

Supporting Information

Palladium-catalysed dual ring-opening [3 + 4] annulation of isatoic anhydrides with cyclic iodoniums to build tribenzo[*b,d,f*]azepines and mechanistic DFT study

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I Computational Details

All density functional theory calculations were performed with the Gaussian 09 program.^[1] Geometry optimizations were carried out at the BP86^[2]/def2-SVP^[3] level of theory and frequency calculations were carried out to confirm stationary points as local minima (showing no imaginary frequencies) or transition states (showing one imaginary frequencies) at the same level of theory. For every transition state, intrinsic reaction coordinate (IRC) calculations were employed to confirm the connection between two corresponding minima. Single-point energy calculation is performed to refine the relative energy results at the BP86-L/def2-TZVP level of theory. The solvation effect of acetonitrile was simulated by the SMD continuum solvent model.^[4] A correction of 4.3 kcal/mol applies to per component change for a reaction at 298.15 K and 1 atm, i.e., a reaction from m to n components has an additional correction of $(n-m) \times 4.3$ kcal/mol.^[5] The 3D optimized structural figures in this paper were displayed by the CYLview visualization program.^[6]

II Reference

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[5] R. L. Martin, P.J. Hay and L. R. Pratt, Hydrolysis of Ferric Ion in Water and Conformational Equilibrium, *J. Phys. Chem., A* 1998, **102**, 3565–3573.

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III The DFT calculated energies of all optimized structures.

Table SX. The DFT calculated energies of all optimized structures

Species	G _c hartree	E _{SP} + G _{SOL} hartree	Final G hartree
1a	0.108739	-627.9218924	-627.8063009
CO₂	-0.009384	-188.6783446	-188.6808761
2a	0.131086	-1721.907797	-1721.769858
CO	-0.014248	-113.3539174	-113.3613129
PPh₃	0.219084	-1036.622002	-1036.396065
1	0.454197	-2201.383358	-2200.922309
TS1_A	0.590432	-2829.309408	-2828.712123
IM1_A	0.59124	-2829.336483	-2828.738391
TS2_A -1	0.342015	-1792.615782	-1792.266914
TS2_A -2	0.342654	-1792.62856	-1792.279053

IM2_A-1	0.342135	-1792.640972	-1792.291984
IM2_A-2	0.337853	-1792.655821	-1792.311116
TS1_B	0.592132	-2829.31519	-2828.716206
IM1_B	0.5913	-2829.318814	-2828.720662
TS2_B-1	0.342262	-1792.618911	-1792.269797
TS2_B-2	0.342629	-1792.644926	-1792.295444
IM2_B-1	0.343536	-1792.647199	-1792.29681
IM2_B-2	0.336797	-1792.662088	-1792.318439

- The **G_C** designates the Gibbs Free Energy at BP86/def2-SVP level.
- The **E_{SP} + G_{SOL}** designates the sum of single point energy at BP86/def2-TZVP level and the solvation free energy calculated by SMD continuum solvent mode.
- The **Final G** designates the sum of **E_{SP} + G_{SOL}, G_C** and the 4.3 kcal/mol entropy correction.

IV The Cartesian coordinates (xyz) for all optimized structures

				H	-1.14952800	-2.87836700	0.90415100	C	4.72760400	-1.32164900	-3.12424200
1a								H	4.73428900	-1.54962400	-0.96130000
								C	2.90655600	-0.00836200	-4.06092800
C	3.09922400	-0.02142100	-0.00001200	I				H	1.45462300	0.76364000	-2.62644800
C	2.67235300	-1.36485700	-0.00001400					C	4.07706700	-0.76877600	-4.24067200
C	1.31050700	-1.69679900	-0.00000600	Pd	0.00019000	-0.02942300	0.06311200	H	5.64005200	-1.92474900	-3.25890700
C	0.33282600	-0.67147600	0.00000400	P	2.29084700	-0.01108200	0.02308700	H	2.38614600	0.42036500	-4.93242300
C	0.76484500	0.68242200	0.00000100	P	-2.29013400	-0.01312200	0.01903000	H	4.47744300	-0.93694600	-5.25332700
C	2.14020500	0.99580100	-0.00000400	C	3.07597200	1.59726600	0.52442900	C	3.13108000	-1.25124100	1.12294500
N	-1.03744100	-0.95593800	0.00002200	C	4.24504300	2.11708000	-0.07294700	C	4.31878300	-0.98279800	1.83765700
C	-2.02003600	0.04487600	-0.00001300	C	2.44741100	2.32946600	1.55806500	C	2.52671700	-2.52380100	1.24715200
O	-1.56658900	1.34670400	-0.00002400	C	4.77902700	3.34355100	0.36343200	C	4.89467400	-1.97274300	2.65507000
C	-0.22601800	1.77022300	0.00001300	H	4.73774400	1.56517800	-0.88906400	H	4.79420200	0.00776500	1.76162700
O	-0.00411000	2.95821500	0.00003000	C	2.98954800	3.54735500	1.99945600	C	3.11055100	-3.51367300	2.05427500
O	-3.21134700	-0.17498000	-0.00003200	H	1.51620100	1.93742200	2.00188600	H	1.58229200	-2.72347900	0.71249500
C	-1.50631800	-2.34295100	0.00003100	C	4.15642800	4.05833800	1.40143200	C	4.29565100	-3.23963800	2.76215300
H	4.17223800	0.22212300	-0.00001800	H	5.68827900	3.74291000	-0.11428800	H	5.81833200	-1.74926300	3.21304800
H	3.41674800	-2.17694400	-0.00002100	H	2.49102300	4.10713900	2.80706600	H	2.63045000	-4.50166800	2.14086100
H	1.01268600	-2.75350000	-0.00000900	H	4.57611700	5.01938400	1.73957000	H	4.74763700	-4.01243300	3.40443000
H	2.41997100	2.06034700	-0.00000400	C	3.04537600	-0.34683300	-1.64174700	C	-3.03505100	1.38152300	-0.95726200
H	-2.60968800	-2.31812200	0.00001200	C	4.21820100	-1.11037800	-1.82963000	C	-2.39279300	2.63934900	-0.88199500
H	-1.14950600	-2.87838800	-0.90406800	C	2.38835500	0.19364900	-2.77155300	C	-4.18532900	1.24544700	-1.76488500

C	-2.90340500	3.74309000	-1.58397600	H	-1.63489000	-1.15146800	2.58875700	F	-4.73578900	-0.11845300	-1.23305700
H	-1.47535000	2.73715500	-0.27677300	C	-4.29957100	0.26056000	4.24178500	H	4.18851600	2.69128600	0.20836700
C	-4.68725000	2.35056700	-2.47689900	H	-5.76873800	1.58733800	3.33386300	C	3.28719400	0.01782000	0.08402300
H	-4.68937000	0.26937400	-1.84505100	H	-2.68694600	-1.06695600	4.86533700	C	2.53206300	-1.17526600	-0.01024200
C	-4.05145600	3.60069300	-2.38536600	H	-4.75277700	0.31378200	5.24467600	C	4.68543000	-0.10198900	0.26649800
H	-2.39411800	4.71776000	-1.51521700					C	3.11271600	-2.44650000	0.07061500
H	-5.58201700	2.23065400	-3.10890900					C	5.28319900	-1.36736400	0.34919700
H	-4.44560300	4.46374400	-2.94557800	2a				H	5.30937100	0.80165300	0.34536400
C	-3.08466200	-1.52226900	-0.71975300					C	4.50472200	-2.53755900	0.25270700
C	-4.30901400	-2.05865900	-0.26502600	C	1.13892500	1.22534600	-0.19186600	H	2.50352900	-3.36140000	-0.00302600
C	-2.40865000	-2.15779300	-1.78673200	C	0.29716200	2.33112400	-0.28814200	H	6.37212100	-1.44513700	0.49199300
C	-4.85094700	-3.20537100	-0.87377900	C	2.54037300	1.28342000	-0.01214000	H	4.98208100	-3.52763200	0.32036000
H	-4.83917300	-1.58251600	0.57495100	C	0.90004300	3.60059900	-0.19958300	I	0.42218900	-0.79906200	-0.28810900
C	-2.95796000	-3.29572000	-2.39996200	H	-0.79016900	2.21715800	-0.41551400				
H	-1.43575700	-1.75615900	-2.11832100	C	3.10220400	2.58119900	0.06790200				
C	-4.18012900	-3.82314700	-1.94354500	C	2.29182200	3.72073900	-0.02544100	CO₂			
H	-5.80406300	-3.61909500	-0.50656700	H	0.26444700	4.49702700	-0.26560900				
H	-2.42189800	-3.78120400	-3.23125300	H	2.75116700	4.71901300	0.04242300	C	0.00000000	0.00000000	0.00000000
H	-4.60565700	-4.72240500	-2.41720600	O	-3.15263500	1.80738600	0.48962900	O	0.00000000	0.00000000	1.17537900
C	-3.13159200	0.13354000	1.66964500	S	-2.71208600	0.39404300	0.45475100	O	0.00000000	0.00000000	-1.17537900
C	-4.29026300	0.90977900	1.89065100	O	-2.23619400	-0.25983100	1.69843400				
C	-2.55750600	-0.56936200	2.75428000	O	-1.75582700	0.11996100	-0.75157700				
C	-4.86790400	0.97349400	3.17223300	C	-4.22776100	-0.60607600	-0.09103700	CO			
H	-4.74137700	1.47457300	1.05941500	F	-3.88420900	-1.89409300	-0.28286000				
C	-3.14331400	-0.51315000	4.02919400	F	-5.16833500	-0.54739100	0.86509500	C	0.00000000	0.00000000	-0.65281700

O	0.00000000	0.00000000	0.48961300	H	-3.41563000	-2.39500600	-3.19903200	C	2.57310900	1.54451700	1.00677400
				H	-3.39468800	-4.01041800	-2.37426500	C	2.12791200	2.81389500	0.56853900
				H	-4.48832900	-2.69502300	-1.78710800	C	3.29821400	1.45638200	2.21583300
IM1_A				C	3.13119100	0.30002100	-1.55970400	C	2.41375500	3.96733800	1.31623400
				C	4.10157500	1.31961700	-1.68874100	H	1.55772700	2.90434400	-0.36946200
Pd	-0.21210400	-0.58338400	-0.60792700	C	2.91039500	-0.59038700	-2.63832100	C	3.57070000	2.61309600	2.96880100
P	2.13182800	0.05728700	-0.01172700	C	4.83307000	1.45349900	-2.88246900	H	3.65742000	0.47847400	2.57121600
P	-1.54862500	1.16440700	0.08514100	H	4.29165500	2.01477400	-0.85704600	C	3.13230100	3.87080600	2.52188100
C	-1.54665500	-4.85640900	2.02044400	C	3.65004500	-0.44961900	-3.82460800	H	2.06530600	4.94775000	0.95454300
C	-2.84381500	-4.35929500	1.79941100	H	2.16872700	-1.40094000	-2.53109700	H	4.13844300	2.52718900	3.90928100
C	-3.09652700	-3.54856900	0.68358900	C	4.60798500	0.57183900	-3.95351900	H	3.35047800	4.77582600	3.11092200
C	-2.06109900	-3.20138000	-0.21454800	H	5.58590400	2.25335600	-2.97115700	C	-1.48362300	1.66665000	1.86809900
C	-0.74989100	-3.70610700	-0.00136200	H	3.47095100	-1.14960700	-4.65629400	C	-0.47167200	1.15878000	2.70826000
C	-0.52482800	-4.54574100	1.11303600	H	5.18179700	0.67968500	-4.88807200	C	-2.46470600	2.52737700	2.41642900
N	-2.39629900	-2.43003300	-1.37314900	C	3.00186100	-1.31678700	0.87221900	C	-0.42632000	1.51641400	4.06718000
C	-1.76724100	-1.25331800	-1.72187400	C	2.27677600	-2.07619000	1.81657500	H	0.28060600	0.47134700	2.29336500
O	0.68987200	-2.30577700	-1.37882700	C	4.36537300	-1.60888700	0.65111300	C	-2.41428200	2.88724600	3.77293400
C	0.41073100	-3.52547100	-0.97439900	C	2.91281800	-3.09406000	2.54777200	H	-3.28303600	2.90389700	1.78236400
O	1.05737700	-4.51374700	-1.31781800	H	1.20174500	-1.88215800	1.96602300	C	-1.39385300	2.38386400	4.60074100
O	-2.03063700	-0.63736400	-2.75250600	C	4.99538500	-2.63433200	1.37634500	H	0.37017500	1.10997300	4.70982000
C	-3.49148000	-2.91646700	-2.22666500	H	4.93513300	-1.03518700	-0.09658000	H	-3.18348900	3.55792500	4.18812700
H	-1.34042500	-5.50747600	2.88494000	C	4.27284600	-3.37476800	2.32889300	H	-1.35982400	2.66250600	5.66608900
H	-3.66386600	-4.61000900	2.49117100	H	2.33669200	-3.68052900	3.28086300	C	-1.18792000	2.69452400	-0.90006400
H	-4.11365600	-3.17276200	0.49579300	H	6.05775700	-2.85967200	1.19110600	C	-1.11159900	3.98608000	-0.33565600
H	0.48200000	-4.97590600	1.22885600	H	4.76819700	-4.18071700	2.89346900	C	-0.97496700	2.52588600	-2.28969300

C	-0.82716800	5.09636600	-1.15131800	P	1.21682000	1.46183200	0.05597600	H	-5.09939100	-0.21252400	-0.77456500
H	-1.26042400	4.12844100	0.74548700	C	1.94255200	-1.12494800	-1.63653600	C	-3.60420700	-2.99357400	-3.07829700
C	-0.69700000	3.64172000	-3.09773000	O	0.16869200	-2.59684500	-1.25831800	H	-1.69469100	-2.58440200	-2.10083200
H	-1.04552900	1.51726000	-2.73192600	C	0.21361300	-3.36222300	-0.19780600	C	-4.96988400	-2.67568000	-3.15747800
C	-0.61953300	4.92732800	-2.53152300	O	-0.69954500	-4.08088400	0.20547800	H	-6.57226300	-1.41991300	-2.37611600
H	-0.76713900	6.10068700	-0.70188600	O	2.01605100	-0.64802800	-2.75543600	H	-3.17891300	-3.77638400	-3.72641900
H	-0.53480300	3.50113600	-4.17813800	C	3.86846400	-3.72228800	0.46879400	H	-5.62279900	-3.20449600	-3.87059800
H	-0.39505300	5.79886000	-3.16706600	C	2.71569500	-3.03981700	-0.02236600	C	-3.04369200	1.21741100	-0.05899700
C	-3.38166100	0.94361900	-0.13681800	C	2.93169600	-2.08648800	-1.07795100	C	-3.91211900	1.60510700	0.98349900
C	-4.13179800	1.67368900	-1.08118800	C	4.23000200	-1.94031300	-1.63239100	C	-2.83153000	2.10266400	-1.14182700
C	-4.03401900	-0.01759200	0.66861600	C	5.33571500	-2.64170600	-1.14796400	C	-4.55301100	2.85754500	0.94421200
C	-5.51546300	1.45340100	-1.20998600	C	5.14367300	-3.52685200	-0.07281700	H	-4.09041600	0.92563800	1.83111500
H	-3.63795900	2.41787100	-1.72374600	H	3.75469700	-4.45995100	1.27275200	C	-3.47634000	3.34959900	-1.18079000
C	-5.41648000	-0.22817900	0.54247100	H	4.34071500	-1.22228000	-2.45878200	H	-2.15234200	1.81250400	-1.96040800
H	-3.45774400	-0.60307200	1.40337000	H	6.33065400	-2.49822300	-1.59643600	C	-4.33760600	3.73228900	-0.13489800
C	-6.16202700	0.50680700	-0.39872200	H	5.99267400	-4.09453400	0.34164800	H	-5.23133300	3.14703400	1.76313700
H	-6.08943600	2.03031200	-1.95254600	N	1.46641000	-3.35616400	0.53740000	H	-3.30079700	4.02761800	-2.03088300
H	-5.91590000	-0.97040700	1.18590200	C	1.43135400	-4.12217700	1.78552700	H	-4.84225100	4.71120500	-0.16371200
H	-7.24636000	0.33965500	-0.49829700	H	1.71053800	-5.19058900	1.64339700	C	-2.54669300	-1.21265600	1.50183100
				H	2.11616700	-3.66806000	2.52943900	C	-3.29036700	-2.40678900	1.61097000
				H	0.39536100	-4.10057900	2.16357300	C	-1.97597100	-0.64481800	2.66670300
IM1_B				C	-3.29363400	-1.31516300	-1.33358800	C	-3.48087400	-3.00847400	2.86733500
				C	-4.67084000	-0.99784500	-1.41624400	H	-3.70865800	-2.87767400	0.70938800
Pd	0.28192500	-0.53482400	-0.63071500	C	-2.76293700	-2.32008600	-2.17327800	C	-2.17919200	-1.24495100	3.92006000
P	-2.18320700	-0.42569500	-0.13305900	C	-5.50199400	-1.67674800	-2.32169500	H	-1.37053200	0.27354100	2.59615800

C	-2.93299600	-2.42864900	4.02390900	H	-0.85442600	3.66284300	5.00808100	H	3.88975400	2.83345100	-1.86119400
H	-4.05855300	-3.94380700	2.93751100	C	3.04574600	1.39399200	0.37304000	H	2.14138100	3.17686500	-1.80561700
H	-1.73694600	-0.78755900	4.81949700	C	3.93318900	2.40486300	-0.05466200	H	3.15884700	3.45331200	-0.34382800
H	-3.08497100	-2.90328200	5.00658200	C	3.55596100	0.28755600	1.09000700	C	3.76380100	0.65840800	-0.30224800
C	1.03702600	2.83067700	-1.18211800	C	5.30454000	2.31400900	0.24246200	C	4.99521100	1.29267000	0.06086600
C	0.94669100	2.47276500	-2.54701900	H	3.55563800	3.26564400	-0.62705700	C	3.70109800	-0.77427800	-0.15344100
C	1.03166400	4.19799500	-0.82253000	C	4.92401600	0.20900400	1.39989300	C	6.09988900	0.56023000	0.51110700
C	0.84308000	3.47034100	-3.53235300	H	2.87546800	-0.52371800	1.39483400	H	5.08398100	2.38520900	-0.00890800
H	0.98176300	1.40899500	-2.83621400	C	5.80138700	1.22211100	0.97503100	C	4.83710300	-1.48334500	0.28462600
C	0.92104800	5.18951000	-1.81303100	H	5.98870300	3.10540900	-0.10329500	C	6.03534700	-0.84004500	0.62415400
H	1.11010000	4.49381200	0.23508000	H	5.30605300	-0.66084900	1.95644200	H	7.02443400	1.09717500	0.78106200
C	0.82394100	4.82835400	-3.16874400	H	6.87651100	1.15461800	1.20573100	H	4.73967500	-2.57877200	0.33986500
H	0.77638600	3.17933100	-4.59273000					H	6.90522000	-1.41979800	0.96960100
H	0.91277000	6.25198500	-1.52114300					C	-1.35487300	-1.15300800	1.50680600
H	0.73702600	5.60780700	-3.94266300	IM2_A-1				C	-0.43806500	-0.87806300	2.54476400
C	0.58315200	2.19969100	1.64644600					C	-2.24926100	-2.23910500	1.63342400
C	1.26946200	2.01025700	2.86815200	P	-1.37414700	-0.07425600	0.01582700	C	-0.42549900	-1.67309600	3.70248500
C	-0.63333400	2.92213300	1.65740900	C	0.29420100	2.61939700	0.14799700	H	0.28068000	-0.05006900	2.43435100
C	0.75227400	2.52924200	4.06765200	O	0.02172600	3.67838000	0.52644200	C	-2.23168100	-3.03075500	2.79403900
H	2.22408100	1.46383400	2.88808900	C	2.50414600	-1.61544400	-0.48884300	H	-2.95291300	-2.47185400	0.81890600
C	-1.14108600	3.44756700	2.85810300	O	1.29800800	-1.04655900	-0.52458700	C	-1.32198200	-2.74888200	3.82877300
H	-1.18876700	3.08868000	0.72280500	O	2.59347500	-2.82866200	-0.69180800	H	0.29894500	-1.45797400	4.50350600
C	-0.45362200	3.25118300	4.06816100	Pd	0.80183100	0.88461100	-0.32785000	H	-2.92773000	-3.87957300	2.88527300
H	1.30558300	2.37315100	5.00752600	N	2.72093700	1.38196000	-0.86408700	H	-1.30418400	-3.37765500	4.73308200
H	-2.08610000	4.01249300	2.83971200	C	2.98526300	2.77160800	-1.21422900	C	-1.99480100	-1.14803800	-1.35707700

C	-1.17767100	-2.21074700	-1.81645700	Pd	1.04763500	0.07869900	0.36004200	C	-2.04345400	-0.74236500	-3.89827400
C	-3.26678700	-0.94039100	-1.93890200	O	1.56035700	3.09873700	-1.16148600	H	-0.69643600	-1.45180600	-2.33450500
C	-1.64129600	-3.04700600	-2.84489400	O	2.64215500	1.68315100	-2.69590100	C	-3.64241600	0.96889000	-3.23867600
H	-0.17813200	-2.36460300	-1.37800500	C	2.10203600	2.37139800	-1.91352200	H	-3.57078400	1.59853400	-1.15854000
C	-3.71665800	-1.78494500	-2.96889100	C	3.01590100	0.29801700	0.73032200	C	-3.09807700	0.12952500	-4.22585500
H	-3.91457600	-0.12368700	-1.58684900	C	3.64756000	1.34813700	1.41300900	H	-1.60983800	-1.39935800	-4.66912800
C	-2.90598600	-2.83855600	-3.42412900	C	3.81192600	-0.76890200	0.24191900	H	-4.46667800	1.65594400	-3.48903000
H	-0.99822000	-3.86910700	-3.19684000	C	5.05014600	1.33932700	1.60688200	H	-3.49360700	0.15766300	-5.25381200
H	-4.71024400	-1.61597300	-3.41383900	H	3.05468400	2.19342000	1.80298600	C	-2.16254800	-1.52092400	0.85809900
H	-3.26054200	-3.49826500	-4.23219600	C	5.20538900	-0.79568900	0.42539600	C	-3.39839600	-2.02897700	0.40203500
C	-2.72409300	1.15448800	0.29942100	C	5.81722700	0.27314400	1.11501700	C	-1.50465100	-2.15720700	1.93417000
C	-2.89723700	2.19129200	-0.64801000	H	5.53626100	2.16979900	2.14390500	C	-3.97202700	-3.15183400	1.02372500
C	-3.56596200	1.10665200	1.43113900	H	5.81879600	-1.62641300	0.04431900	H	-3.91017900	-1.54952500	-0.44742700
C	-3.90447600	3.15302900	-0.47161200	H	6.90877600	0.26304100	1.26420300	C	-2.08505300	-3.27422400	2.55750200
H	-2.24080300	2.24581500	-1.53253000	P	-1.35516600	-0.03840100	0.10648300	H	-0.52402700	-1.77795000	2.26837200
C	-4.56721000	2.07870200	1.60820700	N	3.08101500	-1.77316500	-0.43199200	C	-3.31908600	-3.77321100	2.10313500
H	-3.43834400	0.30851800	2.17842300	C	3.71668500	-2.94139300	-1.02872700	H	-4.93428800	-3.54556300	0.65909500
C	-4.74054500	3.09975000	0.65881500	H	4.46232800	-2.63525800	-1.79351300	H	-1.56400600	-3.76485600	3.39495400
H	-4.03210500	3.95297700	-1.21791600	H	4.23288100	-3.54966700	-0.25503700	H	-3.76926900	-4.65505100	2.58639600
H	-5.21568400	2.03435500	2.49751400	H	2.93168600	-3.55289800	-1.50863400	C	-2.10597800	1.39973800	1.00258000
H	-5.52555900	3.85923300	0.80072800	C	1.71194400	-1.58604700	-0.51416800	C	-3.20301400	1.28317100	1.88372700
				O	0.94083600	-2.35740600	-1.06766300	C	-1.50644600	2.66813400	0.81121500
				C	-2.08056000	0.06239000	-1.59393600	C	-3.69599500	2.41693000	2.55449400
IM2A-2				C	-1.52912400	-0.77595900	-2.59165600	H	-3.67256900	0.30128900	2.05071500
				C	-3.13886700	0.93679100	-1.92558900	C	-2.00713100	3.79836600	1.47827400

H	-0.64103100	2.77492000	0.13486500	H	-3.73567500	-3.28527500	2.90902200	C	5.31083800	0.01218400	-0.14566200
C	-3.10214700	3.67486700	2.35280200	H	-2.50191100	-2.57806100	4.97848900	C	5.86033400	1.26901200	-0.43622000
H	-4.55124400	2.31349800	3.24138200	C	-1.93098000	-1.13767800	-1.36380000	C	5.02188100	2.37099600	-0.65213100
H	-1.53261300	4.77958700	1.31850600	C	-1.27135900	-2.38343100	-1.51231400	C	3.62858200	2.19568500	-0.55071700
H	-3.48953500	4.56021100	2.88169500	C	-2.99295600	-0.80044000	-2.23403500	C	3.05758800	0.94769000	-0.23320300
				C	-1.68880200	-3.27245300	-2.51691500	H	5.98574800	-0.84626400	-0.01919500
				H	-0.41955500	-2.65835800	-0.87061200	H	6.95477700	1.37654900	-0.50437300
IM2_B-1				C	-3.39704300	-1.69846500	-3.23682800	H	5.43833000	3.36407000	-0.88357400
				H	-3.51315900	0.16370700	-2.12865000	H	2.98013900	3.07057800	-0.71301900
P	-1.36345000	0.02253200	-0.04601700	C	-2.74682000	-2.93615300	-3.37979000	N	3.42105100	-1.48236600	0.24160600
C	0.77052000	2.37997000	0.62252400	H	-1.16629900	-4.23584300	-2.62654100	C	4.31592800	-2.46277600	0.85119000
O	0.63716300	3.41019600	1.13149800	H	-4.22759900	-1.42612400	-3.90748200	H	5.06187400	-2.86989500	0.13104800
C	2.20337100	-1.99567700	-0.27219900	H	-3.06353700	-3.63870500	-4.16727200	H	4.85710900	-2.00565800	1.70422600
O	1.37779100	-1.13838500	-0.84133100	C	-2.55408700	1.43524700	-0.11500300	H	3.69551300	-3.30808200	1.19833800
O	1.94706400	-3.20098300	-0.19913700	C	-2.30269200	2.46847100	-1.04794800				
Pd	1.02609500	0.69190000	-0.12054400	C	-3.68744900	1.52201500	0.72183500				
C	-1.74014700	-0.84184900	1.54172500	C	-3.18009300	3.56047900	-1.15179800	IM2_B-2			
C	-1.04215500	-0.45538000	2.70830400	H	-1.41342000	2.41600100	-1.69848100				
C	-2.70983600	-1.86656300	1.62347800	C	-4.55652600	2.62289300	0.62264400	Pd	-0.91366500	0.34145500	-0.54508400
C	-1.32063900	-1.07259500	3.93900000	H	-3.89029700	0.72770800	1.45666700	O	-1.06832100	3.47778400	0.67479600
H	-0.26591200	0.32494100	2.65081000	C	-4.30743200	3.64062600	-0.31436100	O	-2.22323200	2.26134400	2.32316600
C	-2.98153800	-2.48403200	2.85640800	H	-2.97646500	4.35714600	-1.88470400	C	-1.64623500	2.84581100	1.48475200
H	-3.24609400	-2.19005500	0.71780800	H	-5.43538500	2.68375200	1.28406200	P	1.30322000	-0.15594700	-0.06806400
C	-2.29058700	-2.08770100	4.01499500	H	-4.99005100	4.50190600	-0.38921600	C	-1.87936500	-1.13826100	0.43667200
H	-0.76748700	-0.76584000	4.84065900	C	3.90663500	-0.18568400	-0.04954300	O	-1.25330400	-1.94695200	1.08974100

C	1.92269000	0.12002600	1.65789800	C	4.20303100	1.38534800	-2.65627300	PPh₃			
C	1.18442000	-0.43430000	2.72989600	H	3.72793800	-0.57817800	-1.85029100				
C	3.08936000	0.86747200	1.93229000	C	2.78055200	3.22048900	-1.92934700	P	-0.00065200	-0.00087000	-1.22601300
C	1.61529000	-0.24420400	4.05293500	H	1.17363800	2.70558800	-0.55968900	C	-1.59431700	-0.50492000	-0.41016700
H	0.27396000	-1.01769500	2.52000800	C	3.86820800	2.74996100	-2.68779300	C	-1.68304000	-1.36176800	0.70962600
C	3.51068400	1.05827100	3.26074200	H	5.05119400	1.01063400	-3.25133500	C	-2.79026600	-0.01951200	-0.99125000
H	3.67150500	1.30669000	1.10745800	H	2.50931800	4.28791800	-1.95176500	C	-2.93711800	-1.71542300	1.23984700
C	2.77629700	0.50359500	4.32252200	H	4.45251700	3.44815700	-3.30801800	H	-0.76388300	-1.75687200	1.17024200
H	1.03340000	-0.68026800	4.88050100	C	-5.59219700	-1.83409600	0.53165700	C	-4.04104900	-0.36249700	-0.45246700
H	4.42050100	1.64571200	3.46368400	C	-4.22499800	-1.95626600	0.78257300	H	-2.73702000	0.63303900	-1.87908000
H	3.10705700	0.65607400	5.36229800	C	-3.31500100	-1.03309300	0.20904600	C	-4.11788300	-1.21511300	0.66416600
C	1.86441400	-1.86414900	-0.48967200	C	-3.76366200	0.05393400	-0.62784700	H	-2.98988100	-2.38615900	2.11274700
C	2.94027700	-2.49472500	0.17207000	C	-5.17476800	0.14607700	-0.87662700	H	-4.96193600	0.02864400	-0.91431100
C	1.18872100	-2.54768600	-1.52462100	C	-6.04783300	-0.77783700	-0.30271800	H	-5.09878700	-1.49373700	1.08137600
C	3.33826200	-3.78932300	-0.20507600	H	-6.30816900	-2.54649500	0.96854700	C	0.35948700	1.63122800	-0.41006900
H	3.46420400	-1.97598300	0.99038900	H	-3.82792800	-2.76364200	1.41741000	C	1.37370000	2.42691100	-0.99464000
C	1.59383600	-3.83822100	-1.90250900	H	-5.56764800	0.94941800	-1.51667200	C	-0.33457000	2.13347900	0.71337600
H	0.33141000	-2.06386300	-2.02226300	H	-7.12798200	-0.68310500	-0.50562400	C	1.70167400	3.68163300	-0.45569100
C	2.66834300	-4.46136800	-1.24275000	N	-2.81344700	0.88600300	-1.10213100	H	1.90929900	2.05656000	-1.88505200
H	4.17491800	-4.27718800	0.32010600	C	-3.14978600	1.96781100	-2.00234000	C	-0.01426800	3.39656400	1.24356500
H	1.05828400	-4.36473400	-2.70834600	H	-3.61112400	1.60889800	-2.95502000	H	-1.13274500	1.53233000	1.17675000
H	2.97899900	-5.47794300	-1.53227100	H	-3.85912700	2.70206200	-1.54755700	C	1.00539600	4.17166000	0.66436600
C	2.36743700	0.95480000	-1.10254500	H	-2.23197500	2.52904200	-2.27132600	H	2.49749800	4.28587800	-0.92031300
C	3.45896100	0.48941800	-1.86741800					H	-0.56605100	3.77576100	2.11898900
C	2.02946200	2.32914300	-1.14586600					H	1.25412200	5.16058400	1.08153600

C	1.23307500	-1.12853600	-0.41008700	C	-1.39192000	-1.45011300	-1.88650800	C	1.98120500	-1.51948600	2.36791900
C	1.41265800	-2.40698400	-0.99050400	O	0.09815400	-2.41741800	-1.63407400	C	4.26130100	-1.49890700	1.50766100
C	2.01956400	-0.77450000	0.70864500	C	0.16026500	-3.35189800	-0.66025900	C	2.39974100	-2.29776400	3.46094500
C	2.33762200	-3.31611600	-0.45169400	O	1.21350300	-3.94315800	-0.43194700	H	0.91891500	-1.24451200	2.25708200
H	0.82034200	-2.68930100	-1.87724300	O	-1.38715500	-0.87587400	-2.96743800	C	4.67526600	-2.28206900	2.59826000
C	2.95552400	-1.68102200	1.23881200	C	-3.72512000	-2.12562800	-2.18574700	H	4.98961400	-1.20437500	0.73546600
H	1.89968700	0.21911800	1.16845600	H	-2.15586100	-5.70652400	2.62757500	C	3.74749700	-2.67852500	3.57871300
C	3.11478700	-2.95379800	0.66384000	H	-4.39166000	-4.85798600	1.82819200	H	1.66455700	-2.61971100	4.21548800
H	2.46133400	-4.30915700	-0.91308700	H	-4.52953900	-3.24801800	-0.04603800	H	5.72998400	-2.59043000	2.67938200
H	3.56329200	-1.38923500	2.11064700	H	-0.05880800	-4.93894200	1.41913800	H	4.07496900	-3.29694700	4.42976100
H	3.84864300	-3.66212100	1.08049400	H	-3.49991500	-1.61867100	-3.14081000	C	2.84178800	1.66149500	0.43843400
				H	-4.14282000	-3.13186600	-2.39484400	C	2.30368500	2.73279700	-0.31216900
				H	-4.47727400	-1.52769000	-1.62848200	C	3.74589100	1.94418600	1.48591300
TS1_A				C	3.43329000	-0.49976200	-1.40570100	C	2.68129300	4.05720600	-0.03553900
				C	4.29321200	0.43910100	-2.01794000	H	1.57715600	2.52544400	-1.11508800
Pd	-0.10019600	-0.43881500	-0.57291500	C	3.39424000	-1.82899300	-1.89339100	C	4.10939200	3.27303200	1.77015200
P	2.29366400	-0.05413700	-0.00926000	C	5.10456400	0.05585200	-3.10088600	H	4.16821000	1.12255700	2.08494500
P	-1.55531200	1.20595500	0.08843500	H	4.33612800	1.47511600	-1.64875700	C	3.58338000	4.33096700	1.00863200
C	-2.21517800	-4.99411500	1.79038300	C	4.21451600	-2.20191000	-2.97087300	H	2.25583600	4.87900200	-0.63261700
C	-3.46289500	-4.51823600	1.34174800	H	2.72514100	-2.57845700	-1.43600900	H	4.81301800	3.48046600	2.59251600
C	-3.54483600	-3.61059000	0.27807300	C	5.06818000	-1.26448500	-3.57997400	H	3.87164300	5.37049800	1.23261700
C	-2.37144900	-3.14229700	-0.37039700	H	5.77175600	0.79775800	-3.56874700	C	-1.40776700	1.91109500	1.80438700
C	-1.10953100	-3.64632700	0.06683100	H	4.17614500	-3.23905600	-3.34051700	C	-0.17387000	1.82284500	2.48258400
C	-1.05483400	-4.56324100	1.13895300	H	5.70388400	-1.56272700	-4.42918700	C	-2.49389400	2.55401200	2.44464500
N	-2.46547000	-2.25440900	-1.44658400	C	2.90990300	-1.10197100	1.38884300	C	-0.02294900	2.36626700	3.76989300

H	0.67636100	1.32477000	1.99500700	C	-6.15191100	0.28053700	0.02670500	H	6.18027600	-3.57998700	0.33419600
C	-2.34172400	3.09459900	3.73295200	H	-6.29947600	1.74192800	-1.58161700	N	1.58291000	-3.61259500	0.47830600
H	-3.46805300	2.62832200	1.93705600	H	-5.68403300	-1.12158500	1.63038200	C	1.63361000	-4.51193500	1.63127100
C	-1.10669800	3.00171500	4.39939000	H	-7.23106100	0.05903100	0.03554900	H	2.12486900	-5.47796200	1.38190000
H	0.94881200	2.28600700	4.28181800					H	2.18164400	-4.03958100	2.47247100
H	-3.19733800	3.58974900	4.21967600					H	0.59059900	-4.71563000	1.92859100
H	-0.99125800	3.42222100	5.41118700	TS1_B				C	-3.39390100	-1.37822500	-1.17579000
C	-1.36508900	2.68287800	-1.02456000					C	-4.77955300	-1.10561600	-1.26870200
C	-1.39795300	4.01242000	-0.55038400	Pd	0.15347700	-0.53195900	-0.55345700	C	-2.84620500	-2.44533000	-1.92027900
C	-1.16198200	2.44226500	-2.40538400	P	-2.28842000	-0.35209600	-0.08539200	C	-5.60379500	-1.89420500	-2.08699900
C	-1.23702400	5.08670900	-1.44418900	P	1.30292400	1.36241700	0.05367900	H	-5.21843100	-0.26950700	-0.70217800
H	-1.54125800	4.21323200	0.52225500	C	1.64963600	-1.45254200	-1.67948300	C	-3.67947500	-3.23039900	-2.73895000
C	-1.00977200	3.52174800	-3.29286400	O	0.25833800	-2.67757800	-1.20206500	H	-1.77020700	-2.66853800	-1.85064700
H	-1.12232500	1.40554100	-2.78232800	C	0.30090300	-3.45820700	-0.12682100	C	-5.05467900	-2.95943400	-2.82493200
C	-1.04506200	4.84492700	-2.81579400	O	-0.68019100	-4.04596900	0.31976500	H	-6.68134100	-1.67247300	-2.15113200
H	-1.26116600	6.12013800	-1.06234500	O	1.53135500	-1.09963300	-2.83971000	H	-3.24107900	-4.06170600	-3.31363400
H	-0.85513300	3.32320100	-4.36541900	C	4.02133300	-3.60215200	0.43979700	H	-5.70219100	-3.57564900	-3.46950300
H	-0.91866900	5.68843900	-3.51339300	C	2.78117300	-3.10341100	-0.04710200	C	-3.08917300	1.31133000	-0.28677900
C	-3.38226500	0.86335300	0.01628300	C	2.83302700	-2.10686700	-1.07300700	C	-4.00055700	1.87081100	0.63365200
C	-4.25444500	1.51718200	-0.88069400	C	4.08256900	-1.68756000	-1.58617200	C	-2.77522000	2.02861300	-1.46513300
C	-3.91037200	-0.10032500	0.90722600	C	5.28928400	-2.19680000	-1.09631400	C	-4.58652600	3.12499600	0.37919300
C	-5.63074700	1.22233500	-0.87673600	C	5.24721500	-3.15690900	-0.07136200	H	-4.25439300	1.32650200	1.55645700
H	-3.86009100	2.26831500	-1.58181700	H	4.02832000	-4.37307200	1.22049700	C	-3.36686100	3.27626200	-1.71977100
C	-5.28613900	-0.37946300	0.91998600	H	4.07603900	-0.94117500	-2.39447700	H	-2.05478900	1.60540000	-2.18488700
H	-3.23947400	-0.63407400	1.60002400	H	6.24874000	-1.85414100	-1.51239100	C	-4.27353800	3.82988700	-0.79595500

H	-5.29800400	3.55019400	1.10554900	C	0.59923000	2.34007400	1.47439500				
H	-3.11351400	3.82185800	-2.64260100	C	1.17216800	2.30873200	2.76587600	P	-1.37928100	-0.01326700	0.06377800
H	-4.73541900	4.81035900	-0.99377300	C	-0.57225800	3.10656100	1.26930800	C	1.23304900	2.37635500	-0.27658800
C	-2.73248100	-0.89113400	1.62973100	C	0.58840800	3.02743800	3.82431800	O	1.34418400	3.49801000	0.05711800
C	-3.45924600	-2.07663200	1.87456100	H	2.08770100	1.72703500	2.94949700	C	2.56214300	-1.75734600	-0.76769300
C	-2.23666700	-0.14946200	2.72935400	C	-1.14559200	3.83242100	2.32680300	O	1.30379300	-1.39590600	-0.95095700
C	-3.70654800	-2.49700600	3.19346900	H	-1.03977500	3.14448000	0.27408600	O	2.96752100	-2.87919500	-1.06931000
H	-3.82549600	-2.68081500	1.03138800	C	-0.56963700	3.79408100	3.60925100	Pd	0.77617300	0.55706000	-0.58622700
C	-2.49832700	-0.56753900	4.04419000	H	1.05236900	2.99270500	4.82311300	N	2.61556000	1.36241700	-0.96679600
H	-1.64461600	0.76388700	2.55952900	H	-2.05356800	4.42732500	2.14174000	C	2.96928800	1.66998700	-2.35300700
C	-3.23490800	-1.74271300	4.28088000	H	-1.02109300	4.36274500	4.43778500	H	3.91557500	2.25711300	-2.38536800
H	-4.27257800	-3.42592800	3.36820600	C	3.06031200	1.12383800	0.60419600	H	3.10621900	0.75259000	-2.96884500
H	-2.11475600	0.02711700	4.88860900	C	4.11426600	1.98201400	0.22365500	H	2.16737600	2.28014600	-2.81717700
H	-3.43332700	-2.07360800	5.31291200	C	3.33615200	0.03802500	1.46684500	C	3.57476900	0.63827200	-0.18211200
C	1.42715100	2.62899700	-1.29790800	C	5.41455100	1.76849200	0.71496700	C	4.58206300	1.37770800	0.47873600
C	1.37001200	2.18309300	-2.63815700	H	3.92281100	2.82241300	-0.46079800	C	3.55804200	-0.78666200	-0.09310700
C	1.60093400	4.00775500	-1.03388500	C	4.63197000	-0.16095700	1.97022400	C	5.57320100	0.73137400	1.23211000
C	1.48971900	3.10466600	-3.69391200	H	2.52568200	-0.65803000	1.73967800	H	4.56786000	2.47547100	0.39026300
H	1.23649700	1.11024900	-2.85576500	C	5.67515100	0.70403900	1.59468900	C	4.58730700	-1.41124600	0.64661000
C	1.71672700	4.92310000	-2.09415800	H	6.22923300	2.44340200	0.40675600	C	5.57464700	-0.67207800	1.31447400
H	1.63826500	4.37111500	0.00493600	H	4.83041200	-1.00864800	2.64433800	H	6.34326400	1.32407400	1.75132100
C	1.66137500	4.47372800	-3.42593700	H	6.69435800	0.54136700	1.97986800	H	4.58660600	-2.51173500	0.67080600
H	1.44377900	2.74481100	-4.73415100					H	6.35085700	-1.19342700	1.89708200
H	1.84895200	5.99523400	-1.87679000					C	-1.37988400	-1.17361800	1.49745500
H	1.74973500	5.19363500	-4.25544300	TS2_A-1				C	-0.41995800	-0.97950500	2.51611000

C	-2.30125400	-2.23809400	1.60203600	C	-4.14757400	2.39688800	2.03048200	N	-2.69522300	-1.71165800	0.19833900
C	-0.39189100	-1.83252600	3.63090100	H	-3.37279800	0.38043800	2.28397000	C	-3.37698400	-3.00990400	0.23970600
H	0.31692000	-0.16456300	2.42600700	C	-4.10354900	3.57976800	1.27288600	H	-4.41204300	-2.86522300	0.60565600
C	-2.26599600	-3.09122100	2.71897100	H	-3.19386700	4.59822200	-0.42590700	H	-3.39985300	-3.49575400	-0.76009500
H	-3.04089100	-2.40761100	0.80394000	H	-4.81841200	2.32190200	2.90106500	H	-2.82747200	-3.66996400	0.93507400
C	-1.31431300	-2.88955300	3.73365700	H	-4.73970400	4.43587600	1.54828500	C	-1.37905400	-1.61656500	0.58985900
H	0.36343600	-1.67785000	4.41738800					O	-0.68191800	-2.55321400	0.94029600
H	-2.98358100	-3.92388300	2.79111100					C	2.52778700	-0.46477900	1.19021900
H	-1.28450600	-3.56463500	4.60363400	TS2A-2				C	2.26238900	-1.58992500	2.00640900
C	-2.31143700	-0.88428500	-1.27004400					C	3.73542300	0.25012800	1.35358500
C	-1.63493800	-1.89451900	-1.99618900	Pd	-0.85584600	0.29780800	0.72338500	C	3.20380300	-1.99248200	2.96730000
C	-3.65480400	-0.57386900	-1.57617600	O	-1.91358800	1.57834500	2.28433200	H	1.31650400	-2.14207400	1.88551100
C	-2.31389700	-2.58972300	-3.01066600	O	-3.65128800	0.14080600	2.70300600	C	4.66947400	-0.15994200	2.32151300
H	-0.57823200	-2.12268700	-1.76838800	C	-2.88795300	0.78924100	1.98911600	H	3.94655800	1.13125900	0.72820600
C	-4.32099000	-1.27392600	-2.59770500	C	-3.18050600	0.68826100	0.41061800	C	4.40635500	-1.28008500	3.12841500
H	-4.18205900	0.21585000	-1.01878000	C	-3.66655000	1.87300700	-0.20135200	H	2.99002100	-2.86728700	3.60163500
C	-3.65312700	-2.28252200	-3.31370700	C	-3.36168400	-0.54313000	-0.28795600	H	5.60738900	0.40454500	2.44555300
H	-1.78519000	-3.37530200	-3.57351600	C	-4.40832300	1.82498700	-1.39103000	H	5.13824800	-1.59600900	3.88880800
H	-5.36844900	-1.02702500	-2.83361900	H	-3.49522600	2.83099800	0.31476300	C	1.53646900	-1.08387700	-1.49975000
H	-4.17724500	-2.82862300	-4.11437000	C	-4.11129300	-0.59342700	-1.47695000	C	2.72250900	-1.83398000	-1.65195400
C	-2.46319100	1.39056000	0.57657200	C	-4.65373600	0.58778500	-2.01472400	C	0.53057500	-1.16368300	-2.48881400
C	-2.41743600	2.58556800	-0.17664500	H	-4.81128400	2.75311000	-1.82640700	C	2.89983100	-2.64889600	-2.78427000
C	-3.33373700	1.30338500	1.68487900	H	-4.24331800	-1.55050600	-2.00468000	H	3.50697400	-1.78738700	-0.88070000
C	-3.23878000	3.67109400	0.16701300	H	-5.24506200	0.54108600	-2.94281600	C	0.71677400	-1.97133900	-3.62211600
H	-1.72733900	2.66816000	-1.03190400	P	1.26148700	0.03525700	-0.05849300	H	-0.40550600	-0.59455100	-2.36050400

C	1.90108100	-2.71666700	-3.77087000	Pd	0.93128300	0.39579400	-0.26927200	C	-3.57668500	1.63508200	0.89048300
H	3.82487100	-3.23725100	-2.89230000	C	-1.80134000	-0.95058700	1.40613300	C	-2.66972200	3.98720600	-0.36138300
H	-0.07179300	-2.02654000	-4.38930600	C	-1.34435000	-0.50775100	2.67007700	H	-0.97514900	2.79228100	-1.03295800
H	2.04180200	-3.35830500	-4.65521300	C	-2.51907700	-2.16160400	1.31337300	C	-4.31536100	2.82578000	1.00598700
C	1.79683900	1.70667600	-0.63557100	C	-1.61790800	-1.25994700	3.82261800	H	-3.93017200	0.71854800	1.38876600
C	2.49975400	1.91238800	-1.84279400	H	-0.76923100	0.42871300	2.75340800	C	-3.86548400	4.00112100	0.37890500
C	1.45711400	2.81892300	0.17211200	C	-2.78175000	-2.91538000	2.47186000	H	-2.30858500	4.90762800	-0.84689400
C	2.86472200	3.21377700	-2.23075000	H	-2.86894600	-2.52232900	0.33396900	H	-5.24733000	2.83461500	1.59339800
H	2.76094000	1.05484600	-2.48212400	C	-2.33535100	-2.46703100	3.72585700	H	-4.44468000	4.93332600	0.47421500
C	1.82773900	4.11517400	-0.22048600	H	-1.25896900	-0.90583300	4.80200100	C	3.78377200	-0.05502000	0.06163700
H	0.89348500	2.67033500	1.10956200	H	-3.33817200	-3.86237400	2.38842900	C	5.16282700	0.09246000	-0.25428800
C	2.53155300	4.31461700	-1.42221800	H	-2.54015900	-3.06131500	4.63043700	C	5.65806200	1.26217800	-0.84131300
H	3.41288600	3.36665400	-3.17406000	C	-2.16338500	-0.79617100	-1.50752600	C	4.79637600	2.33156600	-1.16001900
H	1.55793800	4.97387900	0.41416900	C	-1.41315800	-1.80417600	-2.15978400	C	3.44140600	2.23180500	-0.82773300
H	2.81682000	5.33255200	-1.73195100	C	-3.46850700	-0.48895200	-1.95433000	C	2.93792000	1.08291800	-0.16500300
				C	-1.98307000	-2.50462700	-3.23746400	H	5.84263500	-0.75553800	-0.08531700
				H	-0.38087700	-2.02699400	-1.83237100	H	6.73065500	1.32933800	-1.08507800
TS2_B-1				C	-4.02357800	-1.19203700	-3.03693100	H	5.18405200	3.24199900	-1.64227000
				H	-4.05272700	0.30305800	-1.46060400	H	2.76448200	3.07905600	-1.02289800
P	-1.38333600	0.07201800	-0.07592100	C	-3.28388300	-2.20234600	-3.67744500	N	3.28544000	-1.28602500	0.52880300
C	1.59333200	1.67078200	0.90961600	H	-1.39561800	-3.28880200	-3.74083400	C	4.17614300	-2.09224800	1.36944000
O	1.69680100	2.29912600	1.90193300	H	-5.04039900	-0.94590700	-3.38244400	H	4.92949400	-2.66850500	0.78627700
C	2.33347200	-2.10725300	-0.26602500	H	-3.72148800	-2.75095100	-4.52691700	H	4.69256300	-1.43177000	2.09376200
O	1.51477000	-1.47552700	-1.05578200	C	-2.37600100	1.61530500	0.14633200	H	3.56235000	-2.83386000	1.91226800
O	2.40854200	-3.32291900	-0.11823300	C	-1.92498600	2.80152300	-0.47273900				

				H	3.61653100	-2.05563400	0.32462100	H	-3.43962200	-3.30127900	0.65374700
				C	1.89064600	-2.71656300	-3.12756600	H	-5.60508100	1.06567000	-0.59111300
				H	0.52776500	-1.10362500	-2.58085500	H	-7.01375700	-0.89490200	0.03380500
Pd	-0.86625600	0.44891300	-0.28680900	C	2.99395500	-3.49388700	-2.73142900	N	-2.83635600	1.05494500	-0.62100100
O	-1.49316500	2.75164700	0.67750400	H	4.47164200	-3.86435700	-1.17421500	C	-3.13680200	1.82887800	-1.83487200
O	-3.74301400	2.65129200	1.26513900	H	1.39539200	-2.90988000	-4.09233200	H	-3.17881000	1.17867900	-2.73654500
C	-2.67553100	2.45945800	0.75972500	H	3.36778400	-4.29638800	-3.38716500	H	-4.10294600	2.37696100	-1.75081500
P	1.37757800	-0.06391100	-0.01207300	C	2.38983500	1.40814400	-0.50148700	H	-2.33931900	2.58486000	-1.98305600
C	-1.64211000	-1.35322200	-0.02183000	C	3.63831800	1.29573000	-1.15256600				
O	-1.01317900	-2.37330100	0.17720700	C	1.86815600	2.69249400	-0.21583600				
C	1.94229300	-0.46288700	1.70555100	C	4.35875100	2.45077500	-1.50270900				
C	1.37782700	-1.58784400	2.35306200	H	4.04717800	0.30180600	-1.39226300				
C	2.87681600	0.33907400	2.39581400	C	2.59725800	3.84287000	-0.56347800				
C	1.75584600	-1.90484000	3.66731900	H	0.88510400	2.79763500	0.27362800				
H	0.64075700	-2.21106800	1.82218200	C	3.84195500	3.72480300	-1.20695000				
C	3.24537400	0.01749900	3.71471700	H	5.33025200	2.35272800	-2.01304900				
H	3.31779000	1.22007400	1.90482400	H	2.18249000	4.83747400	-0.33531200				
C	2.68842800	-1.10363300	4.35211200	H	4.40818700	4.62810300	-1.48481900				
H	1.31238200	-2.78321800	4.16281700	C	-5.32746500	-2.22686200	0.39139700				
H	3.97414300	0.65109000	4.24503600	C	-3.93335100	-2.35352300	0.38993100				
H	2.97794300	-1.35249100	5.38551000	C	-3.13243800	-1.24642200	0.02880500				
C	2.03029900	-1.44710000	-1.04590900	C	-3.71918800	0.00094900	-0.32244700				
C	3.13450100	-2.23305700	-0.64975400	C	-5.13010500	0.10916700	-0.32989100				
C	1.40704200	-1.70102200	-2.28712200	C	-5.91620700	-0.99542200	0.02891800				
C	3.61249300	-3.25232100	-1.49213700	H	-5.96193000	-3.08271000	0.66969300				