100	1.95216600
	C	5.34774700	1.87612100	-0.22054300
	C	6.67044700	1.90664800	0.22915700
	C	4.33060400	2.58352600	0.42937000
	C	6.97624000	2.66602500	1.35639400
	H	7.43991900	1.35784600	-0.30221900
	C	4.66435600	3.32538500	1.55941800
	H	3.29331200	2.55210500	0.09764900
	C	5.98246500	3.38446000	2.03713600
	H	8.00286600	2.70034100	1.71223300
	H	3.87377900	3.86190900	2.07722400
	C	6.32354200	4.22233800	3.24608600
	H	5.54103000	4.15636800	4.00954000
	H	7.27087700	3.91118200	3.69766900
	H	6.42014700	5.28147300	2.97293400
	C1	0.83026600	1.98581900	0.40296700
imb2	C	3.80897500	3.64511500	0.10428700
	C	5.06024600	4.11553700	0.45210000
	C	6.00667500	3.25628600	1.05384200
	C	5.73106100	1.92340100	1.32144700

	C	4.46337200	1.43495100	0.96509700
	C	3.49641000	2.28852000	0.34510900
	C	2.32153900	1.50849700	0.18344700
	C	2.60815800	0.11936900	0.51589100
	N	3.92569700	0.16440800	1.15128800
	C	0.91210400	1.64668600	-0.01223100
	C	0.26820800	0.51850300	0.47926500
	C	1.26599500	-0.40678400	1.16181200
	C	1.27243900	-0.08282600	2.67908300
	C	0.94966500	-1.89306800	0.94452400
	C	0.19889900	2.77711300	-0.65170700
	O	-1.00855600	2.93584400	-0.67406300
	O	1.04831100	3.64437800	-1.25092300
	C	0.42554100	4.73749900	-1.94346900
	S	4.88878400	-1.21373300	1.57126600
	O	5.68147700	-0.79171800	2.72740100
	O	3.93504100	-2.31256400	1.66614600
	H	3.07052600	4.28673900	-0.35735700
	H	5.32223300	5.15285200	0.26684000
	H	6.98075300	3.65270700	1.32777200
	H	6.45567200	1.29102600	1.81596100
	H	2.64784400	-0.42621500	-0.52711400
	H	0.29166300	-0.30561100	3.11179200
	H	2.02215000	-0.70651000	3.17566600
	H	1.50409500	0.96967400	2.87168700
	H	-0.05315300	-2.10826300	1.33144900
	H	0.98155300	-2.14432600	-0.11851100
	H	1.67180900	-2.51694500	1.47346600
	H	1.24492200	5.31790100	-2.36877200
	H	-0.22770800	4.36205900	-2.73502600
	H	-0.16265900	5.34778600	-1.25261100
	Au	-1.72441900	0.11723800	0.27646900
	P	-4.03984600	-0.37207900	-0.05053900
	C	-4.31947000	-2.05291600	-0.73428900
	C	-5.45059100	-2.81871600	-0.41316300
	C	-5.62498400	-4.08267600	-0.97970800
	C	-4.67397300	-4.59147700	-1.86667600
	C	-3.54282400	-3.83670500	-2.18553900
	C	-3.36173100	-2.57470600	-1.61935900
	C	-5.00981900	-0.30611300	1.50942000
	C	-4.42966000	-0.85229600	2.66687500
	C	-5.12479800	-0.84321800	3.87519200
	C	-6.40072500	-0.27777600	3.94505700
	C	-6.97876800	0.27659400	2.80234500
	C	-6.28879200	0.26317000	1.58773400
	C	-4.85652100	0.78668300	-1.21588500

	C	-5.99757300	0.42232600	-1.94921200
	C	-6.60229100	1.34006100	-2.80843300
	C	-6.07169200	2.62507300	-2.94653700
	C	-4.93034900	2.98814600	-2.22982100
	C	-4.31794300	2.07465000	-1.36964000
	H	-6.18870200	-2.43495300	0.28502700
	H	-6.50161400	-4.67118600	-0.72273100
	H	-4.80976000	-5.57778700	-2.30191500
	H	-2.79346700	-4.23145400	-2.86548700
	H	-2.47062800	-1.99966000	-1.85789300
	H	-3.43024900	-1.27743100	2.62054900
	H	-4.66612800	-1.26849900	4.76349300
	H	-6.93862800	-0.26378100	4.88902500
	H	-7.96753100	0.72434500	2.85314900
	H	-6.74434200	0.70259100	0.70600800
	H	-6.40600800	-0.58011300	-1.86004800
	H	-7.48277900	1.04868300	-3.37464600
	H	-6.54134600	3.33669100	-3.62032900
	H	-4.50408700	3.98057900	-2.34612100
	H	-3.41211100	2.35787600	-0.84090700
	C	6.00435500	-1.48424600	0.20122500
	C	7.37625900	-1.33946100	0.42124200
	C	5.49981300	-1.88030000	-1.04137700
	C	8.25604800	-1.59019000	-0.63089400
	H	7.74274600	-1.05036600	1.39987300
	C	6.39940200	-2.11333500	-2.07736000
	H	4.43228000	-1.97721400	-1.22766600
	C	7.78431300	-1.97735400	-1.89236200
	H	9.32539900	-1.48319100	-0.46693700
	H	6.00743700	-2.40169500	-3.04924100
	C	8.73855600	-2.25385100	-3.02953600
	H	8.44752600	-1.70575800	-3.93315900
	H	9.76374100	-1.96854300	-2.77396100
	H	8.74307300	-3.32026200	-3.28871100
	C1	2.31343900	-1.19246900	-2.27883100
tsb2	C	3.73853000	3.67510100	0.24759000
	C	4.99127100	4.13758700	0.61024000
	C	5.96252700	3.25305900	1.12392200
	C	5.70801000	1.89849800	1.28773100
	C	4.43889500	1.42536100	0.92285700
	C	3.44733600	2.30318000	0.39031000
	C	2.28330200	1.50499500	0.17383300
	C	2.59807600	0.13791100	0.40126100
	N	3.91381000	0.13284600	1.00423300
	C	0.85242900	1.62492400	-0.01413900
	C	0.24242400	0.44186900	0.34560800

	C	1. 27654100	-0. 55357700	0. 86584100
	C	0. 11302700	2. 79378600	-0. 53769700
	O	-1. 09915800	2. 92571600	-0. 55768700
	O	0. 94094000	3. 74503800	-1. 03485800
	S	4. 84458600	-1. 23951300	1. 48409100
	O	5. 50501400	-0. 84886100	2. 72981700
	O	3. 91350200	-2. 36245000	1. 43591800
	H	2. 98380500	4. 34123800	-0. 14839800
	H	5. 23218600	5. 19103800	0. 50165300
	H	6. 93612000	3. 64143900	1. 41058600
	H	6. 45400700	1. 24156700	1. 71370800
	H	2. 72272800	-0. 26120200	-0. 91255800
	Au	-1. 75729200	0. 04003000	0. 18823500
	Cl	2. 77503000	-0. 72338600	-2. 44446100
	C	0. 29087900	4. 88984700	-1. 60527900
	H	-0. 34500100	4. 58974000	-2. 44224300
	H	-0. 32176500	5. 40017700	-0. 85692400
	H	1. 09498600	5. 53978400	-1. 95246200
	C	6. 11310900	-1. 46640600	0. 24259000
	C	7. 44902900	-1. 29473700	0. 61209300
	C	5. 76277400	-1. 88288900	-1. 04465500
	C	8. 44613200	-1. 52856300	-0. 33396000
	H	7. 69836700	-1. 00395900	1. 62643500
	C	6. 77529200	-2. 10185500	-1. 97379900
	H	4. 72486800	-2. 01079900	-1. 33273900
	C	8. 12721400	-1. 92767900	-1. 63866800
	H	9. 48802900	-1. 40217700	-0. 05071700
	H	6. 50496100	-2. 41251400	-2. 97963600
	C	9. 20709200	-2. 15099100	-2. 67016200
	H	9. 02222300	-3. 06207900	-3. 25006000
	H	9. 24506600	-1. 31734300	-3. 38344400
	H	10. 19509300	-2. 23591900	-2. 20707100
	P	-4. 09626000	-0. 39591100	-0. 04008200
	C	-4. 46492100	-2. 07170700	-0. 69739400
	C	-5. 59019400	-2. 80951300	-0. 30002900
	C	-5. 83127400	-4. 07134600	-0. 84716000
	C	-4. 95363900	-4. 60617400	-1. 79214000
	C	-3. 82892600	-3. 87886800	-2. 18874300
	C	-3. 58125900	-2. 62017900	-1. 64125900
	C	-5. 00324700	-0. 28688100	1. 55520400
	C	-4. 37860700	-0. 80314900	2. 70301500
	C	-5. 02557000	-0. 76044400	3. 93729600
	C	-6. 29704600	-0. 19080200	4. 04216900
	C	-6. 91931500	0. 33418500	2. 90860800
	C	-6. 27774700	0. 28710600	1. 66876000
	C	-4. 92540800	0. 77702900	-1. 18310400

	C	-6.09036600	0.43218300	-1.88751800
	C	-6.70162300	1.36041600	-2.73088500
	C	-6.15399700	2.63676900	-2.88126600
	C	-4.98969000	2.98067900	-2.19236300
	C	-4.37013900	2.05677100	-1.34851200
	H	-6.27281700	-2.40523300	0.44150100
	H	-6.70300900	-4.63734700	-0.53002600
	H	-5.14117700	-5.59032500	-2.21278200
	H	-3.13716300	-4.29397900	-2.91619700
	H	-2.69566600	-2.06509600	-1.93983500
	H	-3.38169700	-1.23005900	2.62857300
	H	-4.53225200	-1.16192500	4.81807000
	H	-6.79710200	-0.14991400	5.00597700
	H	-7.90462100	0.78567000	2.98660800
	H	-6.76685400	0.70476100	0.79435200
	H	-6.51315200	-0.56329000	-1.78767200
	H	-7.60082500	1.08390800	-3.27478100
	H	-6.62875400	3.35673500	-3.54253000
	H	-4.55108800	3.96663200	-2.31770200
	H	-3.44810300	2.32668500	-0.84074400
	C	1.01582800	-1.98034800	0.35127500
	H	0.04137300	-2.32268100	0.71688500
	H	1.00650000	-2.01128500	-0.74048100
	H	1.78684600	-2.66152200	0.71433000
	C	1.22400900	-0.53858900	2.41804800
	H	1.41299500	0.46317100	2.81688500
	H	0.23474800	-0.86421900	2.75633600
	H	1.97361400	-1.22843100	2.81586100
imb3	C	-4.01209500	3.50597600	-0.38589300
	C	-5.30082800	3.91822000	-0.70490300
	C	-6.21670100	3.03359900	-1.29702000
	C	-5.86598000	1.71687100	-1.58584700
	C	-4.57241800	1.30428600	-1.25768500
	C	-3.63101300	2.18145100	-0.65218700
	C	-2.41545700	1.41116500	-0.47857000
	C	-2.63860100	0.13504200	-0.93867800
	N	-3.94386000	0.04379800	-1.45987500
	C	-0.96982800	1.54221900	-0.19458100
	C	-0.32964800	0.37361800	-0.50550000
	C	-1.34011800	-0.65291800	-1.04630200
	C	-1.01813900	-0.96934500	-2.52780900
	C	-1.28090300	-1.94113400	-0.19333500
	C	-0.28644500	2.71140000	0.38854200
	O	0.91949900	2.87275700	0.49277700
	O	-1.16589000	3.64051700	0.84605500
	C	-0.57799800	4.79275400	1.46288600

	S	-4.84390000	-1.40090700	-1.73104500
	O	-5.82372200	-1.08390000	-2.76751800
	O	-3.85270300	-2.45667400	-1.92336500
	H	-3.30192100	4.18809600	0.06310100
	H	-5.60174600	4.94227700	-0.50049100
	H	-7.21437900	3.38155300	-1.55027900
	H	-6.55982500	1.04975600	-2.08028700
	H	-2.83861600	0.75112300	1.70304900
	H	-0.02935700	-1.43538400	-2.59590600
	H	-1.76406000	-1.65551600	-2.93743000
	H	-1.00727800	-0.05391100	-3.12851500
	H	-0.27463600	-2.36866100	-0.25138000
	H	-1.48885500	-1.72294100	0.86049200
	H	-1.99630100	-2.67982500	-0.56026300
	H	-1.41538200	5.42200600	1.76762100
	H	0.01594000	4.50140000	2.33347000
	H	0.06508800	5.32483800	0.75619700
	Au	1.66792900	0.00500100	-0.25964500
	P	4.01155900	-0.34570500	0.05253600
	C	4.44037300	-2.03331900	0.64338700
	C	5.60271400	-2.70639500	0.23862900
	C	5.88531200	-3.98138100	0.73356500
	C	5.01299500	-4.59375000	1.63507900
	C	3.85165600	-3.93084700	2.03951800
	C	3.56238300	-2.66023900	1.54268400
	C	4.98851900	-0.11039300	-1.48760400
	C	4.43443800	-0.56638800	-2.69540800
	C	5.13679700	-0.42461900	-3.89167000
	C	6.39372000	0.18524100	-3.89762700
	C	6.94593900	0.65129000	-2.70351500
	C	6.24869300	0.50508800	-1.50220000
	C	4.73351500	0.80175700	1.29200600
	C	5.87526900	0.47177000	2.04010100
	C	6.40148100	1.38235500	2.95705200
	C	5.79140800	2.62606600	3.13743300
	C	4.65004700	2.95469200	2.40401000
	C	4.11511500	2.04819700	1.48647400
	H	6.28297600	-2.24062000	-0.46813700
	H	6.78607700	-4.49618400	0.41033400
	H	5.23332500	-5.58724800	2.01604800
	H	3.16489700	-4.40644200	2.73419600
	H	2.64913500	-2.15413100	1.84525100
	H	3.44780800	-1.02253200	-2.69749700
	H	4.69706100	-0.77963600	-4.81953600
	H	6.93659500	0.30400800	-4.83138500
	H	7.91924600	1.13451100	-2.70440900

	H	6.68226900	0.87919700	-0.58006700
	H	6.34683200	-0.49879700	1.91587300
	H	7.28355500	1.11744900	3.53390400
	H	6.20015000	3.33226900	3.85530800
	H	4.16313700	3.91472400	2.55051700
	H	3.21021700	2.30565000	0.94235500
	C	-5.71899900	-1.69492100	-0.19887500
	C	-7.09396900	-1.46438200	-0.14325700
	C	-5.02040000	-2.16751000	0.91670700
	C	-7.77140000	-1.70298300	1.05234300
	H	-7.62228000	-1.12257900	-1.02577400
	C	-5.71402600	-2.39230700	2.10097700
	H	-3.95559900	-2.36348100	0.85943300
	C	-7.09618300	-2.16079100	2.19069200
	H	-8.84358400	-1.53052300	1.09844700
	H	-5.17264400	-2.75294800	2.97153800
	C	-7.82648000	-2.38913100	3.49220100
	H	-7.58668900	-1.60131100	4.21788800
	H	-8.91142800	-2.39020800	3.34970200
	H	-7.54135800	-3.34433100	3.94745900
	Cl	-2.92015700	0.50078500	2.98002400
imb4	C	4.18082700	3.54138400	-0.04735600
	C	5.47635000	3.97658400	0.20918400
	C	6.39026700	3.15945400	0.89297200
	C	6.03075300	1.88754900	1.33412300
	C	4.73278100	1.44925500	1.06319900
	C	3.79047000	2.26005000	0.37217700
	C	2.56724400	1.49009800	0.31018600
	C	2.78403200	0.27417100	0.90200700
	N	4.09705400	0.22450400	1.41712500
	C	1.13160200	1.58571000	-0.01034800
	C	0.48457900	0.45534100	0.41630000
	C	1.48950500	-0.50459900	1.07875100
	C	1.15211800	-0.66164000	2.58269900
	C	1.43484100	-1.88040700	0.37533300
	C	0.44007000	2.69892800	-0.69259100
	O	-0.76653300	2.81511300	-0.84480800
	O	1.30438100	3.62418000	-1.17735400
	C	0.70284300	4.72304100	-1.87458200
	S	4.99582100	-1.19826700	1.77130000
	O	6.03751800	-0.80084900	2.71592700
	O	4.00847200	-2.21758100	2.11943900
	H	3.47198200	4.17511600	-0.56381900
	H	5.78265600	4.96758000	-0.11546500
	H	7.39245800	3.52577800	1.09824000
	H	6.72283400	1.27606100	1.89807500

	H	-0.04969500	-0.14685600	-1.97985400
	H	0.17559100	-1.14490400	2.69505800
	H	1.91051500	-1.27842600	3.07269900
	H	1.11200300	0.31418300	3.07768000
	H	0.41855300	-2.28290100	0.44432300
	H	1.68612800	-1.79044400	-0.68751900
	H	2.12073400	-2.58398500	0.85078500
	H	1.53130200	5.35863300	-2.19013600
	H	0.14255200	4.36623600	-2.74303300
	H	0.02551400	5.27436000	-1.21644400
	Au	-1.52641700	0.07963600	0.26639200
	P	-3.87991800	-0.30710400	0.08146900
	C	-4.30349800	-2.00382700	-0.48486100
	C	-5.37769500	-2.73265400	0.04604000
	C	-5.66074300	-4.01425000	-0.43183800
	C	-4.87669600	-4.57596800	-1.44065600
	C	-3.80371500	-3.85554000	-1.97186700
	C	-3.51271300	-2.57822000	-1.49408800
	C	-4.76463100	-0.09093500	1.67884300
	C	-4.14357400	-0.56992300	2.84478500
	C	-4.77195000	-0.44112800	4.08276500
	C	-6.02068700	0.17908300	4.17292300
	C	-6.63906300	0.66723500	3.02095200
	C	-6.01654300	0.53317100	1.77774600
	C	-4.69313000	0.82106100	-1.11619100
	C	-5.89377400	0.47825000	-1.75969000
	C	-6.49169700	1.36960500	-2.65063500
	C	-5.89466500	2.60587700	-2.91041200
	C	-4.69515300	2.94597700	-2.28315800
	C	-4.08897600	2.05864500	-1.39134300
	H	-5.98764100	-2.30581300	0.83642500
	H	-6.49236600	-4.57329200	-0.01140200
	H	-5.09679600	-5.57455600	-1.80830400
	H	-3.18594600	-4.29021400	-2.75264300
	H	-2.66856700	-2.02826700	-1.90243900
	H	-3.16364500	-1.03615800	2.78159400
	H	-4.28115200	-0.81450500	4.97720800
	H	-6.50569300	0.28785900	5.13916100
	H	-7.60647100	1.15767200	3.08690300
	H	-6.50262000	0.92239900	0.88880500
	H	-6.35421000	-0.48818600	-1.57540900
	H	-7.41880300	1.09535000	-3.14676000
	H	-6.35917700	3.29662300	-3.60910700
	H	-4.21814700	3.89881000	-2.49439100
	H	-3.13917900	2.32177000	-0.93401000
	C	5.78278700	-1.65470300	0.22883300

	C	7.13208400	-1.35437700	0.03475600
	C	5.04222600	-2.31084700	-0.75887300
	C	7.73795400	-1.70835600	-1.17007900
	H	7.69823700	-0.87026900	0.82186200
	C	5.66513100	-2.65206800	-1.95565200
	H	4.00203700	-2.56366400	-0.58976200
	C	7.01729900	-2.35240500	-2.18431500
	H	8.79027000	-1.48197400	-1.32162500
	H	5.09245400	-3.16507400	-2.72421500
	C	7.67045800	-2.70211200	-3.49989900
	H	7.43265100	-1.95213200	-4.26577700
	H	8.76033300	-2.74407100	-3.40863400
	H	7.32155400	-3.66994700	-3.87613100
	Cl	-0.01069000	-0.58839400	-3.20953400
tsb3	C	3.91127800	3.58068000	0.56658600
	C	5.12378700	4.04497100	1.06481500
	C	6.02987900	3.16992900	1.68443200
	C	5.74898700	1.81147000	1.82080800
	C	4.53466800	1.34808500	1.31057800
	C	3.60509100	2.21760100	0.68152500
	C	2.47589300	1.39386000	0.31761300
	C	2.73216500	0.09062200	0.69071300
	N	3.97853300	0.03280300	1.32455400
	C	1.12493200	1.45205400	-0.19092200
	C	0.52841400	0.19915200	-0.16351300
	C	1.51463500	-0.80054800	0.49824400
	C	0.98420400	-1.23868200	1.89148200
	C	1.70673600	-2.04371600	-0.39783900
	C	0.45458900	2.63517800	-0.79336400
	O	-0.74900300	2.80621300	-0.85577900
	O	1.34448400	3.51158300	-1.30542400
	C	0.77356200	4.63698600	-1.99328900
	S	4.93552300	-1.37588100	1.63484100
	O	5.77572200	-1.04767600	2.78327400
	O	3.99678100	-2.49243000	1.67594300
	H	3.20813800	4.25258000	0.08965400
	H	5.37070600	5.09968400	0.97952900
	H	6.96583100	3.55579900	2.07870200
	H	6.43426300	1.15017100	2.33392700
	H	0.20915300	-0.11897700	-1.44887200
	H	0.07206700	-1.83094500	1.76791800
	H	1.73513700	-1.85189700	2.39679200
	H	0.74937800	-0.36977200	2.51498600
	H	0.72831500	-2.49846300	-0.58280800
	H	2.11672100	-1.77025500	-1.37393300
	H	2.34967500	-2.77855100	0.08922700

	H	1. 62255400	5. 22312500	-2. 34580100
	H	0. 16544800	4. 29517200	-2. 83444900
	H	0. 15056700	5. 22677900	-1. 31519000
	Au	-1. 59577200	0. 00678100	0. 01818000
	P	-3. 92240400	-0. 28131900	0. 12983900
	C	-4. 44664900	-1. 77143200	-0. 80654700
	C	-5. 54476100	-2. 55289900	-0. 41563600
	C	-5. 92084800	-3. 66178800	-1. 17579300
	C	-5. 20453300	-3. 99766800	-2. 32654600
	C	-4. 10700900	-3. 22631600	-2. 71566900
	C	-3. 72197400	-2. 11881500	-1. 95924700
	C	-4. 56941600	-0. 50816700	1. 83461900
	C	-3. 83511000	-1. 32209500	2. 71347900
	C	-4. 28496300	-1. 54048000	4. 01452200
	C	-5. 46554500	-0. 93831900	4. 45785200
	C	-6. 19474500	-0. 12030900	3. 59423000
	C	-5. 75174800	0. 09477400	2. 28674300
	C	-4. 85059700	1. 12240500	-0. 60108200
	C	-6. 15670500	0. 96376500	-1. 09342700
	C	-6. 84275300	2. 05413000	-1. 62799900
	C	-6. 22994500	3. 30858300	-1. 68270300
	C	-4. 92706100	3. 46838000	-1. 20891600
	C	-4. 23376000	2. 38141000	-0. 67268400
	H	-6. 09848600	-2. 30402700	0. 48508800
	H	-6. 76952600	-4. 26500600	-0. 86457800
	H	-5. 49644300	-4. 86401600	-2. 91410300
	H	-3. 53866600	-3. 48856300	-3. 60334900
	H	-2. 85309200	-1. 53805700	-2. 26182600
	H	-2. 90679200	-1. 77733700	2. 37823100
	H	-3. 70831400	-2. 17181000	4. 68477400
	H	-5. 81087500	-1. 10149600	5. 47507800
	H	-7. 10942800	0. 35643100	3. 93598900
	H	-6. 32373800	0. 73757700	1. 62521300
	H	-6. 63243600	-0. 01247100	-1. 07367100
	H	-7. 85152400	1. 92142000	-2. 00946700
	H	-6. 76364400	4. 15548800	-2. 10563300
	H	-4. 43877400	4. 43700000	-1. 26687000
	H	-3. 20781000	2. 50926600	-0. 34006600
	C	5. 97819400	-1. 52895500	0. 19041000
	C	7. 32370200	-1. 17108200	0. 28080200
	C	5. 43782200	-2. 01817500	-1. 00333600
	C	8. 13277400	-1. 29699900	-0. 84838600
	H	7. 72999300	-0. 81835400	1. 22174200
	C	6. 26148100	-2. 13116900	-2. 11815500
	H	4. 39652600	-2. 31383300	-1. 05809800
	C	7. 61770700	-1. 76952200	-2. 06202700

	H	9.18279900	-1.02454800	-0.78183300
	H	5.84497300	-2.51022700	-3.04789100
	C	8.49001000	-1.88178800	-3.28904600
	H	8.22013400	-1.12056300	-4.03216400
	H	9.54778100	-1.74712000	-3.04397800
	H	8.37389900	-2.85851800	-3.77249000
	Cl	0.01536700	-0.50290200	-3.04100200
imb5	C	-2.92890200	3.24291000	-0.14488600
	C	-3.77142100	4.10500500	-0.83838800
	C	-4.77830100	3.60702600	-1.68191400
	C	-4.96803600	2.23690400	-1.85236100
	C	-4.12763600	1.37292400	-1.14638400
	C	-3.10352100	1.85726000	-0.28576900
	C	-2.43736000	0.68992700	0.23831800
	C	-3.04789400	-0.43096000	-0.26336300
	N	-4.07298400	-0.04956800	-1.15094100
	C	-1.23838200	0.26250700	0.97887800
	C	-1.13220800	-1.08456100	0.87236400
	C	-2.25574800	-1.69315400	0.04990900
	C	-1.67837700	-2.34088400	-1.23579300
	C	-2.97301900	-2.76312600	0.90886600
	S	-5.41550700	-1.02230600	-1.61928500
	O	-5.89967200	-0.46341800	-2.87924900
	O	-4.95147100	-2.40367500	-1.52402900
	C	-6.65834200	-0.73884800	-0.36264700
	C	-7.70682600	0.14545200	-0.62364900
	C	-6.57202900	-1.41431000	0.85787000
	C	-8.67075100	0.36021700	0.35983800
	C	-7.54381500	-1.18330300	1.82753300
	C	-8.60239800	-0.29059100	1.59930300
	C	-9.63301300	-0.02676400	2.67072700
	H	-2.14523500	3.62079800	0.50028200
	H	-3.64560200	5.17938500	-0.73240600
	H	-5.41525400	4.29912000	-2.22583900
	H	-5.71720400	1.85673800	-2.53476400
	H	-0.36440200	-1.69837300	1.32983800
	H	-0.97236300	-3.13227000	-0.96550200
	H	-2.49000700	-2.76452700	-1.83329400
	H	-1.14699500	-1.59885600	-1.84116900
	H	-2.25024200	-3.52801500	1.21122500
	H	-3.39695300	-2.31892900	1.81657100
	H	-3.76745900	-3.24489500	0.33544800
	H	-7.77496000	0.63670400	-1.58719300
	H	-5.77015100	-2.12089000	1.03869700
	H	-9.49312700	1.04157600	0.15726600
	H	-7.48374700	-1.71163700	2.77564000

	H	-9.81150000	-0.91665000	3.28319800
	H	-9.29882100	0.77183700	3.34637200
	H	-10.58834500	0.28895700	2.23953500
	P	3.87977300	0.17722000	-0.18719900
	C	5.11426500	-0.07351400	-1.52357800
	C	5.47082100	0.95328600	-2.41135500
	C	6.42773900	0.72452400	-3.40130200
	C	7.03635000	-0.52725700	-3.51372400
	C	6.68381200	-1.55458700	-2.63603200
	C	5.72397300	-1.33225100	-1.64841000
	C	2.78584400	1.53756400	-0.75152100
	C	1.58816900	1.21959200	-1.40994300
	C	0.73918200	2.23372300	-1.85466500
	C	1.07870800	3.57221400	-1.64612000
	C	2.26938800	3.89657100	-0.99136900
	C	3.11967000	2.88490400	-0.54061200
	C	4.80280100	0.85545200	1.24773400
	C	6.15441100	1.21807300	1.16816600
	C	6.81278600	1.71612800	2.29540300
	C	6.12779500	1.85532500	3.50273700
	C	4.77948000	1.49578400	3.58428700
	C	4.11489000	0.99256400	2.46659600
	Au	2.73826500	-1.76378600	0.33723900
	H	4.99499500	1.92640100	-2.33942900
	H	6.69216300	1.52368600	-4.08831200
	H	7.77716800	-0.70403000	-4.28868500
	H	7.14617000	-2.53349000	-2.72525800
	H	5.43778300	-2.13952300	-0.97948100
	H	1.31217800	0.17876800	-1.55436800
	H	-0.19394800	1.97853000	-2.34776400
	H	0.41110500	4.35911100	-1.98577700
	H	2.53507300	4.93704400	-0.82442300
	H	4.03468600	3.14255600	-0.01515000
	H	6.69686700	1.10803700	0.23453400
	H	7.86209900	1.99004100	2.22706700
	H	6.64329800	2.23792600	4.37954400
	H	4.24375200	1.59697300	4.52411800
	H	3.06668600	0.71396300	2.53783300
	C	-0.27516400	1.06422900	1.75583300
	O	0.76154200	0.63799000	2.23608900
	O	-0.67221100	2.35031900	1.90682800
	C	0.21350600	3.18429300	2.66780500
	H	0.37287300	2.76592800	3.66504900
	H	1.17739000	3.28245800	2.16125800
	H	-0.28282600	4.15323100	2.73472700
	Cl	1.57036300	-3.74966100	0.87379200

imc1	C	3.47157100	-3.19715700	1.98521700
	C	4.62460900	-3.82852700	2.43751800
	C	5.85752500	-3.63276500	1.78855800
	C	5.96933200	-2.80520200	0.67387500
	C	4.80911300	-2.16351700	0.23365500
	C	3.55641800	-2.34612000	0.87403200
	C	2.58567400	-1.55311900	0.14786600
	C	3.24816500	-0.93258100	-0.87487000
	N	4.59058800	-1.30304500	-0.86117000
	C	1.14822600	-1.34771500	0.40937000
	C	0.26193900	-1.58744200	-0.55403500
	C	-0.17368700	-2.02524700	-1.76061800
	C	-0.63619500	-3.46078400	-1.92026200
	C	0.00349400	-1.21776500	-3.02860300
	C	0.68136100	-0.73159600	1.69401200
	O	-0.49084000	-0.65073600	2.03313800
	O	1.69839100	-0.30284400	2.43844500
	C	1.34328000	0.50343500	3.57452100
	S	5.76981000	-0.39121700	-1.73276700
	O	5.08126100	0.02659900	-2.94913300
	O	6.97269200	-1.22143700	-1.76624000
	C	6.07423200	1.03595100	-0.70221100
	C	5.09429700	2.02916900	-0.58621700
	C	7.29923900	1.13716800	-0.04170000
	C	5.36419600	3.13406900	0.21598700
	C	7.54664100	2.25836200	0.74964200
	C	6.58830400	3.27051000	0.89031100
	C	6.86642100	4.49334000	1.73170100
	H	2.52001100	-3.35474700	2.48545600
	H	4.57393400	-4.48684300	3.30058900
	H	6.74256100	-4.14369900	2.15749000
	H	6.91254500	-2.66923800	0.15963500
	H	2.88126000	-0.19692800	-1.57509700
	H	0.13639900	-4.00325100	-2.48268800
	H	-0.78266700	-3.95676900	-0.95865800
	H	-1.56225300	-3.51547100	-2.50206200
	H	0.88962800	-1.61830100	-3.54336400
	H	-0.85425500	-1.34191200	-3.69803000
	H	0.15953700	-0.15995400	-2.81844300
	H	2.28594000	0.72996300	4.07250300
	H	0.86030700	1.41711200	3.22064200
	H	0.67216200	-0.04158600	4.24302900
	H	4.13504300	1.95195700	-1.08837500
	H	8.04347100	0.35702200	-0.15672600
	H	4.60346800	3.90388000	0.31689900
	H	8.50015600	2.34631800	1.26433200

	H	6.00743400	4.74602400	2.36341700
	H	7.73576200	4.34616600	2.38014200
	H	7.06854900	5.36744700	1.09899200
	P	-3.93270000	0.20553400	0.06848900
	C	-3.79255500	1.97610700	0.50015000
	C	-2.70897200	2.70778700	-0.00751000
	C	-2.56303200	4.05745100	0.31870900
	C	-3.50282700	4.68188100	1.13918700
	C	-4.58808000	3.95708800	1.64358700
	C	-4.73295500	2.60493300	1.33500300
	C	-4.75860000	-0.60744400	1.49142100
	C	-3.97089200	-0.98622000	2.59207800
	C	-4.57119300	-1.57069100	3.70720400
	C	-5.95106400	-1.78909400	3.73236400
	C	-6.73499500	-1.41919000	2.63844600
	C	-6.14324400	-0.82936600	1.51939800
	C	-5.09938700	0.06951400	-1.34189300
	C	-5.19183400	-1.15288800	-2.02746700
	C	-6.07740000	-1.29606000	-3.09391600
	C	-6.86925500	-0.21648100	-3.49601700
	C	-6.77490500	1.00316000	-2.82538100
	C	-5.89513000	1.14886100	-1.74983100
	Au	-1.83393100	-0.77606900	-0.37830800
	H	-1.96501000	2.23751300	-0.64099400
	H	-1.69236800	4.58403200	-0.05833700
	H	-3.38745200	5.73102900	1.39879700
	H	-5.31529400	4.44133600	2.28992700
	H	-5.56294600	2.04174500	1.75185100
	H	-2.89566300	-0.82748800	2.57709300
	H	-3.95705400	-1.86187700	4.55475600
	H	-6.41317500	-2.25050700	4.60086800
	H	-7.80786400	-1.59072400	2.65177400
	H	-6.75871100	-0.54786300	0.67040600
	H	-4.56506600	-1.98921000	-1.72767400
	H	-6.14254000	-2.24579600	-3.61755300
	H	-7.55164100	-0.32558100	-4.33439200
	H	-7.38218200	1.84745200	-3.13946600
	H	-5.82309100	2.10236100	-1.23659100
	B	0.72647200	2.15979200	-0.80322600
	F	0.71888600	1.68999900	0.52076200
	F	1.95714200	1.86018500	-1.42085100
	F	-0.30116800	1.45651600	-1.53006400
	F	0.45176500	3.52008600	-0.84561400
tsc1	C	-4.18887300	-3.53745700	-0.98179400
	C	-5.49806600	-3.99145200	-0.94668200
	C	-6.48274000	-3.29389700	-0.21956000

	C	-6.18803500	-2.13508500	0.49100600
	C	-4.87182100	-1.66424500	0.43368200
	C	-3.86082600	-2.35134300	-0.29951800
	C	-2.62129200	-1.66424800	-0.04252000
	C	-2.92453900	-0.53312800	0.75967900
	N	-4.27694400	-0.56202800	1.07875700
	C	-1.22022200	-1.94147900	-0.17029400
	C	-0.46991800	-1.37911500	0.85403700
	C	-1.22517800	-1.05180400	2.03687100
	C	-1.86708900	-2.16466500	2.84635400
	C	-0.87067400	0.17076400	2.84668700
	C	-0.59083100	-2.61465000	-1.34322400
	O	0.58040600	-2.92976600	-1.42597400
	O	-1.48426800	-2.84709400	-2.32666900
	C	-0.94490100	-3.42335300	-3.52753300
	S	-5.06416000	0.85519100	1.75117600
	O	-6.48105000	0.50587700	1.81461900
	O	-4.28881000	1.15940200	2.95192800
	C	-4.76535400	2.09427900	0.52097400
	C	-3.70923200	2.99027000	0.70959200
	C	-5.50776000	2.07514600	-0.66365000
	C	-3.37763200	3.85729800	-0.32315100
	C	-5.15164300	2.95025700	-1.68452600
	C	-4.06406200	3.82501900	-1.54446100
	C	-3.57357600	4.66370900	-2.69514400
	H	-3.42515700	-4.06781000	-1.53673900
	H	-5.76917500	-4.89792900	-1.47986100
	H	-7.50048300	-3.67390200	-0.20313400
	H	-6.94250200	-1.61183100	1.06268300
	H	-2.41458800	0.41911800	0.64669500
	H	-1.13236000	-2.50575600	3.58943500
	H	-2.73969900	-1.79668600	3.39560600
	H	-2.15217200	-3.02206700	2.23420200
	H	-0.06476700	-0.08685200	3.54863200
	H	-0.53209300	0.98358000	2.20279300
	H	-1.73284000	0.49959800	3.43628800
	H	-1.79308400	-3.52982600	-4.20399700
	H	-0.19250100	-2.75734500	-3.95651700
	H	-0.48974100	-4.39543700	-3.31850300
	H	-3.14452000	2.98292300	1.63400600
	H	-6.33497600	1.38337100	-0.78554500
	H	-2.52346500	4.51655800	-0.20731300
	H	-5.70446200	2.92965000	-2.61983100
	H	-2.58145300	4.29931400	-2.98771000
	H	-4.24069100	4.60291300	-3.56028700
	H	-3.47000100	5.71812400	-2.41216800

	P	3.64753700	0.11157600	0.13282800
	C	4.81898000	-0.11708200	1.53178500
	C	6.12088200	-0.60911000	1.36804800
	C	6.95996900	-0.76154200	2.47521600
	C	6.50978700	-0.42126500	3.75078100
	C	5.21163700	0.06805600	3.92205400
	C	4.36870800	0.21243100	2.82184100
	C	4.43917000	-0.64211100	-1.34114100
	C	3.97058500	-1.87923700	-1.80967500
	C	4.56755400	-2.47635600	-2.92205800
	C	5.62571700	-1.84416000	-3.57628500
	C	6.08568600	-0.60457400	-3.12354900
	C	5.49354000	-0.00259600	-2.01370300
	C	3.59222800	1.91718200	-0.18147200
	C	4.60810000	2.79329900	0.23189000
	C	4.50121800	4.15817900	-0.04159800
	C	3.38220200	4.65497000	-0.71637100
	C	2.36791900	3.78633200	-1.12418000
	C	2.47106200	2.42008100	-0.86086600
	Au	1.47738900	-0.75131300	0.56858700
	H	6.48081700	-0.87787300	0.38034000
	H	7.96604800	-1.14808200	2.33648900
	H	7.16417000	-0.54129500	4.60992000
	H	4.85279800	0.32915400	4.91387100
	H	3.35481500	0.57913300	2.96133400
	H	3.12568100	-2.36184200	-1.32674900
	H	4.19420500	-3.43120200	-3.28139700
	H	6.08453300	-2.30867800	-4.44510100
	H	6.89899900	-0.10191000	-3.63993800
	H	5.84030200	0.97111100	-1.67960400
	H	5.47082200	2.41729400	0.77453500
	H	5.28865700	4.83420900	0.28154700
	H	3.30008700	5.72061400	-0.91492300
	H	1.47598700	4.14593600	-1.62762700
	H	1.67362700	1.75919300	-1.18549700
	B	-1.03594900	1.60565200	-1.38843400
	F	-2.30004400	1.16338500	-1.77174000
	F	-0.98420200	1.65065600	0.04712200
	F	-0.76956500	2.89101600	-1.88521100
	F	-0.04696800	0.69719400	-1.83140500
imc2	C	4.38143800	-2.99460500	1.42019500
	C	5.68627600	-3.44659200	1.36483700
	C	6.54953400	-3.00687500	0.33783000
	C	6.14129700	-2.11837800	-0.64956500
	C	4.82497800	-1.63653500	-0.59029300
	C	3.94032800	-2.07248600	0.44640400

	C	2.66816200	-1.51180600	0.15610800
	C	2.81018900	-0.56403400	-0.97235000
	N	4.16714800	-0.78571100	-1.49573500
	C	1.29805700	-1.66171300	0.44398900
	C	0.54459200	-1.11738300	-0.60788700
	C	1.45884300	-0.77225700	-1.77387300
	C	1.59139900	-2.00527100	-2.70146700
	C	0.99231000	0.44499900	-2.58114300
	C	0.69974600	-2.15902600	1.71015700
	O	-0.48762800	-2.32442200	1.90523000
	O	1.63846200	-2.39313800	2.65016600
	C	1.13007600	-2.60995500	3.97736200
	S	4.99127700	0.60137300	-2.20018700
	O	6.35912700	0.15687900	-2.46209400
	O	4.10514600	1.03770200	-3.27438000
	C	4.96786700	1.79333500	-0.88024300
	C	3.85537200	2.63403200	-0.75805000
	C	5.94532400	1.73486000	0.11898500
	C	3.69533000	3.37885200	0.40414100
	C	5.77550500	2.50886300	1.26551800
	C	4.63562300	3.30853300	1.44233200
	C	4.37075500	4.04559500	2.73047500
	H	3.69438300	-3.32034200	2.19010800
	H	6.05112300	-4.15037100	2.10651800
	H	7.56779300	-3.38551500	0.30732600
	H	6.80952000	-1.80477800	-1.43964200
	H	2.72186600	0.44177600	-0.53499300
	H	0.61907800	-2.24658000	-3.14266800
	H	2.29509100	-1.77162600	-3.50706500
	H	1.95206000	-2.88848200	-2.16490600
	H	0.04011500	0.21500100	-3.07162100
	H	0.83946200	1.30370600	-1.92471000
	H	1.72781600	0.69832200	-3.34908700
	H	2.00708200	-2.78955100	4.60014500
	H	0.60224000	-1.71256400	4.30863000
	H	0.45534200	-3.46923200	4.00059200
	H	3.10835100	2.67100100	-1.54222400
	H	6.81051000	1.09090400	0.00325500
	H	2.78875700	3.95646100	0.54360000
	H	6.52314200	2.46236100	2.05316400
	H	3.36458800	3.79468900	3.08495000
	H	5.09836000	3.78533200	3.50534500
	H	4.40748300	5.13254600	2.58308300
	P	-3.69162100	0.06695500	-0.19164800
	C	-3.96361000	1.81147800	-0.69917500
	C	-5.06822700	2.20417800	-1.46885000

	C	-5.23495800	3.54555200	-1.82034500
	C	-4.30339500	4.49836100	-1.40547600
	C	-3.20255800	4.10903700	-0.63793300
	C	-3.02238600	2.77110100	-0.28551100
	C	-4.86762500	-0.93226200	-1.19335000
	C	-4.47845900	-1.29771600	-2.49316300
	C	-5.33333300	-2.04288300	-3.30413400
	C	-6.58178100	-2.44470500	-2.82235500
	C	-6.97114900	-2.09598200	-1.52852900
	C	-6.12069100	-1.34214800	-0.71608300
	C	-4.26842800	-0.03355100	1.54500400
	C	-5.35826900	0.72800000	1.99835600
	C	-5.79013200	0.61664400	3.31967100
	C	-5.13324000	-0.24748700	4.19957800
	C	-4.04037700	-0.99406100	3.75746700
	C	-3.60186600	-0.88849900	2.43596800
	Au	-1.42945000	-0.64376500	-0.46860900
	H	-5.79472300	1.46759900	-1.79803600
	H	-6.09172700	3.84223300	-2.41963100
	H	-4.43322100	5.54152100	-1.68168600
	H	-2.47395100	4.84682500	-0.31363500
	H	-2.16176600	2.47983800	0.31256100
	H	-3.50044600	-1.00266800	-2.86502600
	H	-5.02018300	-2.31804500	-4.30753700
	H	-7.24470500	-3.03292500	-3.45109000
	H	-7.93773200	-2.41215400	-1.14563600
	H	-6.43194700	-1.08175900	0.29053200
	H	-5.85914300	1.41716500	1.32424300
	H	-6.63189200	1.21138800	3.66402000
	H	-5.46622600	-0.32751600	5.23102800
	H	-3.51471100	-1.65249400	4.44320900
	H	-2.73100700	-1.45036600	2.11117400
	B	0.69211700	1.65383900	1.68295200
	F	1.16256900	1.53316000	0.33110200
	F	-0.71862300	1.65875300	1.64733300
	F	1.18233800	2.84704600	2.21786900
	F	1.14739400	0.54779400	2.41368700
tsc2	C	4.14201600	-3.55478800	0.62589300
	C	5.45369000	-3.99163100	0.52579300
	C	6.38509500	-3.28578600	-0.25852400
	C	6.03425500	-2.13960700	-0.96309100
	C	4.70642300	-1.69712400	-0.86664400
	C	3.75630900	-2.39175100	-0.06359600
	C	2.50747300	-1.69205900	-0.21520100
	C	2.72262900	-0.55289600	-0.99643400
	N	4.06322200	-0.60978200	-1.50183600

	C	1. 07134500	-1. 84487400	-0. 00217600
	C	0. 39633000	-0. 92526500	-0. 76924700
	C	1. 37853000	-0. 13828300	-1. 64027700
	C	1. 33193400	-0. 71489600	-3. 08240500
	C	1. 05514600	1. 36744600	-1. 67455800
	C	0. 40823000	-2. 73687300	0. 97145600
	O	-0. 79437300	-2. 89818800	1. 09019900
	O	1. 29655700	-3. 38241200	1. 76493100
	C	0. 72059200	-4. 20399500	2. 78969300
	S	4. 90426100	0. 79283800	-2. 09223300
	O	6. 22058200	0. 31767100	-2. 51158000
	O	3. 99374600	1. 42663400	-3. 04243200
	C	5. 05862500	1. 84220800	-0. 65842800
	C	4. 30262200	3. 01330800	-0. 58770800
	C	5. 86816200	1. 43633600	0. 40717200
	C	4. 32623000	3. 75963500	0. 58743600
	C	5. 86457800	2. 18964800	1. 57652300
	C	5. 07072300	3. 34061600	1. 69804500
	C	4. 96308100	4. 06791700	3. 01414300
	H	3. 41270500	-4. 08595600	1. 22259300
	H	5. 76661300	-4. 88844200	1. 05272900
	H	7. 40623100	-3. 65048800	-0. 33083300
	H	6. 75165900	-1. 62158100	-1. 58405800
	H	2. 70468000	0. 28026200	0. 34019600
	H	0. 33918900	-0. 54762800	-3. 51274900
	H	2. 07935300	-0. 21054900	-3. 70171000
	H	1. 53307000	-1. 79071900	-3. 08600900
	H	0. 06148500	1. 51399800	-2. 11043600
	H	1. 04439900	1. 79608300	-0. 67030100
	H	1. 78326300	1. 89769100	-2. 29243000
	H	1. 56540500	-4. 63722800	3. 32677300
	H	0. 11126100	-3. 59713200	3. 46423600
	H	0. 09807200	-4. 98970900	2. 35270400
	H	3. 69639000	3. 31820100	-1. 43281500
	H	6. 47491200	0. 54009000	0. 33110200
	H	3. 72676200	4. 66373400	0. 65502800
	H	6. 47072400	1. 86704700	2. 41894300
	H	4. 10977700	3. 66538400	3. 57522600
	H	5. 86046800	3. 93638000	3. 62722400
	H	4. 79344800	5. 14056200	2. 87343100
	P	-3. 83047100	0. 20520100	-0. 14307600
	C	-3. 93538400	2. 01151700	0. 18074300
	C	-5. 03286200	2. 78694500	-0. 22234500
	C	-5. 07308700	4. 15212100	0. 06830300
	C	-4. 02036600	4. 75217400	0. 76154700
	C	-2. 92210100	3. 98616200	1. 15956100

	C	-2.87207100	2.62281300	0.86758800
	C	-4.99176900	-0.11979000	-1.53084700
	C	-4.51581400	0.06889100	-2.83940500
	C	-5.35259000	-0.14834500	-3.93317100
	C	-6.66994300	-0.56916200	-3.73433700
	C	-7.14659400	-0.77093000	-2.43833500
	C	-6.31353100	-0.54778800	-1.33953800
	C	-4.55241700	-0.59924600	1.34033900
	C	-5.61180600	-0.01972200	2.05796100
	C	-6.14738700	-0.67165700	3.16867700
	C	-5.62587000	-1.90209200	3.57685000
	C	-4.56234600	-2.47438900	2.87754200
	C	-4.02030300	-1.82750100	1.76483100
	Au	-1.58582400	-0.47111200	-0.56876200
	H	-5.85083500	2.32980900	-0.77140800
	H	-5.92552400	4.74548700	-0.25151800
	H	-4.05211200	5.81532900	0.98440400
	H	-2.09482500	4.44874700	1.69033200
	H	-2.00118500	2.04401300	1.16504200
	H	-3.48571900	0.37759000	-2.99815800
	H	-4.97239100	0.00039500	-4.94002700
	H	-7.31928000	-0.74692200	-4.58725700
	H	-8.16749000	-1.10715300	-2.27852500
	H	-6.69160200	-0.71675300	-0.33626500
	H	-6.00824100	0.94637700	1.75885200
	H	-6.96532900	-0.21506800	3.71947800
	H	-6.04066100	-2.40593100	4.44586500
	H	-4.14048200	-3.42143800	3.20197700
	H	-3.16974200	-2.26456600	1.24938000
	B	1.52826700	1.03073500	2.35728600
	F	2.71743500	0.99415600	1.13841700
	F	0.45281700	1.54500100	1.69870600
	F	2.13055000	1.86115300	3.23872400
	F	1.43274000	-0.27076000	2.71055100
imc3	C	4.04005700	-3.46584700	0.51138200
	C	5.30708000	-3.99494800	0.29318100
	C	6.18030200	-3.41295500	-0.63992500
	C	5.80984900	-2.29252300	-1.38081100
	C	4.53693600	-1.75944000	-1.15600800
	C	3.64333900	-2.33186600	-0.21163500
	C	2.42901200	-1.53508100	-0.26994000
	C	2.60657600	-0.54659100	-1.21530700
	N	3.88094500	-0.66717700	-1.80043000
	C	0.99992600	-1.55285600	0.11119700
	C	0.31447400	-0.63484000	-0.63582400
	C	1.27049200	0.07860500	-1.60688500

	C	0. 93979100	-0. 32358300	-3. 06721200
	C	1. 14865900	1. 60877800	-1. 43874500
	C	0. 40384700	-2. 32039700	1. 22074300
	O	-0. 78273200	-2. 39896000	1. 49389400
	O	1. 35088700	-2. 93891400	1. 96995400
	C	0. 87042000	-3. 59201500	3. 15204000
	S	4. 77147200	0. 70177100	-2. 41282600
	O	5. 96906300	0. 14844400	-3. 03861800
	O	3. 80765400	1. 48632300	-3. 17999500
	C	5. 22119000	1. 60081600	-0. 93632100
	C	4. 47067200	2. 71747700	-0. 56193800
	C	6. 26767400	1. 13251700	-0. 13628600
	C	4. 75071700	3. 34457900	0. 64858600
	C	6. 52631700	1. 77225600	1. 07312500
	C	5. 76004200	2. 86778200	1. 49698200
	C	5. 97250500	3. 48634200	2. 85597700
	H	3. 35796100	-3. 91349900	1. 22258100
	H	5. 62275800	-4. 87603300	0. 84518100
	H	7. 16084900	-3. 85118900	-0. 80420600
	H	6. 47209500	-1. 86455400	-2. 12171600
	H	3. 04649500	-0. 16218500	0. 88709900
	H	-0. 06674700	0. 02469800	-3. 32125300
	H	1. 65975000	0. 13508300	-3. 75142700
	H	0. 97101800	-1. 41050100	-3. 19501600
	H	0. 11432500	1. 90702700	-1. 63811400
	H	1. 39598200	1. 91436000	-0. 41803300
	H	1. 80097000	2. 12379300	-2. 14651800
	H	1. 74733800	-4. 05125300	3. 61035700
	H	0. 42715300	-2. 85920300	3. 83161100
	H	0. 12400200	-4. 35048800	2. 90166800
	H	3. 68021700	3. 08127300	-1. 20668200
	H	6. 86234500	0. 28184300	-0. 44910000
	H	4. 15891000	4. 20482600	0. 94980300
	H	7. 32877700	1. 40379200	1. 70669000
	H	5. 23677400	3. 07894500	3. 56090400
	H	6. 97109000	3. 27066600	3. 24875000
	H	5. 83869100	4. 57322800	2. 83047900
	P	-4. 00772400	0. 21331600	-0. 13226700
	C	-4. 52019600	1. 93195400	-0. 53725500
	C	-5. 75493100	2. 23783900	-1. 12816400
	C	-6. 09501600	3. 56512400	-1. 39904100
	C	-5. 20847300	4. 59576800	-1. 08253000
	C	-3. 97513400	4. 29799100	-0. 49764200
	C	-3. 62879100	2. 97363600	-0. 23158100
	C	-5. 08519900	-0. 87381000	-1. 15119800
	C	-4. 63987000	-1. 23240000	-2. 43409000

	C	-5.42665200	-2.04169200	-3.25340000
	C	-6.66059100	-2.51084000	-2.79703000
	C	-7.10546200	-2.16787800	-1.51902100
	C	-6.32303200	-1.35366500	-0.69762400
	C	-4.52454000	-0.05327800	1.60974100
	C	-5.60200000	0.63999700	2.18417600
	C	-5.97165900	0.39146900	3.50660000
	C	-5.26813200	-0.54690000	4.26535300
	C	-4.19056900	-1.23224200	3.70127600
	C	-3.81166600	-0.98746900	2.38000600
	Au	-1.67796100	-0.21249000	-0.44335700
	H	-6.44774800	1.44207400	-1.38440900
	H	-7.05221900	3.79123600	-1.86109000
	H	-5.47414600	5.62728000	-1.29728600
	H	-3.27752700	5.09539300	-0.25714900
	H	-2.66143300	2.74398500	0.20778500
	H	-3.67124100	-0.88556000	-2.78458000
	H	-5.07018900	-2.31422400	-4.24285000
	H	-7.26927900	-3.14849800	-3.43234000
	H	-8.06044100	-2.53806600	-1.15599900
	H	-6.67241600	-1.10189200	0.29896700
	H	-6.14470600	1.38059000	1.60390200
	H	-6.80426000	0.93532300	3.94472300
	H	-5.55415000	-0.73559000	5.29670100
	H	-3.63175500	-1.95316100	4.29132600
	H	-2.95590400	-1.51014200	1.96036200
	B	2.22579100	1.09307100	2.83689300
	F	3.45983100	0.37097600	1.59417400
	F	1.64094900	1.99444200	2.03500200
	F	3.13168700	1.53134000	3.71887500
	F	1.55036900	-0.02785800	3.11753400
imc4	C	-4.16139800	2.88957200	-2.00757900
	C	-5.44373100	3.12908700	-2.48908500
	C	-6.36911400	2.08248300	-2.62939100
	C	-6.03584900	0.77213600	-2.29212500
	C	-4.75067500	0.53739100	-1.79855500
	C	-3.79978500	1.58294200	-1.64684500
	C	-2.59745900	0.95804600	-1.14548200
	C	-2.82991900	-0.38270600	-0.97902900
	N	-4.13690800	-0.68763300	-1.40571700
	C	-1.17194800	1.20136000	-0.89611300
	C	-0.53471100	0.02193100	-0.59952800
	C	-1.54917100	-1.13987900	-0.66029100
	C	-1.18400400	-2.08773600	-1.83140100
	C	-1.54128400	-1.92028600	0.67464700
	C	-0.47670600	2.51456800	-0.91534100

	O	0.72831100	2.67665700	-0.99895000
	O	-1.33950000	3.54707300	-0.80512200
	C	-0.73363000	4.84658500	-0.70504600
	S	-5.05974000	-2.07403400	-0.96643000
	O	-6.06487600	-2.24411600	-2.01275700
	O	-4.08530300	-3.12239800	-0.67406200
	C	-5.89551800	-1.61135600	0.54735000
	C	-5.18882800	-1.59849900	1.75371800
	C	-7.25012500	-1.27792700	0.50351500
	C	-5.85189000	-1.23072000	2.92050200
	C	-7.89655700	-0.91674900	1.68491600
	C	-7.21091800	-0.87871500	2.90603300
	C	-7.90790500	-0.45369300	4.17606300
	H	-3.44314000	3.69329900	-1.90553900
	H	-5.73132300	4.13902700	-2.76890600
	H	-7.36082300	2.28988300	-3.02188300
	H	-6.73714400	-0.03846500	-2.44095900
	H	-0.32871900	0.62638200	1.20341600
	H	-0.21791400	-2.56468700	-1.63494300
	H	-1.94727900	-2.86400500	-1.93412000
	H	-1.10838900	-1.53406100	-2.77286800
	H	-0.52982600	-2.29473000	0.86614000
	H	-1.81895100	-1.27350300	1.51360400
	H	-2.22512700	-2.76952300	0.63066600
	H	-1.56455800	5.54955500	-0.63618500
	H	-0.11165800	4.89517300	0.19104800
	H	-0.12284000	5.05637100	-1.58719200
	H	-4.14357300	-1.88359800	1.78280900
	H	-7.78892300	-1.32088400	-0.43580300
	H	-5.30618100	-1.22184700	3.86061100
	H	-8.95313600	-0.66319500	1.65572700
	H	-7.69860600	0.60011000	4.40249100
	H	-8.99380600	-0.56278900	4.09412700
	H	-7.56885100	-1.04235400	5.03528100
	P	3.85623200	-0.47371300	-0.09524500
	C	4.35133800	-1.43896400	1.38930000
	C	5.30484700	-2.46524300	1.34093900
	C	5.64011300	-3.16645700	2.50199300
	C	5.02907500	-2.84730900	3.71499200
	C	4.07863900	-1.82387400	3.76804500
	C	3.73429100	-1.12400500	2.61243000
	C	4.61471900	-1.34319400	-1.52742500
	C	3.90096600	-2.40368100	-2.11066000
	C	4.43551200	-3.10553100	-3.19056000
	C	5.68259000	-2.74832400	-3.70895700
	C	6.39316200	-1.68905300	-3.14221600

	C	5.86464600	-0.98878400	-2.05569200
	C	4.72929900	1.13131800	0.06116300
	C	5.99211700	1.22439600	0.66937000
	C	6.64040100	2.45635300	0.75494400
	C	6.03150300	3.60416000	0.24089600
	C	4.77060700	3.51889400	-0.35128200
	C	4.11426400	2.28955900	-0.43989300
	Au	1.49791400	-0.22659000	-0.33008300
	H	5.78256100	-2.72171700	0.40054200
	H	6.37768500	-3.96311200	2.45443300
	H	5.28930800	-3.39561300	4.61638700
	H	3.59832600	-1.57259200	4.70959900
	H	2.99454700	-0.32994400	2.66114100
	H	2.92201500	-2.67290600	-1.72239200
	H	3.87304700	-3.92292100	-3.63310200
	H	6.09483500	-3.28906000	-4.55649300
	H	7.35968100	-1.40180900	-3.54726600
	H	6.42168400	-0.16157000	-1.62761600
	H	6.46188900	0.33834200	1.08694600
	H	7.61598500	2.52065600	1.22922500
	H	6.53537400	4.56435100	0.31335200
	H	4.28507300	4.41143100	-0.73550400
	H	3.11923200	2.24169000	-0.87302500
	B	0.63355800	2.22381500	2.81735300
	F	-0.43726100	0.79349800	2.16764500
	F	1.83606200	1.74524100	2.45261400
	F	0.27741600	2.12222700	4.09680300
	F	0.10894000	3.21208900	2.08125000
tsc3	C	-4.01961600	2.79655600	-2.23076000
	C	-5.25369900	2.99750300	-2.83938600
	C	-6.16999500	1.94249300	-2.97672600
	C	-5.87829500	0.66271600	-2.50822400
	C	-4.64316200	0.46789100	-1.88615400
	C	-3.70209600	1.52177900	-1.74067600
	C	-2.55058100	0.93744000	-1.09530300
	C	-2.80303800	-0.38925400	-0.84123100
	N	-4.07257000	-0.72074200	-1.34011400
	C	-1.16348100	1.20400400	-0.74357900
	C	-0.55447500	0.06497800	-0.26751200
	C	-1.56059700	-1.11090800	-0.34022700
	C	-1.09163200	-2.14077800	-1.40197300
	C	-1.68592000	-1.79901200	1.03820100
	C	-0.47399400	2.52380600	-0.81001500
	O	0.72439900	2.67886500	-0.95316200
	O	-1.33830500	3.54734500	-0.67476500
	C	-0.73496400	4.84822000	-0.55519300

	S	-5.02798200	-2.09390500	-0.91275200
	O	-5.93458100	-2.32063600	-2.03483100
	O	-4.07826200	-3.11654500	-0.48334000
	C	-5.99206900	-1.55953600	0.49616300
	C	-5.40861900	-1.53953400	1.76659400
	C	-7.32317400	-1.18249900	0.30920200
	C	-6.17070300	-1.11974200	2.85251700
	C	-8.06944200	-0.76793400	1.41133300
	C	-7.50758400	-0.72139100	2.69407600
	C	-8.31143600	-0.24026600	3.87779800
	H	-3.30743700	3.60624900	-2.12731500
	H	-5.50964300	3.98203000	-3.22135400
	H	-7.12188600	2.11816100	-3.47013400
	H	-6.57010700	-0.15615200	-2.65501900
	H	-0.27630700	0.50753800	1.23838200
	H	-0.16083000	-2.61362200	-1.07224300
	H	-1.85286100	-2.91488300	-1.53146500
	H	-0.90691400	-1.65317900	-2.36459700
	H	-0.69418700	-2.13368400	1.36160200
	H	-2.06502800	-1.10602200	1.79594300
	H	-2.34283100	-2.66841700	0.97968000
	H	-1.56775100	5.54527000	-0.45812100
	H	-0.10313800	4.87246400	0.33466900
	H	-0.13768900	5.07910100	-1.44118400
	H	-4.38303700	-1.86054100	1.90684700
	H	-7.76929300	-1.23355400	-0.67709700
	H	-5.72103500	-1.10640500	3.84207200
	H	-9.10801700	-0.48004600	1.27043600
	H	-8.08411700	0.81012700	4.10243600
	H	-9.38700800	-0.31075500	3.68831500
	H	-8.08373800	-0.82009600	4.77868600
	P	3.87500400	-0.47028900	-0.13025000
	C	4.49526100	-1.25915700	1.40909700
	C	5.45172400	-2.28432000	1.39741600
	C	5.89435700	-2.84329400	2.59875000
	C	5.38761800	-2.38290200	3.81462200
	C	4.43388200	-1.36150000	3.83008100
	C	3.98182700	-0.80169600	2.63547500
	C	4.47218900	-1.52702400	-1.51157300
	C	3.68094000	-2.62138900	-1.89837400
	C	4.09601700	-3.46409900	-2.92893400
	C	5.29945300	-3.21634900	-3.59366000
	C	6.08614000	-2.12468400	-3.22282900
	C	5.67736300	-1.28288400	-2.18618400
	C	4.78032800	1.11878700	-0.25828400
	C	6.09942700	1.24842300	0.20757800

	C	6.77337400	2.46222500	0.07498700
	C	6.13482100	3.55624000	-0.51480700
	C	4.81919600	3.43653900	-0.96460500
	C	4.13738700	2.22485200	-0.83576600
	Au	1.52551100	-0.19083000	-0.15231200
	H	5.84816800	-2.65103100	0.45561100
	H	6.63309400	-3.64010900	2.58070200
	H	5.73113800	-2.82099400	4.74790400
	H	4.03298900	-1.00197700	4.77362700
	H	3.23650600	-0.01119700	2.65868900
	H	2.73444100	-2.80583000	-1.39696700
	H	3.47428200	-4.30641200	-3.21926800
	H	5.61834800	-3.86759500	-4.40288000
	H	7.01880300	-1.92252000	-3.74241200
	H	6.29282800	-0.43210000	-1.91164400
	H	6.59385400	0.40708000	0.68495600
	H	7.79256000	2.55577300	0.44009900
	H	6.65923000	4.50325000	-0.61080800
	H	4.31161300	4.28986700	-1.40515800
	H	3.10211500	2.15444500	-1.15629000
	B	0.51766400	2.07249000	2.81223100
	F	-0.32080700	0.70949200	2.29513000
	F	1.80267600	1.77531200	2.45733100
	F	0.25116600	2.05725800	4.13214200
	F	-0.06442800	3.06269600	2.08546800
imc5	C	2.50894500	3.13387600	-1.09978100
	C	3.26097700	4.15752000	-0.53278900
	C	4.07681500	3.92058800	0.58507500
	C	4.16348300	2.65582100	1.16396700
	C	3.41546700	1.62850500	0.58599300
	C	2.58450200	1.84788500	-0.54514800
	C	1.96543600	0.57484900	-0.82743800
	C	2.41955500	-0.35786100	0.08054900
	N	3.29466000	0.26222800	0.97625000
	C	0.94061700	-0.06032600	-1.64840200
	C	0.70176600	-1.33972100	-1.15274700
	C	1.65054800	-1.66841800	0.00856100
	C	0.92085800	-1.98001700	1.34069500
	C	2.45977700	-2.91371000	-0.44360600
	C	0.42686200	0.38429100	-2.98693200
	O	-0.06942800	-0.35580400	-3.80622600
	O	0.60793800	1.70733200	-3.18349600
	C	0.14913700	2.19933300	-4.45656000
	S	4.49210300	-0.52458700	1.95806400
	O	4.72337900	0.36247000	3.09392300
	O	4.01848300	-1.89263700	2.13490700

	C	5.95790400	-0.54014800	0.93412300
	C	6.05136800	-1.45595400	-0.11858500
	C	7.00078300	0.34194700	1.21908100
	C	7.20191400	-1.46735200	-0.90029900
	C	8.14691700	0.31032900	0.42535300
	C	8.26418800	-0.58412600	-0.64651000
	C	9.49558200	-0.59474000	-1.51964300
	H	1.87087400	3.31404800	-1.95585300
	H	3.21043200	5.15715100	-0.95573000
	H	4.64276900	4.73924700	1.02055600
	H	4.76075800	2.48664300	2.05033700
	H	0.21029500	-2.12650700	-1.71752200
	H	0.19854200	-2.77982600	1.17183200
	H	1.65208800	-2.28337100	2.09310500
	H	0.38598700	-1.09876200	1.71411200
	H	1.75663500	-3.73600300	-0.59894500
	H	2.99107500	-2.72410800	-1.38376400
	H	3.17695300	-3.19776600	0.32891700
	H	0.37468700	3.26578900	-4.45502400
	H	0.67281700	1.69333200	-5.27132600
	H	-0.92547300	2.03130500	-4.56191500
	H	5.24628200	-2.15579500	-0.31304100
	H	6.92230000	1.02290500	2.05872000
	H	7.28134000	-2.18031600	-1.71699700
	H	8.96517900	0.99004900	0.64804500
	H	9.30725800	-0.07315400	-2.46717400
	H	10.33852600	-0.09666400	-1.03113300
	H	9.80016900	-1.61702600	-1.76873000
	P	-3.27795700	0.53114900	0.40826100
	C	-3.22643500	0.45827200	2.24211600
	C	-3.53976800	1.56252400	3.04682500
	C	-3.50218100	1.44502900	4.43822200
	C	-3.15502900	0.22992500	5.02972500
	C	-2.84468900	-0.87239300	4.22862300
	C	-2.87501300	-0.76603500	2.83855300
	C	-3.47923800	2.30506100	-0.02989400
	C	-2.37344300	3.15641700	0.14227400
	C	-2.47015100	4.51039600	-0.17250700
	C	-3.66504600	5.02816400	-0.68112400
	C	-4.76073000	4.18619800	-0.86996500
	C	-4.67278400	2.83000600	-0.54377900
	C	-4.80413300	-0.34759200	-0.07722200
	C	-6.01417900	-0.07588500	0.58720400
	C	-7.17685000	-0.75128600	0.22274300
	C	-7.13712700	-1.71356000	-0.79139800
	C	-5.93388200	-2.00191300	-1.43423000

	C	-4.76389700	-1.32362000	-1.08279300
	Au	-1.28729600	-0.32500000	-0.50275700
	H	-3.80669500	2.51251500	2.59463500
	H	-3.74316800	2.30545100	5.05666700
	H	-3.12372000	0.14168700	6.11235100
	H	-2.57291300	-1.82003500	4.68497100
	H	-2.63189300	-1.62543200	2.21966700
	H	-1.43467500	2.75638200	0.51738100
	H	-1.60941000	5.15783100	-0.02991300
	H	-3.73742800	6.08227700	-0.93466700
	H	-5.68967200	4.58055500	-1.27260200
	H	-5.53162600	2.18512900	-0.69591000
	H	-6.04472900	0.64999600	1.39530700
	H	-8.10907700	-0.53753700	0.73847100
	H	-8.04245700	-2.24862200	-1.06540300
	H	-5.88940000	-2.77153500	-2.19878400
	H	-3.82748800	-1.59501100	-1.55852600
	B	-1.95106800	-3.62844100	-0.69429400
	F	-0.63458900	-4.10793100	-0.58753200
	F	-2.22856300	-2.81772900	0.46041300
	F	-2.87441600	-4.63844700	-0.80169300
	F	-2.01979200	-2.75606900	-1.82812400
(PPh ₃)AuOTf	P	1.47865400	0.03976100	0.01900200
	C	2.76578400	-0.51632000	-1.16039600
	C	3.98610100	0.16191300	-1.29904300
	C	4.95359000	-0.31419700	-2.18604900
	C	4.71066000	-1.46457900	-2.93853400
	C	3.49536200	-2.14104700	-2.80727300
	C	2.52409400	-1.66849700	-1.92568500
	C	1.82113300	1.80604300	0.36825900
	C	1.28144400	2.77771900	-0.49022500
	C	1.53929200	4.12997000	-0.26953200
	C	2.32886200	4.52444100	0.81332400
	C	2.86114600	3.56382400	1.67494300
	C	2.60995100	2.20788600	1.45645400
	C	1.76313500	-0.88178900	1.57612000
	C	3.05074800	-1.29616500	1.95431400
	C	3.24074200	-1.97485100	3.15817800
	C	2.15056600	-2.24913700	3.98763300
	C	0.86764500	-1.84740800	3.61119600
	C	0.66791700	-1.16795800	2.40859100
	Au	-0.66004300	-0.29852100	-0.69826700
	S	-3.64041500	-0.85748700	-0.03793900
	O	-4.72668500	-1.76997300	-0.37969600
	O	-2.91839900	-1.03382700	1.23392600
	O	-2.67486600	-0.64348500	-1.22653200

	C	-4.40256700	0.83654600	0.07379300
	F	-5.28588600	0.87366300	1.07660600
	F	-3.44781400	1.75354800	0.30935400
	F	-5.02402100	1.15122400	-1.06583900
	H	4.17862100	1.06311300	-0.72496200
	H	5.89450800	0.21857200	-2.29153100
	H	5.46370000	-1.82982400	-3.63123800
	H	3.29869400	-3.03173300	-3.39697200
	H	1.57495600	-2.19013800	-1.83501100
	H	0.65194900	2.47594500	-1.32319900
	H	1.11403500	4.87446900	-0.93630400
	H	2.52105800	5.57904300	0.98987700
	H	3.46718100	3.86765200	2.52384000
	H	3.01619800	1.46840900	2.13936400
	H	3.90054200	-1.10240000	1.30624100
	H	4.23865000	-2.29639200	3.44311200
	H	2.30049400	-2.78430200	4.92124100
	H	0.01451000	-2.07031500	4.24502800
	H	-0.33937700	-0.88155900	2.11651900
(PPh ₃)AuCl	P	0.46258900	0.00031200	-0.00184400
	C	1.17212900	-0.19748000	1.67918200
	C	2.36499500	-0.89989800	1.90856700
	C	2.87893300	-1.00494800	3.20246100
	C	2.20868000	-0.41255400	4.27427800
	C	1.01825100	0.28395000	4.05286800
	C	0.49807900	0.38798700	2.76309300
	C	1.17208700	-1.35724200	-1.01262200
	C	0.49827400	-2.58885500	-1.04552200
	C	1.01803900	-3.65420000	-1.78012300
	C	2.20780600	-3.49753900	-2.49507700
	C	2.87825100	-2.27308700	-2.47338400
	C	2.36469200	-1.20468300	-1.73589100
	C	1.17292600	1.55544200	-0.67007400
	C	2.37788500	2.09111700	-0.19072700
	C	2.89087800	3.26644400	-0.74258800
	C	2.20738200	3.91463000	-1.77313600
	C	1.00510800	3.38860700	-2.25146200
	C	0.48595700	2.21722200	-1.70052700
	Au	-1.84927100	-0.00057800	-0.00097600
	H	2.88719500	-1.37394700	1.08310200
	H	3.80031600	-1.55538600	3.37164200
	H	2.60843900	-0.50017300	5.28076700
	H	0.48739400	0.73805100	4.88464800
	H	-0.43736100	0.91583000	2.59708000
	H	-0.43686800	-2.70806400	-0.50467400
	H	0.48756900	-4.60182300	-1.80184300

	H	2.60714800	-4.32561100	-3.07416400
	H	3.79926200	-2.14498300	-3.03536600
	H	2.88663200	-0.25273900	-1.73242600
	H	2.90991700	1.59922200	0.61785500
	H	3.82182800	3.67759400	-0.36202900
	H	2.60631300	4.83208500	-2.19697900
	H	0.46405600	3.89450200	-3.04595600
	H	-0.45918300	1.82101100	-2.06236300
	Cl	-4.20007200	-0.00376600	0.00174000
(PPh ₃)AuBF ₄	P	-0.91382100	0.02149800	-0.01911100
	C	-1.01574800	1.58585800	-0.96469600
	C	-2.21151700	2.32242100	-1.01220700
	C	-2.27871500	3.49872800	-1.75802200
	C	-1.15485300	3.95161800	-2.45384700
	C	0.03852800	3.22994100	-2.39910700
	C	0.11583600	2.05051300	-1.65617200
	C	-1.98878700	0.22502500	1.44967000
	C	-3.33008200	-0.18604700	1.44286000
	C	-4.12837400	0.01622200	2.57035000
	C	-3.59532000	0.62582800	3.70733500
	C	-2.25891200	1.03321800	3.71995700
	C	-1.45577300	0.83096700	2.59851500
	C	-1.67394200	-1.29601400	-1.03990000
	C	-2.49916100	-1.00711900	-2.13629200
	C	-3.06737700	-2.04649900	-2.87593500
	C	-2.81752600	-3.37472600	-2.52828100
	C	-1.99336600	-3.66777600	-1.43857800
	C	-1.41929300	-2.63500300	-0.69950500
	Au	1.24404000	-0.43725700	0.48176900
	H	-3.08365000	1.98720400	-0.45830700
	H	-3.20532200	4.06510700	-1.78797800
	H	-1.20759900	4.87204700	-3.02872300
	H	0.91900500	3.58605900	-2.92557300
	H	1.05983100	1.51450100	-1.60205300
	H	-3.74820100	-0.67219300	0.56668700
	H	-5.16484900	-0.30911800	2.56030700
	H	-4.21737500	0.77673200	4.58512500
	H	-1.83775700	1.50004400	4.60560700
	H	-0.41276000	1.13599200	2.61640600
	H	-2.68903200	0.02242700	-2.42210500
	H	-3.69966200	-1.81481100	-3.72837600
	H	-3.25622400	-4.18069600	-3.10978500
	H	-1.78731000	-4.69994500	-1.17056100
	H	-0.76414000	-2.86744800	0.13605400
	B	4.20342200	0.00354500	-0.04147300
	F	5.04126100	-0.89324100	-0.63165800

	F	3.28234100	0.56009000	-0.95553900
	F	4.80573700	0.95707200	0.72564300
	F	3.30536700	-0.80788600	0.91052000

Table S11. The cartesian coordinates of the optimized stationary points on the reaction channel in Figure 7.

Species	Cartesian coordinates			
imal'	C	-3.52741200	3.51662600	0.35974600
	C	-4.62761000	4.36434600	0.40859900
	C	-5.87197300	3.97297700	-0.11813600
	C	-6.04664900	2.73000400	-0.71977700
	C	-4.94024100	1.87713500	-0.75733600
	C	-3.68004100	2.24512600	-0.21646900
	C	-2.77339700	1.13512000	-0.45327300
	C	-3.47926700	0.16612900	-1.11315400
	N	-4.78668400	0.59814000	-1.33097500
	C	-1.34511600	0.94600300	-0.10109100
	C	-0.46604100	0.66516300	-1.05677400
	C	-0.09245900	0.52005000	-2.35826100
	C	0.36310000	1.71321000	-3.17004500
	C	-0.34645500	-0.77036900	-3.10897800
	C	-0.92995100	0.90421900	1.34692400
	O	-0.32157600	-0.02306200	1.85398900
	O	-1.34592100	1.98108300	2.01242200
	C	-0.89514000	2.09770800	3.37685300
	S	-6.01336500	-0.50158100	-1.82281300
	O	-7.15183200	0.31598600	-2.23408400
	O	-5.34474900	-1.42546400	-2.73298500
	C	-6.43990300	-1.38166100	-0.32654400
	C	-5.61457500	-2.42052900	0.11752200
	C	-7.58799400	-1.01394900	0.37575300
	C	-5.95703500	-3.08747600	1.29053500
	C	-7.91178900	-1.70009900	1.54557200
	C	-7.10613800	-2.74337100	2.02044000
	C	-7.47518000	-3.50004800	3.27416600
	H	-2.56359900	3.82713700	0.74408500
	H	-4.52272400	5.35083200	0.85185800
	H	-6.71295000	4.65941900	-0.07160000

	H	-6.99288600	2.43905300	-1.15806100
	H	-3.16396500	-0.82246500	-1.41878300
	H	1.14771100	1.42734300	-3.87868500
	H	-0.50144600	2.06207700	-3.75364300
	H	0.72652300	2.52434000	-2.53785800
	H	0.53207900	-1.08020000	-3.68447800
	H	-0.66950900	-1.58013000	-2.45236900
	H	-1.15518800	-0.57053700	-3.82725400
	H	-1.35846700	3.00913400	3.75310700
	H	-1.21518100	1.22978100	3.95850600
	H	0.19257200	2.18305600	3.38381700
	H	-4.72310500	-2.70160300	-0.43532400
	H	-8.21852900	-0.21412900	0.00349800
	H	-5.32020200	-3.89438500	1.64485900
	H	-8.80614800	-1.41971300	2.09607500
	H	-6.58957600	-3.73485700	3.87479100
	H	-8.16868700	-2.92844100	3.89874900
	H	-7.96202500	-4.45314100	3.02863300
	P	3.70574600	-0.95242000	-0.11215300
	C	3.62033900	-1.62303100	1.59436600
	C	4.13555600	-2.88497800	1.92710600
	C	4.07421900	-3.33943500	3.24630800
	C	3.50068000	-2.53835400	4.23599000
	C	2.98550500	-1.28238400	3.90566900
	C	3.03793800	-0.81987100	2.59000100
	C	4.00149300	-2.40233300	-1.20586200
	C	2.93631400	-3.29216200	-1.43097900
	C	3.10594200	-4.40039100	-2.25837800
	C	4.33596900	-4.62718200	-2.88346400
	C	5.39376300	-3.74332800	-2.67272500
	C	5.23121600	-2.63537300	-1.83603500
	C	5.20897900	0.08620500	-0.16875000
	C	6.39989900	-0.34768100	0.44138900
	C	7.54263400	0.44715600	0.38305000
	C	7.50215800	1.68425200	-0.26817200
	C	6.31769400	2.12601000	-0.85598600
	C	5.16933800	1.33154400	-0.81154500
	Au	1.65500900	0.09059400	-0.67840500
	H	4.57924900	-3.51423900	1.16123900
	H	4.47614800	-4.31721100	3.49833300
	H	3.45404600	-2.89304900	5.26222600
	H	2.53476400	-0.65825800	4.67193800
	H	2.62485100	0.15454900	2.33949400
	H	1.97129700	-3.11096600	-0.96378000
	H	2.27485600	-5.08013400	-2.42531600
	H	4.46440000	-5.48584400	-3.53667600

	H	6.35008200	-3.90976400	-3.16083200
	H	6.06028600	-1.95274000	-1.68264200
	H	6.43039600	-1.29603500	0.97078300
	H	8.45980700	0.10833000	0.85703400
	H	8.39097200	2.30860500	-0.29960400
	H	6.26992900	3.10026300	-1.33250900
	H	4.24220900	1.70969400	-1.23114200
	S	2.26978500	3.29413400	0.52709900
	O	3.41124400	3.99002000	1.13420600
	O	2.36416800	3.02837900	-0.93711300
	O	1.75029500	2.11828800	1.29645800
	C	0.85648600	4.50278300	0.63184200
	F	1.20782100	5.69402800	0.13532500
	F	-0.20162300	4.05111800	-0.07362400
	F	0.45963900	4.67224200	1.90538300
	O	-2.12631400	-2.94574600	-0.76390200
	C	-1.41034600	-2.84199300	0.23494400
	N	-0.81789300	-3.88053500	0.88108900
	C	-0.00761800	-3.66410100	2.07082800
	C	-1.02435300	-5.24630700	0.42988600
	H	-1.17210400	-1.87186700	0.69507700
	H	-0.45410100	-4.16505200	2.94035000
	H	1.00513200	-4.06120200	1.92900500
	H	0.06538500	-2.59358200	2.27551700
	H	-0.06361800	-5.72689500	0.20480900
	H	-1.53111300	-5.83866400	1.20320200
	H	-1.64040600	-5.21771600	-0.46967100
tsal'	C	3.81389400	3.14257800	-1.24026300
	C	4.94814000	3.92477500	-1.08573700
	C	5.94453100	3.57868300	-0.15187500
	C	5.83359600	2.45045000	0.65450700
	C	4.70618800	1.64453500	0.47387900
	C	3.69226200	1.96906000	-0.47239100
	C	2.64516400	0.99347600	-0.30822400
	C	3.07473200	0.05934400	0.66897500
	N	4.31377700	0.48338000	1.16798100
	C	1.26042100	0.86571700	-0.66819200
	C	0.50673900	0.27725300	0.32831600
	C	1.15170800	0.24530600	1.62608800
	C	1.33269100	1.54806900	2.37667900
	C	0.98398100	-0.96858000	2.50867700
	C	0.69474500	1.17532100	-2.02007200
	O	0.02397900	0.38528300	-2.65756900
	O	1.05213000	2.38757200	-2.46002300
	C	0.37126100	2.85167800	-3.64439000
	S	5.35562200	-0.60553400	2.02282500

	O	6.31411000	0.23826400	2.73165200
	O	4.43301200	-1.49786800	2.71724600
	C	6.21175700	-1.51173200	0.74506500
	C	5.54304500	-2.52523400	0.04871600
	C	7.54178700	-1.18971500	0.46727900
	C	6.23393500	-3.21210000	-0.94577300
	C	8.21167600	-1.89734800	-0.52932300
	C	7.57234800	-2.91569400	-1.24927400
	C	8.31057900	-3.69642400	-2.30987100
	H	3.02397900	3.41688200	-1.92676500
	H	5.06244300	4.82829800	-1.67708600
	H	6.81510000	4.21926000	-0.04145400
	H	6.57897100	2.20902200	1.40143300
	H	2.86629700	-1.00511900	0.62244200
	H	2.09949900	1.45552700	3.15232900
	H	1.54974500	2.38890800	1.71908600
	H	0.37064000	1.77027200	2.85718400
	H	0.07262200	-0.84928900	3.11001900
	H	0.90104900	-1.88728700	1.92355000
	H	1.83102500	-1.05678200	3.19646300
	H	0.81904400	3.81892000	-3.87277500
	H	0.51474700	2.15028800	-4.46968600
	H	-0.68842600	2.96272500	-3.40969900
	H	4.50825000	-2.77445700	0.26217600
	H	8.04170400	-0.41072900	1.03191100
	H	5.72040700	-3.99666100	-1.49563900
	H	9.24812100	-1.65443500	-0.74857100
	H	7.66473900	-3.91579300	-3.16686900
	H	9.18736100	-3.15137400	-2.67288700
	H	8.66118000	-4.65853300	-1.91370400
	P	-3.75562000	-0.94573600	0.18272100
	C	-4.77407000	-0.18390100	-1.13488100
	C	-6.17031400	-0.35011500	-1.16060800
	C	-6.92781600	0.24526200	-2.16655800
	C	-6.30109700	1.02259000	-3.14598700
	C	-4.91968300	1.20694600	-3.11216700
	C	-4.15094500	0.60791800	-2.11050700
	C	-3.94165500	-2.77143600	0.00942400
	C	-4.63829800	-3.37160800	-1.04822500
	C	-4.70001600	-4.76491000	-1.15325300
	C	-4.07354100	-5.57099100	-0.20337100
	C	-3.37338000	-4.97996000	0.85382100
	C	-3.29997100	-3.59154100	0.95459300
	C	-4.58551900	-0.52206200	1.76521000
	C	-5.56848300	-1.34094900	2.34250500
	C	-6.20145900	-0.94893400	3.52300800

	C	-5.86105300	0.26120800	4.13124000
	C	-4.88252800	1.07758200	3.56018500
	C	-4.23781400	0.69157700	2.38366600
	Au	-1.46483400	-0.32026900	0.19199100
	H	-6.66588100	-0.93384100	-0.38970700
	H	-8.00643900	0.11387100	-2.18004000
	H	-6.89492000	1.49580400	-3.92353500
	H	-4.43232300	1.83400300	-3.85279300
	H	-3.08315900	0.79694100	-2.06692400
	H	-5.13656800	-2.75566700	-1.78961100
	H	-5.24443600	-5.21587900	-1.97860000
	H	-4.12804400	-6.65330400	-0.28364600
	H	-2.88333800	-5.60045300	1.59942800
	H	-2.74251300	-3.14025700	1.77147200
	H	-5.83398100	-2.28724200	1.88030500
	H	-6.95889600	-1.59006000	3.96633500
	H	-6.35560500	0.56491700	5.05016900
	H	-4.61137600	2.01961100	4.02802600
	H	-3.47018500	1.33611800	1.95870200
	S	-1.90199700	3.38318400	0.04098800
	O	-3.11767800	4.20870000	-0.00901500
	O	-1.64621800	2.68426100	1.33082900
	O	-1.65204700	2.53672300	-1.16143000
	C	-0.50753900	4.61674300	-0.05546300
	F	-0.60145000	5.53922400	0.91138500
	F	0.69684200	4.01000900	0.07142800
	F	-0.51167200	5.24768100	-1.24368300
	O	2.22060900	-2.90156300	-0.26896200
	C	1.39439200	-2.71869200	-1.17017100
	N	0.50700700	-3.63549800	-1.61581900
	C	-0.47822400	-3.29337000	-2.63234000
	C	0.44518600	-4.96105100	-1.02197000
	H	1.30531500	-1.76004700	-1.70011700
	H	-0.35013100	-3.92198300	-3.52331100
	H	-1.49184900	-3.44281700	-2.24193400
	H	-0.36940200	-2.24200100	-2.90953700
	H	-0.53220000	-5.12214200	-0.55045600
	H	0.59372600	-5.73136700	-1.78932200
	H	1.23163100	-5.03570200	-0.27029300
ima2'	C	3.97475700	2.81878000	-1.56925900
	C	5.11896100	3.57640400	-1.40256600
	C	5.97530100	3.34099500	-0.30578400
	C	5.72251900	2.35428300	0.64076100
	C	4.58131100	1.56090600	0.46243800
	C	3.70589700	1.78702900	-0.64481800
	C	2.59922100	0.91469500	-0.47103500

	C	2.88236500	-0.02005500	0.65118300
	N	4.08755400	0.53974800	1.28977400
	C	1.26257300	0.75294600	-0.86865600
	C	0.55797400	0.08348500	0.14442700
	C	1.46464700	-0.14388300	1.34567300
	C	1.27323400	1.02278500	2.34858900
	C	1.20661000	-1.48978700	2.03619700
	C	0.63877500	1.20149600	-2.15060000
	O	-0.10341700	0.49703500	-2.80696000
	O	1.04271000	2.42528100	-2.51764600
	C	0.32623700	3.01512300	-3.62356300
	S	5.14451000	-0.50079600	2.18740000
	O	6.07713200	0.38537600	2.88129000
	O	4.24578500	-1.39834500	2.90461400
	C	6.04988200	-1.43698600	0.96228400
	C	5.44032400	-2.52738500	0.33246200
	C	7.35467200	-1.05203800	0.64151800
	C	6.15270200	-3.22285000	-0.64123000
	C	8.05144500	-1.77114700	-0.32704300
	C	7.46439500	-2.86254400	-0.98382700
	C	8.23600400	-3.65081500	-2.01466000
	H	3.28049300	3.00039500	-2.37920400
	H	5.35203300	4.37235300	-2.10268900
	H	6.85612100	3.96545500	-0.18242600
	H	6.36816600	2.21280200	1.49721900
	H	3.10365900	-1.00891200	0.22138100
	H	0.24178800	1.03788200	2.70858800
	H	1.95515500	0.87572200	3.19259500
	H	1.46684100	1.99434700	1.88870500
	H	0.18058300	-1.51104400	2.41763500
	H	1.33582600	-2.32301900	1.33895500
	H	1.89654500	-1.62526700	2.87199600
	H	0.79295100	3.98755300	-3.78031100
	H	0.41473300	2.38944100	-4.51510000
	H	-0.71848100	3.13112300	-3.33248200
	H	4.43189100	-2.83392700	0.58431100
	H	7.81640000	-0.21771500	1.15701200
	H	5.67375000	-4.05962700	-1.14222300
	H	9.06891600	-1.48012400	-0.57541000
	H	9.00599900	-3.03875400	-2.49501300
	H	8.74136700	-4.50896000	-1.55202000
	H	7.57523200	-4.04474800	-2.79375700
	P	-3.76132600	-0.86898900	0.24252700
	C	-4.83322800	-0.04032300	-0.98967300
	C	-6.22902500	-0.21180300	-0.97155100
	C	-7.02607800	0.43558600	-1.91270100

	C	-6.43956900	1.26974700	-2.87019700
	C	-5.05847100	1.45862800	-2.87878300
	C	-4.25000900	0.80755500	-1.94273400
	C	-3.98331000	-2.68306000	0.00081700
	C	-4.68643700	-3.22691400	-1.08265300
	C	-4.76561400	-4.61327800	-1.24966700
	C	-4.14896000	-5.46883100	-0.33743300
	C	-3.44208500	-4.93430800	0.74484900
	C	-3.35257200	-3.55283600	0.90848500
	C	-4.50175300	-0.50231600	1.88186000
	C	-5.48138200	-1.32122000	2.46517700
	C	-6.04753900	-0.97005300	3.69130900
	C	-5.64338200	0.19917700	4.33959900
	C	-4.66887800	1.01545100	3.76199200
	C	-4.09067000	0.67040600	2.53880000
	Au	-1.43803500	-0.32010500	0.14069600
	S	-1.80095100	3.41068400	0.10774800
	O	-2.92532900	4.35656500	0.06155000
	O	-1.64666300	2.63843400	1.37038400
	O	-1.60271600	2.59075200	-1.12327600
	C	-0.28924000	4.50064000	0.09662000
	F	-0.32337800	5.39841600	1.08971700
	F	0.84284400	3.77138100	0.24067300
	F	-0.18884200	5.16583000	-1.06975800
	H	-6.69326600	-0.84170700	-0.21766300
	H	-8.10402900	0.29937100	-1.89282900
	H	-7.06415100	1.78244500	-3.59699200
	H	-4.60098700	2.12830300	-3.60091900
	H	-3.18152300	0.99912100	-1.93144500
	H	-5.17649100	-2.57253800	-1.79604800
	H	-5.31590000	-5.01993500	-2.09394500
	H	-4.21655300	-6.54570300	-0.46621200
	H	-2.95998500	-5.59338900	1.46197500
	H	-2.79273200	-3.14649100	1.74680900
	H	-5.79561700	-2.23637300	1.97192200
	H	-6.80282900	-1.61073100	4.13895100
	H	-6.08575300	0.47093300	5.29445300
	H	-4.34890500	1.92576800	4.26079700
	H	-3.32770800	1.31572100	2.10594000
	O	2.41052700	-2.85091700	-0.96919900
	C	1.47005400	-2.65625400	-1.74585200
	N	0.45019800	-3.51215600	-1.98143700
	C	-0.65376500	-3.14365700	-2.85690800
	C	0.38048500	-4.79309500	-1.29746200
	H	1.37734900	-1.73013900	-2.33280200
	H	-0.69964500	-3.80943700	-3.72889400

	H	-1.60362900	-3.21243300	-2.31381800
	H	-0.52866600	-2.11060200	-3.18966200
	H	-0.52092600	-4.84486800	-0.67454000
	H	0.34828100	-5.61359700	-2.02563900
	H	1.26699200	-4.89508100	-0.67089500
tsa2'	C	3.96125500	3.25526500	-1.56033300
	C	5.18888600	3.89787300	-1.54731100
	C	6.17772200	3.52654500	-0.61504000
	C	5.97350100	2.51908800	0.32234300
	C	4.73510400	1.86069500	0.30754300
	C	3.73523100	2.21578800	-0.64115100
	C	2.59938900	1.39355000	-0.35307100
	C	2.93174200	0.45344100	0.64661100
	N	4.22839600	0.84500600	1.14817900
	C	1.19384700	1.29692900	-0.64736500
	C	0.57537900	0.50744200	0.29781100
	C	1.58533900	0.14330500	1.39213100
	C	1.44585400	1.16538800	2.55736800
	C	1.39023400	-1.27616000	1.95063600
	C	0.57306300	1.79926300	-1.90787600
	O	0.10139300	1.05344000	-2.75528300
	O	0.68250000	3.12055800	-2.04938000
	C	-0.01418500	3.70328100	-3.17332100
	S	5.23562600	-0.19909000	2.07857100
	O	6.33128000	0.63614500	2.56369500
	O	4.33648600	-0.89517200	2.99317700
	C	5.90356200	-1.39974600	0.93032600
	C	5.32545000	-2.66788400	0.85789500
	C	7.01037200	-1.06536800	0.14279400
	C	5.86362500	-3.60669800	-0.02153200
	C	7.52561500	-2.01425900	-0.73503000
	C	6.96519700	-3.29813600	-0.83031300
	C	7.56017900	-4.32756100	-1.76105400
	H	3.17483900	3.54840000	-2.24634000
	H	5.38708700	4.70498400	-2.24608300
	H	7.12570800	4.05769500	-0.60909100
	H	6.72667900	2.28082900	1.06112600
	H	2.95823100	-0.71883500	-0.31826900
	H	0.46380400	1.05161000	3.02627200
	H	2.22301200	0.97376800	3.30402600
	H	1.53054700	2.19424700	2.19866900
	H	0.39415100	-1.34922600	2.39808700
	H	1.46139100	-2.03860800	1.16971400
	H	2.13669400	-1.49022000	2.71785700
	H	0.20206900	4.76957000	-3.11704300
	H	0.35049900	3.27610700	-4.11131200

	H	-1.08138800	3.51846100	-3.04808700
	H	4.48021400	-2.91330300	1.49076700
	H	7.46757100	-0.08587400	0.22524100
	H	5.42377200	-4.59956200	-0.07380600
	H	8.38510000	-1.75811600	-1.34949800
	H	8.47248600	-4.76273900	-1.33267400
	H	6.86230600	-5.14899400	-1.95069900
	H	7.83597000	-3.88421900	-2.72416500
	P	-3.49549000	-1.23788900	0.18501900
	C	-4.75410300	-0.61280400	-0.99024800
	C	-6.05596400	-1.14464000	-1.01087500
	C	-6.99995200	-0.64788500	-1.90683700
	C	-6.65798500	0.39281300	-2.77709000
	C	-5.37445800	0.93584500	-2.74521900
	C	-4.41748700	0.43703500	-1.85632200
	C	-3.20615400	-3.00533800	-0.27444900
	C	-3.73781600	-3.58857000	-1.43289200
	C	-3.42703100	-4.91085900	-1.76879700
	C	-2.59057200	-5.66792300	-0.94855700
	C	-2.05456600	-5.09422300	0.21006000
	C	-2.35083600	-3.77148900	0.53811200
	C	-4.33595000	-1.30092900	1.81801000
	C	-4.98477700	-2.44885200	2.29806900
	C	-5.63509200	-2.42078500	3.53306700
	C	-5.64520600	-1.24877100	4.29197800
	C	-5.00266400	-0.10410600	3.81489300
	C	-4.34343500	-0.12231900	2.58453800
	Au	-1.36096900	-0.15470500	0.24424100
	S	-2.73224200	3.30475600	0.04253400
	O	-3.88169300	4.17842000	-0.23707500
	O	-2.85038600	2.42659900	1.23662700
	O	-2.15188600	2.61550000	-1.14888000
	C	-1.37236500	4.48198700	0.52368200
	F	-1.74595500	5.26042800	1.54942300
	F	-0.25811700	3.81834500	0.89274500
	F	-1.04643600	5.28196600	-0.51102800
	H	-6.33420400	-1.93576600	-0.31975600
	H	-8.00493300	-1.06149400	-1.91722500
	H	-7.40026100	0.78856300	-3.46540900
	H	-5.11246000	1.76649100	-3.39373600
	H	-3.43737800	0.90344200	-1.80696400
	H	-4.39964400	-3.01386400	-2.07249800
	H	-3.85078000	-5.34853600	-2.66891200
	H	-2.36103200	-6.69907200	-1.20405500
	H	-1.40967300	-5.67891300	0.86131400
	H	-1.91918100	-3.32926200	1.43224100

	H	-4.97869400	-3.36626300	1.71693600
	H	-6.13275700	-3.31471400	3.90007800
	H	-6.15161200	-1.22871900	5.25352200
	H	-5.00816900	0.81081900	4.40068600
	H	-3.84821100	0.77501100	2.21845000
	O	2.75664700	-1.68149200	-0.94494400
	C	1.79309700	-1.57438900	-1.78370800
	N	1.12561900	-2.61655900	-2.23401400
	C	-0.01279300	-2.41860400	-3.13996600
	C	1.40350400	-3.97939700	-1.78452000
	H	1.47662800	-0.60955100	-2.17499000
	H	0.18498500	-2.91366300	-4.09672400
	H	-0.90941100	-2.85176400	-2.68594000
	H	-0.17501900	-1.34974200	-3.29084900
	H	0.53589800	-4.36530100	-1.23908000
	H	1.58996000	-4.61626900	-2.65554200
	H	2.27913100	-3.97283300	-1.13707200
ima3'	C	-4.30825600	-2.46547700	-2.21401900
	C	-5.57544400	-3.03481500	-2.27433300
	C	-6.49663900	-2.85239700	-1.23044500
	C	-6.17846100	-2.09147800	-0.10658600
	C	-4.91361900	-1.50073600	-0.06027800
	C	-3.96469400	-1.68309600	-1.10227700
	C	-2.78156100	-0.96843000	-0.69186100
	C	-3.01954400	-0.35685600	0.50980800
	N	-4.31533300	-0.69158600	0.95166000
	C	-1.38778300	-0.71833500	-1.06260400
	C	-0.75513900	0.00483000	-0.08208400
	C	-1.75216000	0.26558500	1.07521000
	C	-1.29524000	-0.52212100	2.33273400
	C	-1.82380600	1.77558800	1.39027100
	C	-0.70384500	-1.26969900	-2.26254200
	O	0.12264900	-0.67412700	-2.94535700
	O	-1.11513400	-2.50965900	-2.53629000
	C	-0.36812700	-3.22518000	-3.54132300
	S	-5.24396600	0.14621500	2.13153700
	O	-6.24256500	-0.80372200	2.61364500
	O	-4.27970000	0.76753800	3.03549000
	C	-6.09715400	1.44175600	1.23262700
	C	-5.47561100	2.67922300	1.05324900
	C	-7.37978300	1.20375700	0.73136200
	C	-6.14643700	3.67962600	0.35252200
	C	-8.03250100	2.21624300	0.03241700
	C	-7.43016600	3.46676200	-0.16925100
	C	-8.16362100	4.56518300	-0.90135600
	H	-3.58366600	-2.63164400	-3.00258700

	H	-5.85037500	-3.64409900	-3.13109000
	H	-7.47224200	-3.32752300	-1.28524900
	H	-6.87387000	-1.99593200	0.71696700
	H	-0.60502500	1.55221300	-1.20809900
	H	-0.35920100	-0.10193700	2.71521400
	H	-2.06023700	-0.45051800	3.11118600
	H	-1.11542000	-1.57183000	2.08780700
	H	-0.81493200	2.14396300	1.60646400
	H	-2.21927300	2.34603900	0.54017900
	H	-2.45464400	1.96021500	2.26169100
	H	-0.84759500	-4.20148100	-3.60721600
	H	-0.41716800	-2.70044800	-4.49942600
	H	0.66440200	-3.32135100	-3.20351300
	H	-4.49107000	2.85955600	1.46836000
	H	-7.86111400	0.24786700	0.89920700
	H	-5.66637100	4.64541800	0.21511600
	H	-9.03030200	2.03277800	-0.35833800
	H	-8.74442100	4.16788100	-1.74074400
	H	-8.86809200	5.07905800	-0.23408100
	H	-7.47246100	5.31903900	-1.29136400
	P	3.59478000	0.78128300	0.52539100
	C	4.87307300	-0.20834800	-0.33606700
	C	6.23799200	-0.04343000	-0.03821900
	C	7.19478300	-0.81147600	-0.69796400
	C	6.79756900	-1.76088500	-1.64580600
	C	5.44444000	-1.94139900	-1.92791900
	C	4.47781900	-1.16671100	-1.27964200
	C	3.88626800	2.53261600	0.00566500
	C	4.81440300	2.89249000	-0.98170500
	C	4.94420600	4.22706300	-1.38229000
	C	4.15486800	5.21859400	-0.79682800
	C	3.22476600	4.86861500	0.18847900
	C	3.08527900	3.53711800	0.57858700
	C	4.04565300	0.72443700	2.30477000
	C	4.81516700	1.71495000	2.93319900
	C	5.14453800	1.59233700	4.28449200
	C	4.71273900	0.48178200	5.01210600
	C	3.95060800	-0.50799500	4.38706100
	C	3.60993600	-0.39354300	3.03841700
	Au	1.29029500	0.26586700	0.15703900
	S	1.87160200	-3.42579700	0.12251200
	O	2.90887100	-4.46774400	0.07237600
	O	1.87350700	-2.55962100	1.33281500
	O	1.66824600	-2.66972200	-1.14945600
	C	0.27510200	-4.36953400	0.28268500
	F	0.31375100	-5.21508800	1.32180500

	F	-0.76766100	-3.53487900	0.46429000
	F	0.03595100	-5.08477000	-0.83323400
	H	6.55063800	0.67205800	0.71769200
	H	8.24766000	-0.68214100	-0.46165100
	H	7.54474400	-2.37137100	-2.14612500
	H	5.12578000	-2.70438500	-2.63170100
	H	3.42491900	-1.35866500	-1.46786300
	H	5.44495500	2.13372500	-1.43359500
	H	5.67918200	4.49039200	-2.13896200
	H	4.27112600	6.25761200	-1.09449700
	H	2.61053600	5.63359300	0.65638600
	H	2.35206100	3.27276000	1.33618800
	H	5.15307300	2.58397900	2.37646600
	H	5.73789300	2.36515500	4.76624600
	H	4.96905100	0.38884600	6.06421700
	H	3.61341900	-1.37501400	4.94803500
	H	3.01967300	-1.17159600	2.55734800
	O	-0.42615700	2.40981400	-1.74107600
	C	0.52321200	2.16944100	-2.58453700
	N	1.09208000	3.13738000	-3.25575600
	C	2.17886200	2.84105600	-4.19437500
	C	0.75254800	4.54870100	-3.04922900
	H	0.81147100	1.12912300	-2.75521500
	H	1.92807300	3.23958600	-5.18204900
	H	3.10198800	3.30564400	-3.83490600
	H	2.32042400	1.76153200	-4.26432500
	H	1.62124600	5.06540700	-2.62962300
	H	0.48646200	4.99873700	-4.01030200
	H	-0.08730600	4.62347800	-2.36090800
tsa3'	C	-4.21906400	-2.55612100	-2.12068600
	C	-5.46038000	-3.18259600	-2.10606900
	C	-6.35763200	-2.97811600	-1.04602200
	C	-6.04192600	-2.13662200	0.01925700
	C	-4.80396600	-1.49116500	-0.01096100
	C	-3.87822900	-1.69507700	-1.06824400
	C	-2.71889400	-0.90089600	-0.73794100
	C	-2.95547700	-0.22517800	0.43579700
	N	-4.21799000	-0.58847300	0.92767000
	C	-1.36403600	-0.59746200	-1.16338600
	C	-0.74402900	0.25085800	-0.26822300
	C	-1.71469800	0.50685900	0.91805300
	C	-1.17989800	-0.18912500	2.20209700
	C	-1.87186300	2.02292900	1.16477500
	C	-0.70002100	-1.13796400	-2.38498300
	O	0.09589800	-0.52309900	-3.07967400
	O	-1.10204300	-2.38368600	-2.64912000

	C	-0.36468500	-3.08868100	-3.66757700
	S	-5.13843300	0.21374000	2.14499700
	O	-6.01598300	-0.79781300	2.72563000
	O	-4.17426500	0.94793300	2.95873500
	C	-6.15403100	1.39068000	1.25402500
	C	-5.61791000	2.62796000	0.88850400
	C	-7.47678000	1.06197600	0.94899100
	C	-6.41825000	3.53359400	0.19668500
	C	-8.26086800	1.98283100	0.25718400
	C	-7.74784100	3.22843900	-0.13070100
	C	-8.61705400	4.22999000	-0.85274100
	H	-3.51257800	-2.73468200	-2.92209300
	H	-5.73269900	-3.85299000	-2.91664000
	H	-7.31201800	-3.49729500	-1.04146900
	H	-6.71747500	-2.02168300	0.85631200
	H	-0.44573700	1.52037700	-1.08040800
	H	-0.28002400	0.32472000	2.55515000
	H	-1.93800700	-0.14458300	2.98894300
	H	-0.91668100	-1.23052100	1.99926700
	H	-0.88011500	2.45817900	1.33117100
	H	-2.31909200	2.52663800	0.29968500
	H	-2.48464600	2.21339200	2.04739400
	H	-0.82191900	-4.07653200	-3.71468600
	H	-0.44910600	-2.57125900	-4.62701700
	H	0.67769600	-3.16045700	-3.35503000
	H	-4.59774200	2.88196300	1.15175800
	H	-7.88598700	0.10886500	1.26221400
	H	-6.00476700	4.49762700	-0.08888200
	H	-9.29064800	1.72951000	0.01835600
	H	-9.35024200	3.73292800	-1.49633800
	H	-9.17672500	4.84923400	-0.13918200
	H	-8.02016500	4.90601900	-1.47338100
	P	3.64184900	0.67102700	0.57368400
	C	4.91313200	-0.41950400	-0.16688400
	C	6.25618600	-0.34112000	0.24359800
	C	7.21082800	-1.17933300	-0.32797100
	C	6.83138400	-2.11190100	-1.29936200
	C	5.49785200	-2.20482100	-1.69449400
	C	4.53517200	-1.35953900	-1.13530000
	C	4.07292200	2.38439200	0.02696800
	C	5.08003200	2.64979100	-0.91100100
	C	5.31509800	3.95775100	-1.34846400
	C	4.55426200	5.01520900	-0.84800200
	C	3.54771800	4.75968000	0.09010400
	C	3.30278300	3.45492700	0.51616000
	C	3.95775800	0.64333700	2.38226900

	C	4. 74766200	1. 60336900	3. 03247700
	C	4. 97277200	1. 50905700	4. 40720900
	C	4. 41584400	0. 45709600	5. 13678200
	C	3. 63295300	-0. 50244500	4. 49035700
	C	3. 39626900	-0. 41535000	3. 11766500
	Au	1. 35311200	0. 30032600	0. 06427100
	S	1. 70501600	-3. 36361900	0. 06275300
	O	2. 71272400	-4. 43261900	-0. 01147200
	O	1. 71689900	-2. 53552400	1. 29883000
	O	1. 54133300	-2. 56052300	-1. 18691800
	C	0. 07923200	-4. 26248100	0. 17931500
	F	0. 08447300	-5. 14045700	1. 19160300
	F	-0. 93583200	-3. 39931100	0. 38238200
	F	-0. 17461400	-4. 93500700	-0. 95922100
	H	6. 55195900	0. 36288100	1. 01675900
	H	8. 24668200	-1. 11664500	-0. 00521800
	H	7. 57504000	-2. 77666300	-1. 73099900
	H	5. 18932100	-2. 95234300	-2. 41893400
	H	3. 49194000	-1. 47632600	-1. 41472400
	H	5. 68619500	1. 83730600	-1. 29796000
	H	6. 10526800	4. 14735800	-2. 07051000
	H	4. 74918800	6. 03283300	-1. 17667800
	H	2. 95537400	5. 57742200	0. 49254900
	H	2. 50976900	3. 26281900	1. 23425400
	H	5. 18194800	2. 42686200	2. 47344700
	H	5. 58270400	2. 25804900	4. 90556100
	H	4. 59099100	0. 38605000	6. 20708500
	H	3. 19899000	-1. 32386400	5. 05346400
	H	2. 79012500	-1. 16851400	2. 61803000
	O	-0. 29728600	2. 51474400	-1. 65798400
	C	0. 60144600	2. 34732900	-2. 54403800
	N	1. 12875300	3. 35241100	-3. 21738900
	C	2. 18781300	3. 11494500	-4. 19790400
	C	0. 75800400	4. 74236500	-2. 95359300
	H	0. 93372100	1. 33371200	-2. 77701500
	H	1. 90107900	3. 54123300	-5. 16476800
	H	3. 11761000	3. 58274100	-3. 85731300
	H	2. 34839100	2. 04163300	-4. 31347500
	H	1. 62145500	5. 27709500	-2. 54381300
	H	0. 44521900	5. 22107300	-3. 88712600
	H	-0. 06058300	4. 76361200	-2. 23587200
ima4'	C	2. 77059600	2. 79367900	-0. 68800700
	C	3. 57013900	3. 78107600	-0. 12280800
	C	4. 42972500	3. 49228800	0. 94973400
	C	4. 50796000	2. 21137800	1. 49396800
	C	3. 71152800	1. 22028900	0. 91758600

	C	2.85020700	1.49136100	-0.17711400
	C	2.17885100	0.24696800	-0.46591200
	C	2.62177100	-0.71584800	0.40477100
	N	3.54982000	-0.14945900	1.29478300
	C	1.06009400	-0.30866700	-1.23779400
	C	0.77091400	-1.57256200	-0.72841800
	C	1.77184700	-1.97846800	0.35971900
	C	1.11733800	-2.29937100	1.72171800
	C	2.49564400	-3.23891600	-0.18816400
	C	0.53351000	0.14891100	-2.56373900
	O	-0.36718700	-0.41432300	-3.16313000
	O	1.19326700	1.21109600	-3.02727300
	C	0.65899600	1.79962400	-4.23464000
	S	4.80126000	-1.01933800	2.10604200
	O	5.18400700	-0.20558200	3.25603800
	O	4.29134100	-2.37990300	2.26780400
	C	6.16902200	-1.05096900	0.95280000
	C	6.17102000	-1.98412000	-0.08882200
	C	7.22003500	-0.14642000	1.11017900
	C	7.23566700	-1.99424700	-0.98431000
	C	8.27853100	-0.17507400	0.20284000
	C	8.30414800	-1.09223800	-0.85560600
	C	9.46274800	-1.13321200	-1.82285600
	H	2.07638200	3.02149100	-1.48541400
	H	3.51078600	4.79706000	-0.50264700
	H	5.02913800	4.28672800	1.38584100
	H	5.12898500	2.00512700	2.35638700
	H	0.18434400	-2.32817300	-1.24498900
	H	0.38014900	-3.09984800	1.60184100
	H	1.88154800	-2.62001300	2.43361900
	H	0.60526400	-1.42015600	2.12576700
	H	1.76608300	-4.03894500	-0.35174900
	H	2.98708700	-3.02700500	-1.14445000
	H	3.24067700	-3.58384300	0.53115500
	H	1.32034400	2.63622000	-4.45781500
	H	0.66997100	1.06818700	-5.04635800
	H	-0.35907500	2.14630500	-4.04534900
	H	5.36053400	-2.69697700	-0.18835900
	H	7.21468300	0.55507600	1.93598700
	H	7.24104300	-2.71826600	-1.79532900
	H	9.09910700	0.52747700	0.32267100
	H	10.06893600	-0.22450500	-1.76109700
	H	10.12086800	-1.98597400	-1.61099900
	H	9.11600600	-1.24198600	-2.85651400
	P	-3.00340100	-0.38182000	1.25541400
	C	-4.48267600	0.31425100	0.42605400

	C	-5.67697900	0.51749000	1.13758100
	C	-6.80133200	1.02050300	0.48736900
	C	-6.74252400	1.33216500	-0.87451700
	C	-5.55661700	1.14330400	-1.58236700
	C	-4.42872800	0.63350100	-0.93654000
	C	-3.41977500	-2.13211500	1.63005800
	C	-4.35538000	-2.47835900	2.62090600
	C	-4.69296000	-3.81453700	2.83221600
	C	-4.11120400	-4.81886300	2.05281800
	C	-3.19028500	-4.48179900	1.06108300
	C	-2.84231700	-3.14557000	0.85175300
	C	-2.84297500	0.50753600	2.84960200
	C	-2.49228100	-0.15436100	4.03644400
	C	-2.28364400	0.57467100	5.20862600
	C	-2.41329600	1.96428300	5.20232800
	C	-2.74232100	2.62707100	4.01743100
	C	-2.95251700	1.90968900	2.83989300
	Au	-1.03161400	-0.13512000	-0.00518900
	S	-1.68062800	3.11635500	-1.17155000
	O	-2.20501900	2.76870500	-2.50822100
	O	-2.67382500	3.44807900	-0.13414800
	O	-0.57659200	2.20747700	-0.70059200
	C	-0.73915100	4.69718800	-1.44875200
	F	-1.55802000	5.66541400	-1.87832200
	F	-0.14313900	5.10872700	-0.32312500
	F	0.21784000	4.51504800	-2.38591100
	H	-5.72627000	0.30100400	2.20058200
	H	-7.72023700	1.17932000	1.04521500
	H	-7.61773600	1.73634200	-1.37613000
	H	-5.49016900	1.41433300	-2.63150000
	H	-3.50382200	0.52020500	-1.49286600
	H	-4.81279100	-1.71044100	3.23720900
	H	-5.41166400	-4.07107400	3.60584900
	H	-4.37788300	-5.85890800	2.22121500
	H	-2.73229400	-5.24661000	0.44084900
	H	-2.12714800	-2.90426300	0.07213100
	H	-2.38173700	-1.23401600	4.05187800
	H	-2.01682500	0.05367800	6.12412800
	H	-2.24800300	2.52998400	6.11533400
	H	-2.82651500	3.70996000	4.00140400
	H	-3.16921900	2.44208900	1.91741500
	O	-1.18000500	-3.98421000	-1.92964500
	C	-1.62865500	-3.48807600	-2.96610200
	N	-2.39369800	-4.14635300	-3.87466700
	C	-2.89539300	-3.47918500	-5.06310600
	C	-2.75073500	-5.54051200	-3.67445100

	H	-1.42820300	-2.44186000	-3.24209300
	H	-2.53970800	-3.98194200	-5.97197800
	H	-3.99315300	-3.47878600	-5.07749100
	H	-2.54617600	-2.44350300	-5.07651500
	H	-3.83850700	-5.65348400	-3.57950200
	H	-2.41137100	-6.14939900	-4.52203700
	H	-2.26719300	-5.88621000	-2.76044200