

Supplementary Information

Predicting an unconventional facile way to metallaanthracenes

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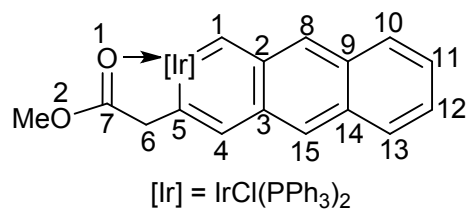
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Content

1. **Table S1. Comparison of the selected bond lengths (Å) of synthesised iridaanthracene in experiment and calculation at B3LYP-D3(BJ)/6-31+G(d)-LANL2DZ-SMD(DCM) level.**
2. **Fig. S1. Selected short H...H distances in the substituted reactants and products.**
3. **Cartesian coordinates and electronic energies for all the species calculated in this study.**

1. Table S1. Comparison of the selected bond lengths (Å) of synthesized iridaanthracene in experiment and calculation at B3LYP-D3(BJ)/6-31+G(d)-LANL2DZ-SMD(DCM) level.



	exp.	calc.
Ir-C1	1.913	1.900
Ir-C5	2.017	1.994
Ir-O1	2.228	2.24
C1-C2	1.413	1.416
C2-C3	1.444	1.452
C3-C4	1.446	1.446
C4-C5	1.327	1.349
C5-C6	1.526	1.520
C6-C7	1.488	1.500
C7-O1	1.241	1.244
C2-C8	1.410	1.406
C8-C9	1.399	1.403
C9-C10	1.432	1.426
C10-C11	1.363	1.376
C11-C12	1.399	1.422
C12-C13	1.377	1.380
C13-C14	1.418	1.421
C14-C15	1.414	1.415
C3-C15	1.378	1.387
C9-C14	1.426	1.440

2.

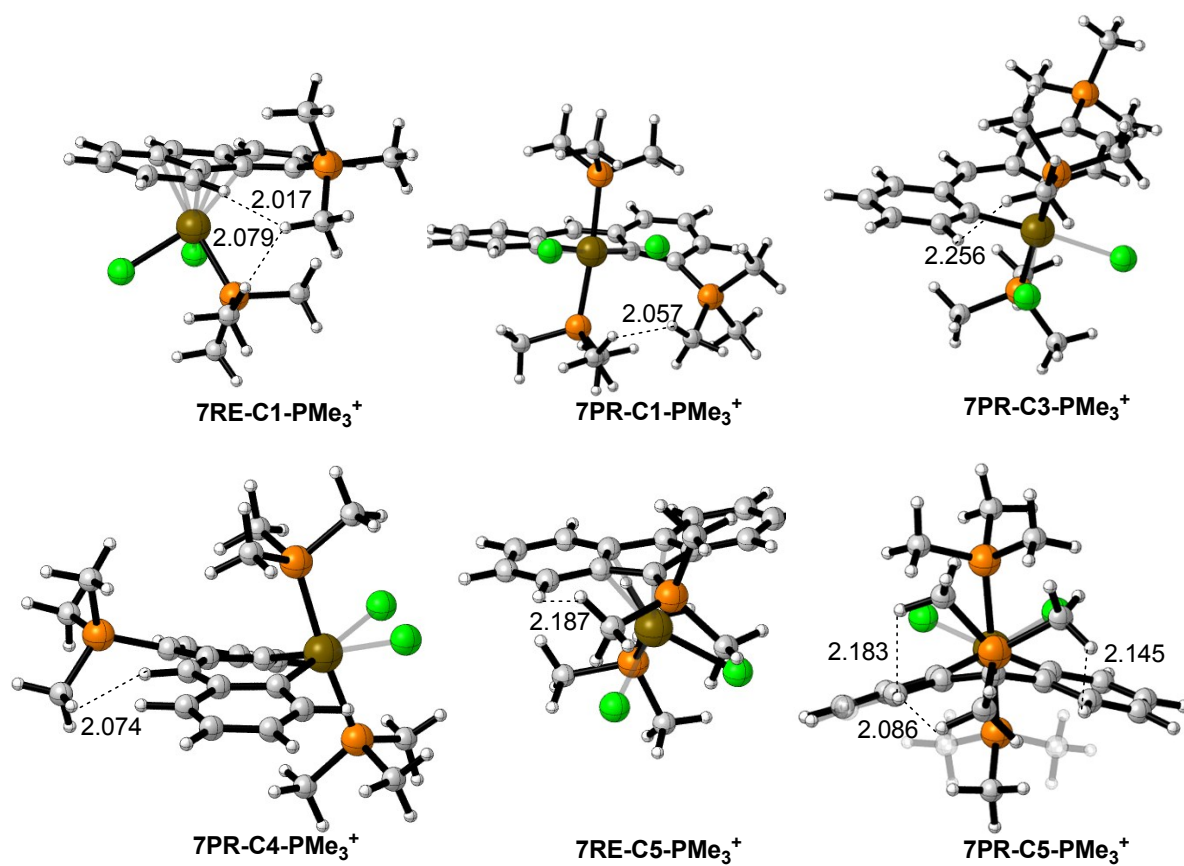


Figure S1. Selected short H...H distance in the substituted reactants and products.

3. Cartesian coordinates and electronic energies for all the species calculated in this study.

PMe₃

E = -126.281544 a.u.

P	0.00006300	0.00003000	-0.60846800
C	-0.91386500	1.36979700	0.28182800
H	-0.49400500	2.33961400	-0.01009400
H	-1.97039300	1.35445700	-0.01058900
H	-0.84403400	1.26452000	1.37210600
C	-0.72978300	-1.47605600	0.28182800
H	-1.77923900	-1.59745000	-0.01124700
H	-0.18803700	-2.38354300	-0.00969000
H	-0.67470200	-1.36246700	1.37208400
C	1.64359500	0.10622400	0.28186200
H	2.27301500	-0.74277500	-0.00970200
H	2.15903600	1.02843800	-0.01113100
H	1.51772800	0.09896900	1.37217000

1RE

E = -594.755421 a.u.

Os	-0.17626200	-0.51789400	-0.07419200
C	2.05027100	-0.82549100	0.01900200
C	1.75156200	0.09290400	-1.07186800
C	2.33924000	1.39482500	-1.07635900
C	3.16756000	1.76430900	-0.04119200
C	3.43763100	0.87399200	1.04432900
C	2.89528000	-0.39052900	1.08481400
C	1.38757000	-2.08958200	-0.25445600
C	0.66978900	-1.92235300	-1.48665200
C	0.85093300	-0.58318500	-1.98974300
H	2.14072300	2.07191300	-1.90326300
H	3.61930400	2.75333800	-0.03742000
H	4.08142700	1.21010100	1.85343700
H	3.10953000	-1.06497700	1.90945300
H	0.05976200	-2.68188800	-1.95948400
H	0.50218600	-0.20430700	-2.94187000
Cl	-2.36911600	-1.68536000	-0.23274600
H	1.45750200	-2.99299900	0.33708700
Cl	-0.55502100	-0.44634700	2.43546000
P	-1.26339700	1.54432700	-0.13388100
C	-3.05445600	1.65661100	0.33706500
H	-3.18098800	1.24996400	1.34479600
H	-3.39501100	2.69866300	0.31510800
H	-3.65260100	1.05765700	-0.35450300
C	-1.26817000	2.40108700	-1.78217900
H	-1.76140400	3.37858900	-1.71778700
H	-0.23854700	2.54157700	-2.12555800
H	-1.79765100	1.77741400	-2.51014000
C	-0.52429500	2.85078200	0.95812500

H	0.54016400	2.95355300	0.72498900
H	-1.02537300	3.81667100	0.82163100
H	-0.61933900	2.52854700	1.99883600

1PR

E = -721.099951 a.u.

C	-0.97420500	-0.28016000	2.77409100
C	-2.05623200	-0.92715800	2.22761900
C	-2.19432400	-1.34278100	0.85678200
C	-1.18387600	-1.07509600	-0.14028900
C	0.16679500	0.11324900	2.00976800
H	-4.09651100	-2.26635600	1.32214100
H	-0.96670300	-0.12982700	3.85634100
H	-2.85953700	-1.23267600	2.89978800
C	-3.34576000	-2.12099500	0.54569000
C	-1.38482600	-1.75658700	-1.37948400
H	1.02962200	0.38159600	2.64428800
C	-2.50610400	-2.52445800	-1.66347500
C	-3.52107600	-2.69999400	-0.69866700
H	-0.64369800	-1.61691800	-2.15889600
H	-2.60944900	-2.98377600	-2.64591600
H	-4.40806400	-3.28830400	-0.92174300
Os	0.35089200	0.22285400	0.11916100
Cl	0.68290000	0.58843100	-2.48920800
P	-1.22084700	2.01114400	-0.16399600
P	2.09308300	-1.40758100	0.05567100
Cl	2.32276000	1.92603300	0.52727700
C	-0.52659200	3.57538200	-0.86539700
H	-0.03832800	3.34746500	-1.81621100
H	-1.32256500	4.31317600	-1.01965700
H	0.22262800	3.97382200	-0.17651200
C	-2.09562900	2.64393800	1.34193300
H	-2.76155600	3.47278400	1.07497400
H	-2.68014900	1.84141100	1.79817100
H	-1.35328000	2.99191500	2.06734600
C	-2.63009000	1.65960900	-1.31251400
H	-3.24828700	0.85604400	-0.90235300
H	-3.24405300	2.55658600	-1.45425200
H	-2.22426300	1.33475300	-2.27424800
C	3.47325800	-1.08532700	-1.12988100
H	3.90120000	-0.10510400	-0.90375900
H	4.24239200	-1.86180000	-1.04593900
H	3.07139900	-1.06279700	-2.14577400
C	2.99744800	-1.64492200	1.65523200
H	3.82271100	-2.35625800	1.53478100
H	3.39164800	-0.68003200	1.98681400
H	2.30142200	-2.02134800	2.41164900

C	1.62416200	-3.15152200	-0.36447100
H	1.19656900	-3.18394600	-1.37086700
H	2.50172100	-3.80738900	-0.32417200
H	0.86986900	-3.50829300	0.34387600

2RE

E = -748.419230 a.u.

C	1.52123100	3.36925300	-0.48044900
C	1.09062900	2.44921100	-1.40155900
C	-0.02509400	1.60158100	-1.07989600
C	-0.70001900	1.78723700	0.20395800
C	-0.19845700	2.74104900	1.14090900
C	0.89203400	3.50609700	0.80329600
C	-0.75653300	0.60970700	-1.84761500
C	-1.96119800	1.05226800	0.13671300
C	-2.00977600	0.37286400	-1.13569400
C	-3.11091000	-0.46584700	-1.43045300
H	-3.14834500	-0.99641000	-2.37789000
C	-4.12733800	-0.60218400	-0.49983300
C	-4.07238100	0.06307200	0.75183800
C	-2.99938200	0.87610900	1.07824800
H	-0.57256900	0.34501200	-2.88220100
H	2.36224400	4.01589300	-0.72088900
H	1.55993400	2.37158900	-2.37851200
H	1.28918000	4.22925700	1.51092000
H	-4.97743600	-1.24243600	-0.72250000
H	-4.87902400	-0.07916300	1.46642600
Os	-0.01587000	-0.31853300	-0.03847800
H	-2.95010400	1.37406300	2.04253800
H	-0.69391300	2.86617000	2.10044200
Cl	-0.37710200	-2.71615100	-0.57359600
P	2.23595300	-0.64075900	-0.08862400
C	3.22993600	0.49611100	0.98604500
H	4.30187300	0.28047600	0.90048700
H	3.04252800	1.53239800	0.69366800
H	2.90934300	0.36192600	2.02331800
C	2.86677100	-2.29677800	0.45657200
H	2.50232000	-3.06608700	-0.22804400
H	3.96287000	-2.29910100	0.47252400
H	2.47976000	-2.50814100	1.45681400
C	3.08528700	-0.46404500	-1.73090400
H	2.95064500	0.55094200	-2.11371200
H	4.15757900	-0.67545900	-1.63886100
H	2.63613800	-1.16928900	-2.43806000
Cl	0.04680700	-0.96890800	2.41948800

2PR

E = -874.762430 a.u.

C	-2.77758800	-2.99922200	-2.01554800
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C	-3.03238400	-1.65094700	-1.95067400
C	-2.07271800	-0.73281700	-1.40304800
C	-0.83996100	-1.21291000	-0.80000200
C	-0.59499900	-2.61550300	-0.99910900
C	-1.52114600	-3.47749200	-1.55035800
C	-2.32753900	0.63823000	-1.58478800
C	-0.16735400	1.54523000	-0.69636600
C	-1.46595700	1.72153100	-1.32610000
C	-1.88451100	3.00679400	-1.80927800
H	-2.88905700	3.10045400	-2.22004100
C	-1.04512700	4.09402100	-1.77854800
C	0.27072300	3.92111600	-1.26920500
C	0.68661000	2.69905300	-0.77853600
H	-3.25824400	0.88362000	-2.09887800
H	-3.50880500	-3.68786100	-2.43194400
H	-3.96940400	-1.24900500	-2.33406900
H	-1.29764400	-4.54152000	-1.61169600
H	-1.37100000	5.06343400	-2.14771800
H	0.95182500	4.77055900	-1.24602400
Os	0.35901800	-0.08783400	0.30512600
Cl	1.91940900	1.28858700	1.92243400
P	2.22988700	-0.50772500	-1.10535000
P	-1.39190500	0.24334100	1.91770600
C	-2.74533900	-1.02499700	1.93131400
H	-3.43935900	-0.83765100	2.75896000
H	-3.29302600	-1.00307900	0.98636500
H	-2.29524200	-2.01513200	2.05144600
C	-0.85472400	0.20306800	3.68969600
H	-1.72324000	0.30570200	4.35066900
H	-0.34627400	-0.74478800	3.88090900
H	-0.14919600	1.01804800	3.86692300
C	-2.34223600	1.83791900	1.88264500
H	-2.92212300	1.91586600	0.96079800
H	-3.01980300	1.89262200	2.74269900
H	-1.63630400	2.67380700	1.92310500
C	3.14535900	-2.10490200	-0.88879000
H	3.95575700	-2.17162500	-1.62420200
H	3.56045100	-2.14487900	0.12168700
H	2.46930500	-2.95343300	-1.01799300
C	3.64798100	0.68707700	-1.07824000
H	4.45044900	0.32886000	-1.73331700
H	3.31710600	1.67011500	-1.42337300
H	4.01844400	0.78268300	-0.05475100
C	1.81915900	-0.54586900	-2.91388500
H	2.71386000	-0.72139200	-3.52284500
H	1.09012200	-1.33988600	-3.10202100
H	1.67847700	2.62562700	-0.35041200
H	1.36952800	0.41131600	-3.19596800
H	0.32876200	-3.02855400	-0.61199700

Cl 1.02000600 -2.12970800 1.82707800

3RE

E = -859.629842 a.u.

C 0.15608500 1.07320100 -1.81736000
C -1.01273900 1.64521800 -1.17113600
C 0.85341900 2.16259700 0.14569900
H 0.18004700 0.72431100 -2.84264900
C 1.31261500 1.58956400 -1.09540700
C 2.69621100 1.61074000 -1.39505200
C 1.77959600 2.65754900 1.09286500
C 3.57695500 2.14295800 -0.47148400
H 3.05023000 1.22766100 -2.34782300
C 3.12680500 2.64236500 0.77876500
H 1.42889600 3.06353800 2.03721700
H 4.63966400 2.17019500 -0.69894200
H 3.85184800 3.02934000 1.48971000
C -0.60628700 2.21009000 0.09485900
C -1.56286500 2.79324900 0.95967600
C -2.87732600 2.87826800 0.54209800
H -1.25424500 3.19331600 1.92130800
C -2.37146800 1.75591900 -1.57326900
C -3.27023200 2.37963500 -0.73128600
H -3.62246900 3.33640800 1.18655100
H -2.68241100 1.38338900 -2.54487000
H -4.30692200 2.48675100 -1.04100000
Os 0.03320000 -0.09381600 0.05402000
P -1.77305400 -1.49698700 -0.08418300
C -3.25980900 -0.84695100 0.80760300
H -4.11852300 -1.51138500 0.65718600
H -3.02127400 -0.78924600 1.87359500
H -3.50754200 0.15303500 0.44893100
C -2.42689800 -1.83413000 -1.78729500
H -3.30752600 -2.48552100 -1.74153800
H -2.70161800 -0.89217800 -2.26843100
H -1.64861400 -2.31786700 -2.38474400
C -1.73403900 -3.21301800 0.62366700
H -2.73495500 -3.65116300 0.54074800
H -1.02721600 -3.85130400 0.08894900
H -1.45236800 -3.16195600 1.67854100
Cl 0.01209400 -0.42400500 2.56148900
P 1.50043100 -1.83775400 -0.22101200
C 3.28577800 -1.38969200 -0.45313700
H 3.89092600 -2.30262200 -0.41588100
H 3.43443300 -0.90017200 -1.41705200
H 3.60587100 -0.71032100 0.34153800
C 1.70974800 -3.06608900 1.15834000
H 2.37090900 -3.87505700 0.82709300
H 2.16139000 -2.55286100 2.01157500

H 0.75532200 -3.48304000 1.47735100
C 1.25272400 -2.93681300 -1.69899300
H 2.06150900 -3.67366800 -1.76920300
H 0.29643300 -3.46122000 -1.63434500
H 1.24907700 -2.31706200 -2.60164900

3PR

E = -985.947907 a.u.

C -4.75248500 -0.98219500 -0.24312900
C -4.23293200 0.27253900 -0.46982800
C -2.81929600 0.50023300 -0.48455400
C -1.88122700 -0.55955400 -0.20916600
C -2.48148700 -1.84110200 -0.04003400
C -3.85105600 -2.05314000 -0.03932800
C -2.40503600 1.80560600 -0.84093500
C 0.06535800 1.40909600 -0.99713100
C -1.11365600 2.26555600 -1.10917400
C -1.01413900 3.60871900 -1.61972700
H -1.90887100 4.22847500 -1.60342700
C 0.15643300 4.09291100 -2.14052100
C 1.27616000 3.21569700 -2.20961600
C 1.20831500 1.93974300 -1.69562100
H -3.20828300 2.52002800 -1.02543500
H -5.82627800 -1.15019900 -0.22817400
H -4.89586800 1.11795900 -0.64590600
H -1.83331000 -2.68605000 0.15971900
H -4.23953700 -3.05529900 0.13451000
H 0.22430700 5.10615500 -2.52742100
H 2.20132700 3.56301100 -2.66604800
H 2.09303300 1.32349000 -1.77016500
Os 0.13330200 -0.25709000 0.08014100
Cl 0.23604400 -2.37962700 1.63353700
P 0.64870000 -1.63963600 -1.81208600
P -0.51012100 0.84747100 2.13045700
P 2.54245900 0.02883900 0.65232700
C -2.18673900 0.40703800 2.79215100
H -2.34061400 0.89748600 3.75981700
H -2.97219900 0.71540100 2.10076000
H -2.23798000 -0.67762800 2.92217000
C 0.48619600 0.52552600 3.66417000
H -0.00927900 1.00010400 4.51836100
H 0.54295100 -0.55270800 3.82915400
H 1.49553300 0.93166700 3.57567400
C -0.56841400 2.70364500 2.13871300
H -0.74570200 3.06690000 3.15736000
H 0.37951900 3.10415900 1.76863700
H -1.37150200 3.05604600 1.48873700
C 3.22940300 -1.01615800 2.02804400
H 4.24851700 -0.68785100 2.26291300

H	2.60794700	-0.95623300	2.92017200
H	3.24884200	-2.05900100	1.70138600
C	3.90909100	-0.29310500	-0.58223800
H	4.87535500	-0.19393700	-0.07453900
H	3.82759300	-1.30537600	-0.98487800
H	3.88149100	0.42142600	-1.40806000
C	3.05957500	1.73560200	1.19346300
H	4.12893600	1.75533200	1.43386500
H	2.86052200	2.44722800	0.38757900
H	2.49193300	2.04799100	2.07272500
C	1.54962500	-3.21957300	-1.45954400
H	1.72837800	-3.76845000	-2.39109600
H	2.50462400	-3.01295500	-0.97010300
H	0.94598600	-3.82635300	-0.78061200
C	-0.80067700	-2.27986700	-2.78099800
H	-1.41857200	-2.93122600	-2.16050600
H	-1.41261700	-1.43829000	-3.11972400
H	-0.44279100	-2.84294000	-3.65026700
C	1.62830100	-0.94929300	-3.23296400
H	2.61800700	-0.61716100	-2.91843400
H	1.74024400	-1.72632800	-3.99737600
H	1.09120600	-0.10004100	-3.66485600

4RE

E = -748.419230 a.u.

C	1.52123100	3.36925300	-0.48044900
C	1.09062900	2.44921100	-1.40155900
C	-0.02509400	1.60158100	-1.07989600
C	-0.70001900	1.78723700	0.20395800
C	-0.19845700	2.74104900	1.14090900
C	0.89203400	3.50609700	0.80329600
C	-0.75653300	0.60970700	-1.84761500
C	-1.96119800	1.05226800	0.13671300
C	-2.00977600	0.37286400	-1.13569400
C	-3.11091000	-0.46584700	-1.43045300
H	-3.14834500	-0.99641000	-2.37789000
C	-4.12733800	-0.60218400	-0.49983300
C	-4.07238100	0.06307200	0.75183800
C	-2.99938200	0.87610900	1.07824800
H	-0.57256900	0.34501200	-2.88220100
H	2.36224400	4.01589300	-0.72088900
H	1.55993400	2.37158900	-2.37851200
H	1.28918000	4.22925700	1.51092000
H	-4.97743600	-1.24243600	-0.72250000
H	-4.87902400	-0.07916300	1.46642600
Os	-0.01587000	-0.31853300	-0.03847800
H	-2.95010400	1.37406300	2.04253800
H	-0.69391300	2.86617000	2.10044200
Cl	-0.37710200	-2.71615100	-0.57359600

P	2.23595300	-0.64075900	-0.08862400
C	3.22993600	0.49611100	0.98604500
H	4.30187300	0.28047600	0.90048700
H	3.04252800	1.53239800	0.69366800
H	2.90934300	0.36192600	2.02331800
C	2.86677100	-2.29677800	0.45657200
H	2.50232000	-3.06608700	-0.22804400
H	3.96287000	-2.29910100	0.47252400
H	2.47976000	-2.50814100	1.45681400
C	3.08528700	-0.46404500	-1.73090400
H	2.95064500	0.55094200	-2.11371200
H	4.15757900	-0.67545900	-1.63886100
H	2.63613800	-1.16928900	-2.43806000
Cl	0.04680700	-0.96890800	2.41948800

4PR

E = -874.762430 a.u.

C	-2.77758800	-2.99922200	-2.01554800
C	-3.03238400	-1.65094700	-1.95067400
C	-2.07271800	-0.73281700	-1.40304800
C	-0.83996100	-1.21291000	-0.80000200
C	-0.59499900	-2.61550300	-0.99910900
C	-1.52114600	-3.47749200	-1.55035800
C	-2.32753900	0.63823000	-1.58478800
C	-0.16735400	1.54523000	-0.69636600
C	-1.46595700	1.72153100	-1.32610000
C	-1.88451100	3.00679400	-1.80927800
H	-2.88905700	3.10045400	-2.22004100
C	-1.04512700	4.09402100	-1.77854800
C	0.27072300	3.92111600	-1.26920500
C	0.68661000	2.69905300	-0.77853600
H	-3.25824400	0.88362000	-2.09887800
H	-3.50880500	-3.68786100	-2.43194400
H	-3.96940400	-1.24900500	-2.33406900
H	-1.29764400	-4.54152000	-1.61169600
H	-1.37100000	5.06343400	-2.14771800
H	0.95182500	4.77055900	-1.24602400
Os	0.35901800	-0.08783400	0.30512600
Cl	1.91940900	1.28858700	1.92243400
P	2.22988700	-0.50772500	-1.10535000
P	-1.39190500	0.24334100	1.91770600
C	-2.74533900	-1.02499700	1.93131400
H	-3.43935900	-0.83765100	2.75896000
H	-3.29302600	-1.00307900	0.98636500
H	-2.29524200	-2.01513200	2.05144600
C	-0.85472400	0.20306800	3.68969600
H	-1.72324000	0.30570200	4.35066900
H	-0.34627400	-0.74478800	3.88090900
H	-0.14919600	1.01804800	3.86692300

C	-2.34223600	1.83791900	1.88264500
H	-2.92212300	1.91586600	0.96079800
H	-3.01980300	1.89262200	2.74269900
H	-1.63630400	2.67380700	1.92310500
C	3.14535900	-2.10490200	-0.88879000
H	3.95575700	-2.17162500	-1.62420200
H	3.56045100	-2.14487900	0.12168700
H	2.46930500	-2.95343300	-1.01799300
C	3.64798100	0.68707700	-1.07824000
H	4.45044900	0.32886000	-1.73331700
H	3.31710600	1.67011500	-1.42337300
H	4.01844400	0.78268300	-0.05475100
C	1.81915900	-0.54586900	-2.91388500
H	2.71386000	-0.72139200	-3.52284500
H	1.09012200	-1.33988600	-3.10202100
H	1.67847700	2.62562700	-0.35041200
H	1.36952800	0.41131600	-3.19596800
H	0.32876200	-3.02855400	-0.61199700
Cl	1.02000600	-2.12970800	1.82707800

5RE

E = -970.824454 a.u.

C	0.17607400	-1.18552000	-2.00747900
C	1.38929300	-1.52695400	-1.29876900
C	-0.41598100	-2.28333000	-0.01693200
H	0.13138700	-0.83639200	-3.03022500
C	-0.91488400	-1.81660600	-1.29198900
C	-2.27052400	-2.06621600	-1.63751600
C	-1.28109900	-2.94072700	0.89545100
C	-3.07496400	-2.74313800	-0.74481800
H	-2.65245700	-1.74787600	-2.60281800
C	-2.59103300	-3.16501700	0.52606200
H	-0.90020800	-3.28804700	1.85157300
H	-4.10738700	-2.95506300	-1.01011000
H	-3.26441200	-3.68077400	1.20491300
C	1.03267700	-2.11098900	-0.02574200
C	2.04268800	-2.55946800	0.86203100
C	3.36499400	-2.44378200	0.48575600
H	1.77273300	-3.02494200	1.80408200
C	2.76108800	-1.43563900	-1.65921900
C	3.71782500	-1.89484100	-0.77888000
H	4.14954400	-2.79703100	1.14902700
H	3.04238400	-1.05440900	-2.63541100
H	4.76723500	-1.84885700	-1.05817100
Os	-0.01337900	0.07877300	-0.12871600
P	-1.81912300	1.38404500	-0.72341200
P	1.52437500	1.76815600	-0.45409100
P	-0.21275200	0.50402600	2.16435300
C	-2.04338700	1.48562600	-2.56162800

H	-2.16691600	0.48514600	-2.98254400
H	-2.92091900	2.09372500	-2.80853600
H	-1.14980800	1.94308400	-2.99845600
C	-3.46807600	0.76764300	-0.13017300
H	-3.67288400	1.19299100	0.85558200
H	-4.25147700	1.09463000	-0.82297700
H	-3.48184500	-0.31922300	-0.05726300
C	-2.02035600	3.17428600	-0.28053900
H	-1.34615500	3.80091300	-0.86465300
H	-3.05201100	3.46154900	-0.51277700
H	-1.84013700	3.33935300	0.78390600
C	-1.85225800	0.09700000	2.93614400
H	-1.74911700	0.03972500	4.02564600
H	-2.57955000	0.87537500	2.69189300
H	-2.21856400	-0.86006800	2.55559400
C	0.91713700	-0.52167100	3.22117700
H	0.83630800	-0.20808700	4.26793800
H	0.63002100	-1.57316700	3.14187800
H	1.95203400	-0.41268200	2.88664300
C	0.07807400	2.17900000	2.90943400
H	-0.61136500	2.91023600	2.48134200
H	-0.09067800	2.12563000	3.99075900
H	1.10511100	2.50464400	2.72668000
C	2.11392300	1.93439700	-2.20496900
H	2.84110500	2.75102700	-2.27900100
H	2.57804800	1.00954300	-2.54787100
H	1.25406400	2.15754700	-2.84492400
C	3.08227100	1.47485100	0.50349700
H	3.87708000	2.14550500	0.15769100
H	2.88850700	1.66501300	1.56345200
H	3.40547800	0.43887900	0.38373800
C	1.23465600	3.56944200	-0.09607000
H	2.21258800	4.05556600	-0.00747000
H	0.69971700	4.02648200	-0.93116300
H	0.67301700	3.72979200	0.82272900

5PR

E = -1097.104662 a.u.

C	-3.49719700	-3.32031900	-0.10773100
C	-2.23624500	-3.56836300	-0.59469500
C	-1.17409300	-2.61849500	-0.43198300
C	-1.40038000	-1.30694700	0.14067800
C	-2.70083100	-1.16641500	0.70638100
C	-3.71080400	-2.10728500	0.58647500
C	0.11089800	-3.10199500	-0.73394300
C	1.48786600	-1.20467100	0.14056100
C	1.35814900	-2.52878100	-0.43154300
C	2.48451600	-3.40357000	-0.58268200
H	2.33280300	-4.35872900	-1.08116100

C	3.71929900	-3.07045500	-0.07958700
C	3.84110300	-1.84633200	0.61745000
C	2.76876700	-0.97543300	0.72255700
H	0.14673400	-4.11724800	-1.12900300
H	-4.29884600	-4.04410500	-0.22363600
H	-2.01392000	-4.50971700	-1.09270300
H	-2.94685300	-0.25487900	1.23088500
H	-4.68724400	-1.89976600	1.01950000
H	4.56944400	-3.73845600	-0.18411500
H	4.79544200	-1.57393600	1.06352800
H	2.94615300	-0.04811300	1.24812800
Os	-0.00818600	0.21066200	0.08236200
P	-1.89772000	1.89885900	-0.08696800
P	1.76878600	2.01561600	-0.13068400
P	0.00954300	-0.04346400	2.51851600
P	-0.01685200	0.02032000	-2.33250600
C	1.42343300	-0.84755500	-3.13748000
H	1.31347000	-1.92737900	-3.03186000
H	1.43765700	-0.59820000	-4.20410000
H	2.36819900	-0.54966500	-2.68240600
C	-1.40952800	-0.92997800	-3.12674000
H	-1.40470600	-0.72806200	-4.20343100
H	-1.26983300	-1.99956600	-2.96955900
H	-2.37434300	-0.64227000	-2.70845800
C	-0.06602400	1.55796100	-3.37605300
H	0.82792700	2.16181700	-3.21145200
H	-0.10217600	1.26875300	-4.43167000
H	-0.95048000	2.15478600	-3.14773500
C	3.20744800	1.58611700	-1.23994500
H	4.00856800	2.31943900	-1.09500200
H	3.59335800	0.58760300	-1.03547900
H	2.87908300	1.63263000	-2.28193800
C	1.46674600	3.71951700	-0.83257300
H	0.91379700	4.33141800	-0.11862500
H	2.44342200	4.18527400	-1.00304700
H	0.92615200	3.68891000	-1.77696100
C	2.68031300	2.62999300	1.37880700
H	3.40524200	3.38869500	1.06422800
H	1.96330900	3.09046000	2.06380500
H	3.21306800	1.83712800	1.90315100
C	-1.68189400	3.64796400	-0.70005400
H	-2.67919100	4.08223200	-0.82884900
H	-1.14130100	4.24060000	0.04021400
H	-1.15672300	3.69441400	-1.65222400
C	-3.28946500	1.42823900	-1.23669200
H	-4.12934900	2.11687400	-1.09283100
H	-2.94429300	1.51247000	-2.27050700
H	-3.62782900	0.40709400	-1.05777700
C	-2.87930100	2.39432300	1.42323100

H	-2.21275600	2.88753000	2.13553100
H	-3.65230000	3.10562700	1.11272000
H	-3.36382400	1.55171900	1.91561900
C	-1.41098100	0.46396700	3.60583400
H	-1.22284400	0.07180400	4.61118600
H	-1.48419100	1.55164100	3.66126600
H	-2.35373700	0.05246900	3.24449400
C	0.09205900	-1.84469400	2.97197200
H	1.00082700	-2.29160800	2.56346700
H	0.09612900	-1.95205500	4.06195000
H	-0.77461900	-2.36866300	2.56258000
C	1.37524900	0.60137700	3.60400600
H	1.35418300	1.69224000	3.63828300
H	1.21508900	0.21407400	4.61615700
H	2.35247800	0.26540900	3.25547900

6RE

E = -751.270628 a.u.

C	0.76720400	0.48062500	-1.82535000
C	0.14300000	1.57167900	-1.11380300
C	2.04108100	0.91947500	0.10130800
H	0.52181100	0.16183500	-2.83119400
C	2.01566300	0.18773900	-1.13930600
C	3.06276600	-0.71445700	-1.43145900
C	3.08691800	0.72471100	1.02513100
C	4.09602900	-0.86894100	-0.51932100
H	3.04867500	-1.28323800	-2.35702700
C	4.10852900	-0.15949900	0.70651100
H	3.08938000	1.26184700	1.96985300
H	4.90664200	-1.55933100	-0.74008400
H	4.92423600	-0.31831300	1.40705400
C	0.84672600	1.75997700	0.14011600
C	0.40661300	2.74037200	1.06521400
C	-0.66041000	3.55083300	0.72959700
H	0.92048700	2.85911800	2.01556100
C	-0.93857400	2.44361900	-1.43607600
C	-1.31354700	3.41319400	-0.53012900
H	-1.00812000	4.30697400	1.42860900
H	-1.44147600	2.35165100	-2.39469500
H	-2.13356900	4.08502600	-0.77319600
Cl	0.23935200	-2.79867900	-0.51988300
Ru	-0.00112900	-0.39428300	0.03300900
Cl	-0.28423900	-0.87007700	2.52959900
P	-2.25224300	-0.62382200	-0.15303100
C	-2.98845400	-2.20768700	0.46155100
H	-4.08267900	-2.16200900	0.40890600
H	-2.61882300	-3.03739800	-0.14467000
H	-2.67054400	-2.36035500	1.49591700
C	-2.96545300	-0.52579900	-1.86331200

H	-4.05096800	-0.68073000	-1.84180900
H	-2.75049300	0.45221500	-2.30204900
H	-2.50235200	-1.29901400	-2.48496800
C	-3.24840700	0.62794000	0.77960800
H	-2.95788000	1.63577500	0.47333300
H	-4.32106500	0.48604200	0.60061300
H	-3.03497500	0.51183300	1.84606100

6PR

E = -877.574201 a.u.

C	-3.88652400	0.70086600	-2.17312700
C	-2.87468600	1.62658100	-2.10079500
C	-1.61941700	1.31096800	-1.47599200
C	-1.41200900	0.03803700	-0.81749700
C	-2.47263000	-0.90715000	-1.00101600
C	-3.66150400	-0.59422700	-1.63214700
C	-0.58152100	2.24453500	-1.63730300
C	1.26571100	0.92818200	-0.58448900
C	0.77270600	2.09463900	-1.28695400
C	1.66802200	3.12100600	-1.74287900
H	1.24231600	4.00012600	-2.22422600
C	3.02860100	2.99807400	-1.59862400
C	3.54037300	1.81815700	-0.99627800
C	2.69337400	0.83023200	-0.52882400
H	-0.83453000	3.14974100	-2.19128500
H	-4.83301800	0.94182600	-2.65041500
H	-3.00011600	2.61637200	-2.53725200
H	-2.36111500	-1.88916200	-0.55818500
H	-4.44761600	-1.34466600	-1.70041300
H	3.70211800	3.77672200	-1.94772300
H	4.61701500	1.69938900	-0.88341600
H	3.12194700	-0.02993100	-0.03036200
Cl	2.08808300	-1.02956200	2.07162200
Cl	-1.38317200	-2.05378600	1.85469300
P	0.82071800	-2.16212200	-1.08123200
P	-0.63199900	1.23906100	1.95409900
Ru	0.12005800	-0.38775000	0.35099100
C	0.07394500	2.95593200	1.88156900
H	-0.20620600	3.44046400	0.94322300
H	-0.29257500	3.55792000	2.72149000
H	1.16622000	2.89453000	1.92852000
C	-2.45750100	1.56993000	1.95162300
H	-2.73078400	2.26581600	2.75368400
H	-2.76108600	1.98937900	0.98863100
H	-2.97816800	0.61939000	2.09856700
C	-0.34359600	0.82227900	3.73395500
H	0.73181700	0.77167900	3.91903700
H	-0.80249100	1.57898700	4.38147400
H	-0.77775400	-0.15980200	3.93414000

C	2.58563600	-2.72324100	-0.99021000
H	2.74756100	-3.57158200	-1.66566200
H	3.25137800	-1.90452300	-1.27660400
H	2.81655000	-3.01411900	0.03740100
C	0.64857700	-1.81148600	-2.89597000
H	1.23624000	-0.92183400	-3.14443100
H	0.99775000	-2.65643400	-3.50147000
H	-0.40113900	-1.60862000	-3.12896100
C	-0.06307700	-3.78349200	-0.92171200
H	-1.13159300	-3.64796000	-1.10787500
H	0.34167000	-4.50799600	-1.63843000
H	0.06189400	-4.16078900	0.09657600

7RE

E = -761.953420 a.u.

C	2.17516800	3.15641600	-0.21700600
C	1.29486900	2.71032900	-1.17476400
C	0.10933900	2.04161600	-0.75470400
C	-0.10843500	1.79730200	0.65912100
C	0.81908500	2.28243100	1.62178500
C	1.93276100	2.95530900	1.17665100
C	-1.01876900	1.49806000	-1.49428200
C	-1.39102100	1.11450500	0.78908600
C	-1.98473300	1.04798600	-0.54173000
C	-3.29366500	0.50223600	-0.69654000
H	-3.73044700	0.41868700	-1.68653100
C	-3.97296700	0.10205400	0.42511500
C	-3.40394700	0.20103500	1.73895600
C	-2.14196100	0.70032000	1.93157300
H	-1.15397200	1.54742700	-2.56606400
H	3.07732500	3.68027400	-0.52012500
H	1.47661200	2.87522700	-2.23195400
H	2.65062000	3.34189800	1.89461000
H	-4.97535000	-0.30556600	0.32492500
H	-3.99273500	-0.12890000	2.58994900
Cl	-1.19172000	-2.26994600	-0.88196600
P	1.31852700	-1.35094600	1.09679900
C	3.02089600	-0.65533500	1.19032700
H	3.58565400	-1.14507100	1.99138500
H	3.52205200	-0.81961800	0.23263800
H	2.97039800	0.41945100	1.38262900
C	1.60662900	-3.14446100	0.80245400
H	2.34919300	-3.51301300	1.51887300
H	0.67058200	-3.69356200	0.92297700
H	1.97364400	-3.28617400	-0.21715500
C	0.70475000	-1.28237500	2.83365700
H	1.37354900	-1.84694100	3.49296600
H	0.66242300	-0.24178800	3.16669700
H	-1.71229600	0.78680200	2.92444200

H	-0.29949300	-1.71424500	2.87763700
H	0.63302700	2.13116300	2.68042100
Cl	1.58403300	-0.79755700	-2.17381100
Ir	-0.02098700	-0.21115400	-0.42883500

7PR

E = -888.314640 a.u.

C	-3.56489000	2.55101200	-1.34857000
C	-2.25274800	2.94660500	-1.44947500
C	-1.18226500	2.07466700	-1.06223300
C	-1.44123300	0.77602100	-0.49408800
C	-2.81059800	0.40744900	-0.44974800
C	-3.83266100	1.25450500	-0.85545600
C	0.11311300	2.54157500	-1.34250000
C	1.42586300	0.51044500	-0.72659800
C	1.33216800	1.85295400	-1.23869900
C	2.47674300	2.52407900	-1.78406600
H	2.35845000	3.55144100	-2.12058300
C	3.68386100	1.87983800	-1.90895300
C	3.76466800	0.52932200	-1.49845100
C	2.67747700	-0.12388700	-0.93604100
H	0.17199900	3.53793900	-1.77904800
H	-4.37532500	3.20933200	-1.64740200
H	-2.00018100	3.92829500	-1.84344800
H	-4.86315400	0.91455100	-0.77642700
H	4.54955400	2.38384900	-2.32844800
H	4.70402700	-0.00775000	-1.61141500
Cl	1.66008000	-1.92527300	1.48094800
P	-0.31312200	-1.95700100	-1.50523500
P	0.30973800	1.01551600	2.16169000
C	-0.76206100	2.51564600	2.26595600
H	-0.57345500	3.03651800	3.21113700
H	-0.55183900	3.19226800	1.43469400
H	-1.81254400	2.21294600	2.22069900
C	0.05976100	0.22582000	3.80546900
H	0.36561700	0.92384300	4.59272200
H	-0.99345500	-0.03558300	3.92539200
H	0.65863700	-0.68586900	3.85524900
C	2.02067400	1.69695700	2.27816500
H	2.23654500	2.32112400	1.40723800
H	2.12307400	2.29570300	3.18983900
H	2.72917600	0.86477100	2.30404800
C	-1.95116200	-2.79259600	-1.62422200
H	-1.93659200	-3.49581700	-2.46412000
H	-2.15534600	-3.32587600	-0.69332000
H	-2.73664600	-2.05074500	-1.78792600
C	0.86928400	-3.36863300	-1.53855900
H	0.66101600	-3.99665000	-2.41199100
H	1.89478700	-2.99567400	-1.59173300

H	0.75702800	-3.95500900	-0.62356500
C	-0.12228700	-1.18624600	-3.17148400
H	-0.29522600	-1.92976500	-3.95719700
H	-0.84730700	-0.37328100	-3.27593700
H	2.80363100	-1.14462800	-0.60146900
H	0.88640800	-0.77738300	-3.27524500
H	-3.07189100	-0.55904400	-0.04159300
Cl	-1.73973700	-1.71461600	1.68054500
Ir	-0.02992600	-0.41470500	0.28019400

8RE

E = -873.153736 a.u.

C	0.87025600	1.36265400	-1.62098500
C	0.38216200	2.12886500	-0.50175300
C	2.20431500	0.84049600	0.24910000
H	0.58870400	1.51098700	-2.65483900
C	2.08945200	0.68861200	-1.17673200
C	3.04180900	-0.07727600	-1.88074300
C	3.28995600	0.27286100	0.94385000
C	4.10144500	-0.62398200	-1.17612800
H	2.94674500	-0.21663400	-2.95289200
C	4.23172100	-0.44374200	0.22388500
H	3.39131300	0.41152600	2.01515100
H	4.85672100	-1.19806400	-1.70572800
H	5.08585200	-0.87674700	0.73648300
C	1.07103200	1.66175000	0.69219300
C	0.75540400	2.22111900	1.96471900
C	-0.18392200	3.22213600	2.02837700
H	1.27782900	1.87948700	2.85314500
C	-0.58032200	3.17421900	-0.39041700
C	-0.83063900	3.70982700	0.84995000
H	-0.43204400	3.67062800	2.98600000
H	-1.07778400	3.54933900	-1.27929800
H	-1.54582500	4.52203800	0.94704300
Cl	-0.06741300	-1.98055800	-1.87015300
P	-2.29828000	0.04734300	-0.65117600
C	-3.26702800	-1.51637300	-0.62124500
H	-4.27769000	-1.29579800	-0.98105700
H	-2.79797700	-2.25883500	-1.26835900
H	-3.33031700	-1.90104200	0.39905500
C	-2.63097100	0.74216600	-2.32062500
H	-3.71306900	0.81343500	-2.47673500
H	-2.18546900	1.73613700	-2.40431200
H	-2.19307900	0.08291900	-3.07469600
C	-3.22320400	1.14330600	0.49917400
H	-2.93305200	2.18191700	0.34124400
H	-4.29364700	1.03180900	0.29370500
H	-3.02259700	0.87026700	1.53674800
Ir	-0.05172000	-0.14528300	-0.28744100

P	-0.33207200	-1.61202400	1.55828800
C	-1.57667600	-1.14248700	2.83774100
H	-2.58886000	-1.22086600	2.43338900
H	-1.48381600	-1.81227400	3.69961200
H	-1.39634200	-0.11236800	3.15952200
C	-0.71090400	-3.37770400	1.19163000
H	-0.79029200	-3.92725700	2.13604100
H	-1.64587000	-3.46794800	0.63610800
H	0.09758600	-3.79960400	0.58947700
C	1.21383700	-1.74256200	2.55563400
H	1.06252700	-2.46886700	3.36178500
H	2.03900800	-2.07209300	1.91945300
H	1.45880100	-0.76886400	2.98704400

8PR

E = -999.482909 a.u.

C	4.76056900	-0.71170500	0.17223700
C	4.18706100	0.45770400	-0.27277100
C	2.76730100	0.64154000	-0.23943500
C	1.88584100	-0.40102800	0.20327700
C	2.52661600	-1.56580400	0.67307600
C	3.90985600	-1.72249000	0.66245500
C	2.31652000	1.92329000	-0.60165000
C	-0.11166300	1.71427200	-0.02517600
C	1.02875100	2.47021600	-0.48242500
C	0.94449100	3.88144300	-0.72061200
H	1.82415600	4.39043200	-1.10637200
C	-0.19978000	4.58731500	-0.43294400
C	-1.28293300	3.88420600	0.13259500
C	-1.22541300	2.51029100	0.33240300
H	3.08971900	2.61569800	-0.93233800
H	5.83705900	-0.85219600	0.15400900
H	4.80495900	1.27104500	-0.64435600
H	1.92126600	-2.38941000	1.02672500
H	4.33983700	-2.65133800	1.03061500
H	-0.26004800	5.65732400	-0.60611400
H	-2.18666200	4.42127600	0.41107700
H	-2.09430500	2.04125700	0.76945100
Cl	-0.33145600	-2.84287100	0.15629800
P	-0.11584400	-0.09899800	2.46606800
P	0.13797900	-0.60518600	-2.29492300
C	0.06584800	0.92864800	-3.32170400
H	0.91623500	1.57342800	-3.09092600
H	0.10030900	0.65760800	-4.38237400
H	-0.85844900	1.47387800	-3.11380200
C	1.76687900	-1.34643200	-2.75677600
H	1.77955700	-1.51853000	-3.83813000
H	2.59286300	-0.68659000	-2.48863200
H	1.88609000	-2.29996500	-2.23591900

C	-0.98845800	-1.75629100	-3.20031300
H	-2.00715100	-1.37093100	-3.25264700
H	-0.60517300	-1.87143200	-4.21974300
H	-0.98456700	-2.72693900	-2.70026500
C	-1.44599600	0.77835400	3.40445800
H	-1.09439600	0.91511300	4.43261800
H	-1.64940800	1.75794100	2.96733300
H	-2.35996300	0.18525700	3.42228400
C	1.36947300	0.83740800	3.04606200
H	1.37174000	1.83105400	2.58829500
H	1.32915700	0.94229500	4.13529800
H	2.28520000	0.31351300	2.76724600
C	-0.00227000	-1.69672900	3.37524500
H	0.87807500	-2.25350400	3.04833100
H	0.07039700	-1.49285500	4.44915400
H	-0.89215100	-2.29770700	3.17220200
Ir	-0.16498000	-0.29471900	0.07553900
P	-2.63911900	-0.40430200	-0.21714500
C	-3.78023900	-0.02180400	1.19770900
H	-4.81220900	-0.10502700	0.83988400
H	-3.62380300	-0.75739700	1.99103600
H	-3.62841200	0.98042300	1.60034300
C	-3.34737500	0.69838600	-1.53494800
H	-4.42829600	0.53381500	-1.60175800
H	-3.16124300	1.74735600	-1.29476900
H	-2.89642600	0.48232900	-2.50552300
C	-3.36686200	-2.04798700	-0.66736100
H	-3.24532600	-2.73241500	0.17448800
H	-4.43359400	-1.90627800	-0.87402100
H	-2.88133700	-2.48587000	-1.53665900

9RE

E = -860.167326 a.u.

C	0.65642800	0.45500500	-1.79186500
C	0.15257200	1.63018200	-1.11188300
C	2.06044900	0.87617600	0.04563900
H	0.32189100	0.10040100	-2.75739500
C	1.93672800	0.11770000	-1.17323700
C	2.91609700	-0.83990900	-1.50952700
C	3.15616500	0.66807100	0.91536300
C	3.98880700	-1.00749400	-0.65362500
H	2.82090400	-1.42309400	-2.41931500
C	4.10799200	-0.26494000	0.55184200
H	3.24527900	1.23997700	1.83371900
H	4.76131700	-1.72951800	-0.90232600
H	4.96503400	-0.43977200	1.19523300
C	0.91652100	1.79011300	0.11364900
C	0.60095500	2.83437500	1.02845600
C	-0.41456800	3.69951600	0.70192900

H	1.17675500	2.94986000	1.94134300
C	-0.89139000	2.54904300	-1.41100200
C	-1.14455700	3.56535600	-0.52025200
H	-0.66513500	4.51430800	1.37456000
H	-1.44889100	2.45453700	-2.33653600
H	-1.92145600	4.29076000	-0.74325900
Cl	0.24365400	-2.69973400	-0.28209100
P	-2.31979700	-0.59767300	-0.22466400
C	-3.02634400	-2.15824600	0.42291100
H	-4.11433800	-2.11045900	0.30459100
H	-2.62908300	-3.01053100	-0.13026200
H	-2.77870600	-2.26361400	1.48295300
C	-2.75978000	-0.54660200	-2.00224500
H	-3.83871300	-0.71203900	-2.09657500
H	-2.50417100	0.42586900	-2.42857600
H	-2.22051600	-1.33709800	-2.53079400
C	-3.26837100	0.72253300	0.61944400
H	-2.89141700	1.70604700	0.33212300
H	-4.32614800	0.64033400	0.34689500
H	-3.15787200	0.59357200	1.70076400
Ir	-0.03912900	-0.33751000	0.14909600
C	-0.28709900	-0.61042400	2.00489600
O	-0.41632600	-0.74043200	3.14187500

9PR

E = -986.518858 a.u.

C	-3.26339900	3.07957300	-0.79146800
C	-1.93318900	3.39502500	-0.62086900
C	-0.95724600	2.37023300	-0.40166900
C	-1.32799400	0.98895700	-0.32818900
C	-2.69322000	0.71833400	-0.52439600
C	-3.63486100	1.72316300	-0.75014700
C	0.37352800	2.81427600	-0.30162900
C	1.61663300	0.64907400	0.00026100
C	1.56045100	2.07823700	-0.14137300
C	2.75746300	2.86661000	-0.14776400
H	2.65900100	3.94451500	-0.24366400
C	4.00138600	2.28827500	-0.04254000
C	4.06946200	0.88817100	0.07272300
C	2.91613000	0.10784600	0.09587900
H	0.50996500	3.89092100	-0.39006500
H	-4.00567900	3.85387100	-0.95889400
H	-1.60098600	4.42934300	-0.65710400
H	-3.03578300	-0.30767700	-0.48785200
H	-4.67755400	1.44841600	-0.89142500
H	4.90416000	2.89069000	-0.05215300
H	5.03720900	0.39918700	0.15134700
H	3.05311800	-0.96217800	0.19249900
Cl	-1.87335700	-2.31152300	0.29274400

P	0.13284600	-0.92444100	-2.27582600
P	-0.34990400	-0.09681700	2.42058900
C	0.62392800	1.31397000	3.08707300
H	0.34663800	2.23366500	2.56635000
H	0.40994300	1.42534200	4.15545500
H	1.69200800	1.12793700	2.94529600
C	-2.08986400	0.30920500	2.84963400
H	-2.17663000	0.39928200	3.93768800
H	-2.37575500	1.25426700	2.38163800
H	-2.74768500	-0.48584800	2.49061500
C	0.08159600	-1.50731300	3.51967800
H	1.15095300	-1.72376100	3.43576800
H	-0.15420300	-1.25251000	4.55827800
H	-0.49101500	-2.38986300	3.22089400
C	1.16480600	-2.37250600	-2.74650500
H	1.21392300	-2.45687000	-3.83719300
H	2.17560100	-2.25041500	-2.34561600
H	0.71940300	-3.28241800	-2.33279700
C	0.86499300	0.48868100	-3.19697100
H	1.90958700	0.62227200	-2.90404600
H	0.81128500	0.28735700	-4.27222500
H	0.30742900	1.40117900	-2.96864300
C	-1.48108300	-1.22478000	-3.09942300
H	-2.10896700	-0.33411600	-3.02023300
H	-1.30205000	-1.45266500	-4.15561600
H	-1.98597000	-2.06521500	-2.61777400
Ir	0.00142600	-0.57184400	0.09103600
C	1.04106800	-2.13789300	0.48791500
O	1.57646000	-3.12760300	0.72753700

10RE

E = -864.954990 a.u.

C	0.74115500	0.42196500	-1.76456300
C	0.18306400	1.57276800	-1.10946600
C	2.04458500	0.85209300	0.13896500
H	0.44771500	0.04619600	-2.73589900
C	1.99013800	0.08914200	-1.07700700
C	3.00198600	-0.84464300	-1.37063800
C	3.10820200	0.68692800	1.04513400
C	4.05295500	-0.97589100	-0.47572000
H	2.95862100	-1.43436700	-2.28019100
C	4.10614700	-0.21895800	0.72023000
H	3.14878400	1.26811400	1.96114200
H	4.85501700	-1.67554800	-0.69162900
H	4.94723100	-0.35367700	1.39400500
C	0.87363800	1.73692600	0.15471900
C	0.48508900	2.76402200	1.05116100
C	-0.52996600	3.61372000	0.66858500
H	1.00188200	2.89113700	1.99712100

C	-0.85761200	2.46729500	-1.47013600
C	-1.18486400	3.47610000	-0.59221000
H	-0.83493200	4.41921300	1.33001700
H	-1.34932600	2.36923800	-2.43230100
H	-1.95981900	4.18890700	-0.85848200
Cl	-0.08866800	-2.70333500	-0.82946600
P	-2.33655500	-0.54229500	0.01538200
C	-3.05855200	-2.07916600	0.70500400
H	-4.14931300	-1.98369500	0.66409700
H	-2.73639400	-2.93851600	0.11564500
H	-2.74613700	-2.20996600	1.74465900
C	-2.97791700	-0.40648600	-1.69428300
H	-4.06649400	-0.53039400	-1.66559800
H	-2.73276100	0.57099700	-2.11311900
H	-2.53494400	-1.19602500	-2.30653400
C	-3.06754300	0.81081600	1.00596100
H	-2.69967300	1.77933100	0.66366300
H	-4.15770200	0.77683300	0.89848300
H	-2.79903500	0.66571900	2.05677500
C	-0.07605500	-0.97744800	1.96585300
O	0.01432100	-1.27505600	3.06737700
Rh	-0.02574000	-0.45104500	0.09288400

10PR

E = -991.275389 a.u.

C	-3.21702700	2.94442400	-1.01563500
C	-1.91732200	3.29038500	-0.71830500
C	-0.93822400	2.28421700	-0.43174400
C	-1.28709600	0.89737600	-0.41793200
C	-2.61754800	0.58957100	-0.73961100
C	-3.55808300	1.57837100	-1.03295900
C	0.36992000	2.74558200	-0.21005100
C	1.59576200	0.58157500	0.13453400
C	1.54679400	2.00932000	0.02514000
C	2.74159300	2.79244400	0.12100800
H	2.65414900	3.87269300	0.04214600
C	3.97408300	2.20202000	0.29408200
C	4.03238700	0.80002500	0.37117900
C	2.87641300	0.02211200	0.29240200
H	0.50260200	3.82530300	-0.25827600
H	-3.96107500	3.70341100	-1.23640000
H	-1.61027400	4.33280600	-0.70466200
H	-2.93363700	-0.44633200	-0.74531100
H	-4.57698600	1.28391100	-1.27319900
H	4.87743700	2.79985400	0.36160000
H	4.99198300	0.30494100	0.49706000
H	3.00304000	-1.05142100	0.35554500
Cl	-1.83899800	-2.46529300	0.15520500
P	0.35411200	-0.93104100	-2.24868800

P	-0.56203400	-0.15574300	2.38304900
C	0.29566200	1.28608200	3.14174900
H	0.04291400	2.19932600	2.59711200
H	-0.02586100	1.38774700	4.18407800
H	1.37791200	1.13412700	3.10652400
C	-2.34756600	0.18345300	2.66576500
H	-2.53219300	0.26249200	3.74269600
H	-2.62870800	1.11986800	2.17805900
H	-2.94084400	-0.63316300	2.24751100
C	-0.17837800	-1.54936900	3.52494900
H	0.90034200	-1.73318900	3.53020900
H	-0.50589900	-1.29794700	4.53955300
H	-0.69838400	-2.44982000	3.18613400
C	1.55943600	-2.26955300	-2.63208100
H	1.73574100	-2.31589900	-3.71213300
H	2.50490500	-2.07003900	-2.11859100
H	1.15660400	-3.22768700	-2.28974500
C	1.02227700	0.54547200	-3.12088400
H	2.02396700	0.77580000	-2.74911700
H	1.07242300	0.33896400	-4.19539000
H	0.36692200	1.40251600	-2.94569600
C	-1.15040000	-1.38262800	-3.20236200
H	-1.86497100	-0.55618000	-3.17581700
H	-0.86832800	-1.58857100	-4.24066900
H	-1.60993200	-2.26778800	-2.75664600
C	0.99307200	-2.26955700	0.59767500
O	1.48391700	-3.26061400	0.88940200
Rh	-0.01595300	-0.63326700	0.09295100

TS1

E = -888.210716 a.u.

C	-0.85447400	-1.82308900	3.67252900
C	-1.82594300	-1.10790600	3.04487500
C	-1.77876500	-1.02188600	1.59580100
C	-0.43716300	-1.15806100	0.96979200
C	0.33402400	-2.25151700	1.56368800
C	0.17746700	-2.49105100	2.89427000
C	-2.81748800	-1.03642000	0.72405100
C	-0.98147500	-1.21432700	-0.86392900
C	-2.38754700	-1.30159500	-0.64155100
C	-3.23474000	-1.76902700	-1.64971400
H	-4.30535100	-1.82028100	-1.46676900
C	-2.70255600	-2.21428000	-2.86480500
C	-1.31901600	-2.21927400	-3.05867200
C	-0.46562900	-1.73324400	-2.05981500
H	-3.86249000	-0.95862500	1.00759700
H	-0.88838400	-1.98099300	4.74690800
H	-2.69306300	-0.72729800	3.57838300
H	0.84705300	-3.18311800	3.39860900

H	-3.36520400	-2.58248600	-3.64356200
H	-0.89687900	-2.58007900	-3.99268700
Cl	0.75627100	1.47798300	-2.26194700
P	2.51829600	-0.74109100	-0.26289100
P	-1.41799800	1.95728600	0.22455200
C	-2.21319000	2.22095800	1.87607400
H	-2.75211500	3.17495700	1.86493100
H	-2.91323000	1.41811500	2.10849000
H	-1.43693300	2.25542300	2.64617300
C	-0.80770400	3.66705400	-0.13393600
H	-1.66793600	4.34477900	-0.15759800
H	-0.11079200	3.98219900	0.64344800
H	-0.29608400	3.67499100	-1.09755600
C	-2.84739300	1.85817500	-0.94599800
H	-3.52901200	1.05162500	-0.67740900
H	-3.39243000	2.80798700	-0.91576300
H	-2.46901500	1.68872800	-1.95763100
C	3.43342100	-1.00873700	1.32400100
H	4.47312100	-1.27085700	1.09983400
H	3.40623400	-0.08541900	1.90686600
H	2.97646800	-1.81006800	1.90728600
C	3.70463900	0.31307000	-1.20454500
H	4.68523200	-0.17557000	-1.20953900
H	3.34461000	0.44448000	-2.22593800
H	3.77790700	1.29179600	-0.72698900
C	2.74976000	-2.36327800	-1.13983600
H	3.76794400	-2.71684200	-0.94276700
H	2.03931500	-3.12534600	-0.81178400
H	0.59400100	-1.70128100	-2.26027800
H	2.63751200	-2.21600700	-2.21791500
H	1.10135800	-2.76067100	0.99862200
Cl	1.74068600	2.03064800	1.08661100
Ir	0.35867600	0.33242600	0.00440500

IN1

E = -888.255643 a.u.

C	-1.85020900	-3.48644200	2.05051900
C	-2.76714000	-2.62838900	1.42894000
C	-2.35790700	-1.87403400	0.32233200
C	-1.00250800	-1.96781800	-0.14184900
C	-0.10363800	-2.84403500	0.48145400
C	-0.53475100	-3.60516700	1.57817000
C	-3.07406100	-0.96071300	-0.53948600
C	-0.82469200	-0.98977300	-1.23867800
C	-2.20326200	-0.46685300	-1.48836600
C	-2.45155700	0.31466400	-2.66584900
H	-3.40320500	0.82648800	-2.78460600
C	-1.52396100	0.31821300	-3.66921300
C	-0.32012900	-0.47570300	-3.57885400

C	-0.00992800	-1.15095900	-2.43841200
H	-4.12738300	-0.71760400	-0.44769000
H	-2.16650200	-4.07852400	2.90573600
H	-3.78669100	-2.55545500	1.80021200
H	0.15303100	-4.29794800	2.05539300
H	-1.71681400	0.87468200	-4.58360800
H	0.33348000	-0.53831200	-4.44539000
Cl	0.85190600	2.02600500	-1.32762900
P	2.59708900	-0.64457700	-0.19122500
P	-1.43663200	1.72406900	0.93089600
C	-2.41466500	1.04535400	2.34431200
H	-3.08256700	1.81764900	2.74245700
H	-3.00496700	0.18787600	2.01589700
H	-1.72676000	0.72151800	3.13175000
C	-0.81188800	3.32491500	1.62017600
H	-1.67247600	3.95677200	1.86449400
H	-0.21383900	3.14757800	2.51267500
H	-0.19156900	3.82438800	0.87155500
C	-2.72974000	2.39582200	-0.21202200
H	-3.47114600	1.64048200	-0.46260300
H	-3.22610300	3.22959700	0.29577200
H	-2.25632300	2.76235900	-1.12562500
C	3.26132200	-1.53949300	1.28729500
H	4.31665900	-1.78214500	1.12046400
H	3.16400800	-0.90304400	2.16823900
H	2.70331500	-2.46572700	1.45073800
C	3.82534700	0.70913400	-0.45664800
H	4.83735500	0.29103600	-0.42417500
H	3.64907000	1.16639300	-1.43311800
H	3.70761000	1.46734100	0.31871300
C	3.10680100	-1.80480000	-1.54851300
H	4.17369000	-2.02079900	-1.42103900
H	2.55228200	-2.74619500	-1.50447600
H	0.86163600	-1.78645100	-2.40182800
H	2.95792600	-1.33643700	-2.52497500
H	0.90160300	-2.96985500	0.09649700
Cl	1.63483100	1.34410400	2.12823200
Ir	0.37367100	0.29761800	0.19079700

TS2

E = -761.886436 a.u.

C	-1.10084800	4.00221500	0.11605100
C	-1.57922900	3.19807800	-0.87702400
C	-1.62439400	1.77275900	-0.64516700
C	-0.73962500	1.24796100	0.42520700
C	-0.50783700	2.10213300	1.56575200
C	-0.62722400	3.44855900	1.36949700
C	-2.48080200	0.84249900	-1.17900300
C	-1.50090600	-0.54766900	0.54350700

C	-2.57869300	-0.37318900	-0.37178400
C	-3.68177600	-1.22543000	-0.31605800
H	-4.48792800	-1.12234300	-1.03807200
C	-3.76529200	-2.17807400	0.71134800
C	-2.76393100	-2.26562000	1.68232700
C	-1.62304000	-1.45304200	1.59591700
H	-3.16068800	1.05317800	-1.99903900
H	-1.13017500	5.08230900	0.00398800
H	-2.04730100	3.60920400	-1.76760800
H	-0.33040900	4.13210400	2.16065400
H	-4.63064400	-2.83317300	0.76555600
H	-2.84920600	-2.98673600	2.49066200
Cl	0.30292100	-2.46988100	-1.29134300
P	1.97684800	-0.29810900	1.08715500
C	2.94596100	1.25433600	1.27294300
H	3.76416700	1.08974000	1.98262800
H	3.35040000	1.53759000	0.29844300
H	2.29811900	2.05564700	1.63776000
C	3.21318900	-1.57526200	0.62017800
H	4.00368500	-1.59233400	1.37875300
H	2.72223900	-2.54942900	0.56875900
H	3.63441800	-1.33396100	-0.35704300
C	1.54063800	-0.77859100	2.80996200
H	2.44370400	-0.67185100	3.42149100
H	0.75100300	-0.15072800	3.22577800
H	-0.82652800	-1.57841400	2.31657000
H	1.22562200	-1.82513500	2.82610000
H	-0.12209500	1.70416300	2.49631100
Cl	2.10867900	0.28696200	-2.10279500
Ir	0.33746200	-0.08920200	-0.45403400

IN2

E = -761.968156 a.u.

C	-1.381601	-1.862636	3.993591
C	-2.150361	-1.775065	2.856009
C	-1.657009	-1.124288	1.678298
C	-0.370506	-0.475482	1.673024
C	0.384492	-0.612355	2.860868
C	-0.095808	-1.281328	3.980430
C	-2.449756	-1.268965	0.522929
C	-0.921478	-0.265205	-1.180318
C	-2.135765	-0.942567	-0.809873
C	-3.031947	-1.450864	-1.806535
H	-3.956363	-1.921273	-1.479980
C	-2.718069	-1.377630	-3.143743
C	-1.494834	-0.777756	-3.515159
C	-0.635283	-0.240272	-2.565284
H	-3.386916	-1.805618	0.664213
H	-1.751197	-2.367776	4.881035

H	-3.141975	-2.220089	2.823860
H	0.526481	-1.337720	4.870745
H	-3.389081	-1.776875	-3.898498
H	-1.227359	-0.716104	-4.567617
Cl	0.580646	2.555217	-1.536968
P	2.002926	-0.519719	-0.295328
C	3.265753	-0.603002	1.039005
H	4.166022	-1.059245	0.613171
H	3.490302	0.402681	1.398429
H	2.909833	-1.220092	1.865626
C	2.966326	0.111312	-1.727278
H	3.825250	-0.552533	-1.876315
H	2.356681	0.129371	-2.631313
H	3.311223	1.123804	-1.506628
C	1.647486	-2.280785	-0.678103
H	2.594677	-2.814584	-0.811467
H	1.091413	-2.723101	0.153180
H	0.263620	0.253933	-2.909022
H	1.053424	-2.353738	-1.591715
H	1.351047	-0.133067	2.925792
Cl	1.354525	2.245553	1.798288
Ir	0.182781	0.712901	0.163889

7RE-C1-PM₃⁺

E = -887.496138 a.u.

C	2.325942	2.938942	-0.132423
C	1.389288	2.594370	-1.071192
C	0.165590	2.012115	-0.637973
C	-0.079380	1.721933	0.773969
C	0.888297	2.202071	1.730609
C	2.056874	2.773630	1.251310
C	-0.964368	1.569912	-1.420633
C	-1.397755	1.069641	0.833754
C	-1.960130	1.106562	-0.514788
C	-3.275062	0.620508	-0.763987
C	-4.012247	0.144513	0.287928
C	-3.474883	0.098582	1.612689
C	-2.208601	0.544956	1.890022
H	-1.072466	1.685215	-2.490210
H	3.271394	3.380037	-0.431576
H	1.552611	2.763249	-2.130080
H	2.806676	3.136059	1.943412
H	-5.021878	-0.219070	0.119121
H	-4.084624	-0.307393	2.414307
Cl	-1.222321	-2.180900	-1.151241
P	1.188472	-1.651956	0.955793
C	2.703473	-0.889774	1.671276
H	3.193659	-1.598160	2.348024
H	3.385065	-0.638026	0.852805

H	2.458774	0.025243	2.212334
C	1.829639	-3.195885	0.186781
H	2.337652	-3.792632	0.952155
H	0.997343	-3.762615	-0.235350
H	2.528867	-2.941798	-0.612182
C	0.206783	-2.276807	2.382116
H	0.838078	-2.866534	3.055698
H	-0.239772	-1.446668	2.930137
H	-1.840685	0.484567	2.903715
H	-0.598239	-2.906588	1.991604
Cl	1.627221	-0.687054	-2.184948
Ir	-0.006718	-0.227795	-0.455283
H	-3.667342	0.639325	-1.775488
P	0.616955	2.350721	3.529828
C	-0.913720	3.294094	3.827743
H	-1.772498	2.807216	3.362278
H	-1.072118	3.365071	4.908335
H	-0.787193	4.295206	3.404970
C	0.562770	0.773031	4.445770
H	1.459999	0.189083	4.229618
H	0.540821	1.025406	5.511155
H	-0.326953	0.193777	4.204460
C	1.982260	3.299902	4.274813
H	2.926542	2.758101	4.175460
H	2.058506	4.289645	3.818542
H	1.741277	3.409044	5.337038

7PR-C1-PMe₃⁺

E = -1013.837943 a.u.

C	2.20133100	-3.24129500	-1.76259800
C	0.86619600	-3.09685300	-2.04164100
C	0.14516300	-1.95691200	-1.57950700
C	0.74506100	-0.90692900	-0.77337600
C	2.18593500	-0.98205800	-0.75701400
C	2.84808400	-2.15161300	-1.16900900
C	-1.19671300	-1.93708300	-2.01269200
C	-2.11314600	-0.08089300	-0.64445500
C	-2.24351900	-1.08190900	-1.66496300
C	-3.49070100	-1.32575300	-2.33370900
H	-3.52296600	-2.10002500	-3.09606200
C	-4.61828400	-0.61518800	-2.00701800
C	-4.51483000	0.35252100	-0.98334100
C	-3.31341000	0.60486600	-0.33542900
H	-1.45299300	-2.71477000	-2.72971300
H	2.76083700	-4.12605300	-2.04721300
H	0.33156500	-3.85925800	-2.60150800
H	3.92176500	-2.24244900	-1.04274100
H	-5.56494400	-0.79767000	-2.50652000
H	-5.39795500	0.91588400	-0.68998800

H	-3.29884000	1.35452700	0.44211900
Cl	-1.60168600	1.79717200	2.03386100
Cl	1.49421700	0.57665900	2.03250000
P	-0.18568200	2.27885900	-0.90705000
P	-0.81803700	-1.62007700	1.79172000
C	-2.25783300	-2.67862700	1.33282500
H	-2.09326800	-3.14110600	0.35693000
H	-2.38019200	-3.46512900	2.08548500
H	-3.16509200	-2.06954100	1.29175800
C	0.57142400	-2.83061400	1.88419000
H	0.32343600	-3.61593900	2.60637900
H	0.73970300	-3.28403800	0.90391800
H	1.47857800	-2.31256000	2.20211500
C	-1.16183300	-1.20586400	3.55035300
H	-2.08804100	-0.63078500	3.61250600
H	-1.25893800	-2.13431700	4.12359500
H	-0.34346500	-0.60219200	3.94691300
C	-1.75899400	3.01734200	-1.53749400
H	-1.50144100	3.94272500	-2.06533000
H	-2.26124100	2.33666800	-2.22706300
H	-2.42579700	3.25193100	-0.70556900
C	0.70152300	2.06221300	-2.51822700
H	0.05429300	1.45711500	-3.16202100
H	0.87361600	3.03283100	-2.99538000
H	1.64800700	1.53363300	-2.40679200
C	0.53936000	3.74614100	-0.02702300
H	0.91397700	3.45448100	0.95409200
H	1.33872000	4.20168900	-0.61783600
H	-0.25725100	4.48108500	0.11789800
Ir	-0.41138800	0.27597200	0.37307000
P	3.51903700	0.24385100	-0.32089000
C	4.62452400	0.23051500	-1.79679900
H	4.04009300	0.49057400	-2.68463900
H	5.39774800	0.98925200	-1.64028200
H	5.10535000	-0.73644800	-1.95054900
C	3.28933300	2.04354300	-0.12204500
H	3.02569900	2.49500900	-1.07782400
H	2.57691200	2.28101600	0.65626500
H	4.28091200	2.40691700	0.17064900
C	4.55997900	-0.37643300	1.05264300
H	4.92673300	-1.37811300	0.81245700
H	5.41234200	0.30321200	1.15359800
H	3.98429100	-0.39735800	1.97708600

7RE-C2-PMe₃⁺

E = -887.505118 a.u.

C	-0.746762	3.299331	-0.084214
C	-1.281704	2.501516	-1.062700
C	-1.696719	1.178650	-0.727792

C	-1.532487	0.708854	0.636766
C	-0.984388	1.560244	1.630568
C	-0.590932	2.829612	1.263664
C	-2.228714	0.098012	-1.521939
C	-2.052486	-0.652393	0.701116
C	-2.548147	-0.982179	-0.622839
C	-3.158362	-2.248821	-0.841395
H	-3.511318	-2.515531	-1.832011
C	-3.297219	-3.103773	0.225668
C	-2.833752	-2.764402	1.535630
C	-2.220948	-1.560364	1.783566
H	-2.480554	0.146927	-2.572117
H	-0.429487	4.306883	-0.336363
H	-1.393750	2.862464	-2.079385
H	-3.772757	-4.069327	0.077454
H	-2.972570	-3.477525	2.342866
Cl	0.164444	-2.663660	-1.850832
P	1.614867	-1.020119	0.641679
C	2.429328	0.509657	1.269246
H	3.286404	0.246901	1.899017
H	2.768784	1.104596	0.416988
H	1.716752	1.098006	1.851338
C	2.993878	-1.952107	-0.141366
H	3.842467	-1.992919	0.549798
H	2.660976	-2.963980	-0.380505
H	3.289155	-1.447742	-1.064421
C	1.235253	-1.983382	2.165273
H	2.159916	-2.193869	2.714209
H	0.555166	-1.414050	2.805085
H	-1.874142	-1.294628	2.776974
H	0.754010	-2.925521	1.886642
H	-0.887677	1.197772	2.647911
Cl	1.306272	0.483153	-2.249584
Ir	-0.236070	-0.578449	-0.718532
P	0.192949	3.929243	2.474969
C	-0.748717	5.484185	2.583318
H	-0.263036	6.141272	3.311424
H	-0.763867	5.970420	1.604006
H	-1.771539	5.263864	2.902667
C	1.894089	4.309925	1.945580
H	2.335942	5.006902	2.664783
H	2.479598	3.387482	1.911519
H	1.873746	4.769279	0.953432
C	0.239796	3.145376	4.115098
H	-0.778219	2.942428	4.459343
H	0.818258	2.218830	4.075748
H	0.723402	3.845135	4.803849

7PR-C2-PM₃⁺

E = -1013.867285 a.u.

C	-3.11549000	2.22046400	-1.00472500
C	-1.85973700	2.72209000	-1.25869100
C	-0.68304700	1.95901600	-0.98447000
C	-0.75347500	0.67171100	-0.35591100
C	-2.06945000	0.17187800	-0.16874700
C	-3.20504500	0.91219300	-0.47606700
C	0.53114800	2.50463000	-1.45690700
C	2.07459800	0.61706500	-0.89685200
C	1.79609000	1.91202400	-1.47851300
C	2.81181300	2.65114200	-2.17962500
H	2.55345900	3.63155400	-2.57231600
C	4.06601800	2.13056800	-2.36610300
C	4.33457000	0.83880400	-1.85331200
C	3.37765600	0.11864600	-1.15528200
H	0.45396200	3.47909800	-1.93655600
H	-4.00167400	2.80555300	-1.22404200
H	-1.74860700	3.70949000	-1.69958400
H	4.83307000	2.68493000	-2.89835400
H	5.32093500	0.40313000	-1.99695900
H	3.64918100	-0.84855900	-0.75727000
Cl	2.66290300	-1.84755500	1.25070600
Cl	-0.64910200	-1.60019600	2.01163900
P	0.47502300	-2.09240800	-1.33106400
P	1.15993100	1.16024400	2.08795700
C	2.35178600	2.53429000	1.77567600
H	1.97183000	3.19977900	0.99763200
H	2.49913100	3.10567500	2.69860500
H	3.30902500	2.11615400	1.45049400
C	-0.37356700	2.02925500	2.63277800
H	-0.14961400	2.67273600	3.49051300
H	-0.76980900	2.63834600	1.81607900
H	-1.11911000	1.28282100	2.91886000
C	1.80083400	0.40626100	3.63816200
H	2.80882900	0.02447900	3.46434000
H	1.81862200	1.16582700	4.42734800
H	1.15301500	-0.42375300	3.92698100
C	1.98325700	-2.68692200	-2.20735100
H	1.70860700	-3.52506500	-2.85679100
H	2.40626100	-1.88297100	-2.81440500
H	2.72445400	-3.01703900	-1.47598300
C	-0.64138100	-1.63652200	-2.72998100
H	-0.24747000	-0.74742400	-3.23224700
H	-0.69595000	-2.46330600	-3.44654500
H	-1.64421300	-1.41523500	-2.35603400
C	-0.25667300	-3.64769400	-0.67343900
H	-1.23124800	-3.44462300	-0.22513100
H	-0.36322900	-4.37165500	-1.48882800
H	0.40233000	-4.05322400	0.09831000

Ir	0.81348100	-0.37780700	0.29117300
H	-2.18300000	-0.81483000	0.26315900
P	-4.82125600	0.12449200	-0.17854200
C	-4.87629100	-1.44500500	-1.10020600
H	-4.76232900	-1.23911200	-2.16840800
H	-4.06450300	-2.09156000	-0.75620000
H	-5.83760100	-1.93347800	-0.91434200
C	-5.01155900	-0.21768300	1.59909500
H	-4.20307500	-0.87381600	1.93225200
H	-4.97193400	0.72584200	2.15132400
H	-5.97741800	-0.70625400	1.76257900
C	-6.17597800	1.20107800	-0.73466400
H	-6.07552900	1.40410100	-1.80448300
H	-7.11966300	0.67896300	-0.54834100
H	-6.16134200	2.13765100	-0.17032100

7RE-C3-PMe₃⁺

E = -887.505128 a.u.

C	-2.814224	-0.820437	0.272619
C	-1.978538	-1.155059	-0.771830
C	-0.623775	-1.477202	-0.481384
C	-0.140583	-1.373079	0.884478
C	-1.041843	-1.056739	1.939093
C	-2.353381	-0.797095	1.631149
C	0.480783	-1.876109	-1.335524
C	1.276724	-1.702839	0.864198
C	1.606481	-2.123268	-0.494081
C	2.925464	-2.580043	-0.782776
C	3.831971	-2.648043	0.243393
C	3.498931	-2.265203	1.586295
C	2.248623	-1.805279	1.906292
H	0.424722	-2.053973	-2.400553
H	-2.320118	-1.185699	-1.799940
H	-3.049764	-0.550526	2.427435
Cl	3.123933	0.878542	-1.089440
P	0.816477	1.987514	0.994031
C	-0.916873	2.561877	1.231003
H	-0.945862	3.376534	1.962992
H	-1.299505	2.917794	0.270606
H	-1.539000	1.735144	1.581806
C	1.705846	3.507571	0.466702
H	1.459808	4.325010	1.153133
H	2.782346	3.326542	0.475847
H	1.396867	3.769359	-0.548350
C	1.445353	1.656133	2.691947
H	1.368802	2.559905	3.306675
H	0.862554	0.853153	3.150662
H	1.990254	-1.522330	2.921462
H	2.492920	1.347013	2.628245

H	-0.691900	-1.026053	2.965585
Cl	-0.010719	1.528784	-2.187805
Ir	0.941501	0.144712	-0.423535
H	3.189587	-2.863882	-1.796264
H	4.839760	-3.000841	0.042271
H	4.261344	-2.344164	2.355626
P	-4.536422	-0.345608	-0.048515
C	-5.659793	-1.538661	0.745413
H	-5.457181	-1.572443	1.819756
H	-6.693120	-1.220274	0.576018
H	-5.497239	-2.527915	0.307457
C	-4.820357	1.307451	0.661249
H	-5.863170	1.593066	0.491539
H	-4.617088	1.282008	1.735724
H	-4.153431	2.024238	0.173759
C	-4.863269	-0.302481	-1.834766
H	-4.190271	0.411000	-2.317994
H	-4.729099	-1.299318	-2.263518
H	-5.899949	0.018139	-1.976972

7PR-C3-PMe₃⁺

E = -1013.865779 a.u.

C	-3.68241900	-0.04560500	-0.11612700
C	-2.91772400	1.09306400	-0.28291000
C	-1.49340400	1.02433800	-0.29893300
C	-0.79912000	-0.21343000	-0.06821500
C	-1.63508000	-1.35949800	0.02822200
C	-3.01545200	-1.29042700	0.01505700
C	-0.82860100	2.21953100	-0.64955200
C	1.51044800	1.35279200	-0.77262300
C	0.52994600	2.40422400	-0.92168900
C	0.88947800	3.69276700	-1.44793100
H	0.12015800	4.45913400	-1.50338200
C	2.16197400	3.94530500	-1.89255600
C	3.11314300	2.89944500	-1.82460600
C	2.79501000	1.65960600	-1.29113500
H	-1.47007300	3.08408200	-0.81537900
H	-3.38293800	2.06506900	-0.42654400
H	2.43481000	4.91533800	-2.29699700
H	4.12480600	3.07499800	-2.18374700
H	3.57265900	0.91197100	-1.22272000
Cl	3.65156900	-0.72780000	0.63528000
Cl	0.88636600	-2.50368000	1.56148800
P	1.36187500	-1.59492900	-1.85214600
P	1.04704500	0.71504700	2.31261800
C	1.40052300	2.52694400	2.33289700
H	0.62904700	3.07267300	1.78541700
H	1.42847800	2.88279700	3.36853300
H	2.36983900	2.70970800	1.85934300

C	-0.60513500	0.58035400	3.12352900
H	-0.56929200	1.03714300	4.11856000
H	-1.36379100	1.08524200	2.52007100
H	-0.86690800	-0.47718500	3.21597100
C	2.19855500	0.06173700	3.59041000
H	3.22670000	0.27608800	3.29289700
H	1.97732400	0.54043000	4.55071000
H	2.07041900	-1.01972600	3.66731800
C	3.00635800	-1.56291100	-2.68090200
H	2.96905200	-2.19734900	-3.57312800
H	3.25743400	-0.54096400	-2.97506900
H	3.76806800	-1.93277600	-1.99137000
C	0.21994400	-0.99363700	-3.17170500
H	0.41281700	0.06760800	-3.35628600
H	0.37873100	-1.55711400	-4.09758900
H	-0.81676600	-1.11549800	-2.84619100
C	0.99599700	-3.39586900	-1.73785700
H	-0.01616100	-3.55281400	-1.35802400
H	1.08986900	-3.84617900	-2.73221600
H	1.70468900	-3.86376700	-1.05050600
Ir	1.16867300	-0.36744200	0.18177700
H	-1.17402300	-2.32710200	0.16979000
H	-3.58634400	-2.20758100	0.12622500
P	-5.49249800	0.05198900	-0.13718600
C	-6.08803600	0.16640000	-1.85603700
H	-7.18076500	0.22930300	-1.85405800
H	-5.66462500	1.06066000	-2.32298300
H	-5.76737400	-0.72301200	-2.40659100
C	-6.20992700	-1.42672800	0.64109400
H	-7.29781200	-1.30914700	0.65258700
H	-5.94837300	-2.31886300	0.06528100
H	-5.83736800	-1.51947500	1.66516600
C	-6.04490900	1.53125600	0.76902800
H	-5.69621900	1.47333000	1.80393600
H	-5.64582700	2.42975900	0.29009700
H	-7.13874600	1.56187200	0.74494200

7RE-C4-PMe₃⁺

E = -887.507015 a.u.

C	2.508659	-0.833314	1.951781
C	2.445161	-0.047427	0.816781
C	1.265623	0.735961	0.590341
C	0.194652	0.688183	1.576309
C	0.313920	-0.123126	2.737945
C	1.450958	-0.876195	2.904213
C	0.861944	1.624061	-0.477259
C	-0.833643	1.630562	1.149609
C	-0.370088	2.248656	-0.078208
C	-1.163705	3.251850	-0.701844

C	-2.330340	3.638470	-0.088747
C	-2.770263	3.053667	1.141112
C	-2.043754	2.067556	1.761205
H	1.447209	1.895720	-1.343860
H	3.390482	-1.432628	2.151709
H	1.563872	-1.508716	3.778812
Cl	-2.045839	0.272893	-2.310644
P	-2.086540	-1.715215	0.406372
C	-1.202416	-3.117154	1.208771
H	-1.927649	-3.799930	1.664732
H	-0.617192	-3.650194	0.455709
H	-0.526162	-2.735699	1.978194
C	-3.180197	-2.535775	-0.822844
H	-3.724023	-3.349750	-0.330905
H	-3.887175	-1.809972	-1.230298
H	-2.571847	-2.936653	-1.637282
C	-3.240558	-1.120357	1.712391
H	-3.894657	-1.939004	2.032255
H	-2.663925	-0.760443	2.569348
H	-3.847661	-0.300734	1.317978
H	-0.482431	-0.131420	3.475537
Cl	0.458869	-1.834421	-1.619033
Ir	-0.637712	-0.059560	-0.388542
H	-0.836389	3.698873	-1.634737
H	-2.942243	4.411783	-0.544770
H	-3.697519	3.402888	1.585556
H	-2.370721	1.629868	2.697992
P	3.894078	0.115490	-0.268137
C	4.468506	1.845522	-0.218523
H	5.367179	1.929502	-0.837546
H	3.692945	2.508394	-0.609496
H	4.700586	2.117374	0.815130
C	5.237878	-0.947736	0.342209
H	4.918451	-1.993435	0.335777
H	6.086478	-0.823894	-0.337999
H	5.532204	-0.645820	1.350852
C	3.556989	-0.341343	-1.996680
H	3.303605	-1.401637	-2.046533
H	2.731507	0.246344	-2.400049
H	4.470325	-0.143067	-2.567840

7PR-C4-PMe₃⁺

E = -1013.858098 a.u.

C	0.00739400	4.43009200	-0.76861400
C	1.00030900	3.49313700	-0.63217600
C	0.68910000	2.10558200	-0.43111200
C	-0.67535600	1.65563700	-0.31674400
C	-1.65875500	2.66255300	-0.49228400
C	-1.33735700	3.99431300	-0.70612000

C	1.79133200	1.23815100	-0.41655300
C	0.58824400	-0.92012900	-0.44084200
C	1.81638200	-0.16814000	-0.42442800
C	3.09064400	-0.84923900	-0.55456200
C	3.12889300	-2.19315400	-0.86084800
C	1.91623500	-2.89376100	-1.06002100
C	0.70043900	-2.28030600	-0.85127600
H	2.74226900	1.74876200	-0.51487700
H	0.24205600	5.47859200	-0.92572000
H	2.04678000	3.78338200	-0.68763800
H	-2.13923800	4.72145600	-0.81282400
Cl	-1.87387700	-2.54636400	0.93850500
P	-2.12160300	-0.55710100	-2.01338700
P	-0.37698800	0.01012800	2.39856700
C	0.22458900	1.68430000	2.89214100
H	0.46386300	1.68526200	3.96116000
H	1.11631200	1.95504100	2.32294500
H	-0.55984400	2.42101800	2.69485200
C	-1.61161100	-0.37605700	3.70670200
H	-1.11563400	-0.35660300	4.68321000
H	-2.41181300	0.36583800	3.67812100
H	-2.03655300	-1.36371600	3.51769100
C	1.03678500	-1.10289200	2.81118500
H	1.91251500	-0.83998700	2.21311100
H	1.28244800	-1.01122400	3.87472200
H	0.74960400	-2.13424700	2.58945600
C	-3.47330000	0.59447500	-2.50505200
H	-3.88281800	0.26834700	-3.46717400
H	-4.25660700	0.58404600	-1.74412100
H	-3.08275500	1.60971200	-2.60686900
C	-2.87458000	-2.21200400	-2.29891600
H	-3.25874100	-2.25935800	-3.32387400
H	-2.13259400	-2.99889100	-2.14768200
H	-3.69180400	-2.36048900	-1.58893100
C	-0.90780600	-0.36832800	-3.39114000
H	-1.41442000	-0.47693100	-4.35623500
H	-0.45097000	0.62442500	-3.33097900
H	-0.12433200	-1.12610800	-3.30732700
H	-2.70123300	2.38770600	-0.41340800
Cl	-3.46224500	0.47729600	1.00475800
Ir	-1.17047200	-0.21758400	0.14869000
H	-0.20153200	-2.86767100	-0.95226600
H	1.95366800	-3.94131200	-1.34682500
H	4.06354800	-2.73087900	-0.96355300
P	4.69809700	-0.02939400	-0.24672600
C	6.02021700	-1.28158300	-0.20687900
H	6.13613500	-1.74559600	-1.18961400
H	6.94538100	-0.75916800	0.05538000
H	5.80340900	-2.03960600	0.54975700

C	4.69693600	0.78552800	1.38497400
H	3.91504900	1.54413100	1.45395800
H	4.53995500	0.02251300	2.15323300
H	5.67464000	1.25613700	1.53068900
C	5.15479000	1.16161900	-1.55549300
H	5.06215800	0.66407200	-2.52541600
H	4.52151100	2.05063500	-1.53624800
H	6.19630000	1.45558000	-1.38977600

7RE-C5-PMe₃⁺

E = -887.513050 a.u.

C	2.347797	3.102079	-0.225818
C	1.454957	2.698002	-1.192229
C	0.242771	2.068396	-0.790286
C	0.010187	1.848230	0.622292
C	0.951998	2.279825	1.592965
C	2.098801	2.903588	1.162733
C	-0.915306	1.533579	-1.526608
C	-1.296561	1.224793	0.774405
C	-1.908704	1.149941	-0.537394
C	-3.248636	0.688592	-0.649929
C	-3.922434	0.339179	0.496418
C	-3.319688	0.415689	1.789146
C	-2.030481	0.860592	1.939573
H	3.269944	3.589193	-0.529103
H	1.673225	2.869443	-2.236724
H	2.831652	3.248974	1.885840
Cl	-1.220932	-2.161034	-1.005270
P	1.207966	-1.417795	1.118312
C	2.943742	-0.832578	1.288066
H	3.433984	-1.357081	2.115489
H	3.478239	-1.034113	0.356111
H	2.955880	0.243439	1.478627
C	1.380753	-3.220918	0.807640
H	2.063185	-3.646258	1.551506
H	0.404723	-3.704580	0.880021
H	1.783761	-3.377839	-0.195974
C	0.511948	-1.306939	2.817271
H	1.110260	-1.916900	3.502966
H	0.527166	-0.265488	3.149717
H	-0.519873	-1.669530	2.811945
H	0.748009	2.125576	2.647661
Cl	1.699780	-0.801859	-2.084008
Ir	0.020639	-0.183727	-0.462766
H	-3.736884	0.630488	-1.615941
H	-4.950579	-0.003590	0.421703
H	-3.900663	0.126164	2.659472
H	-1.568347	0.944250	2.917318
P	-1.225958	1.553875	-3.299612

C	-1.735948	-0.091433	-3.885065
H	-2.617843	-0.440703	-3.346775
H	-1.960900	-0.005167	-4.953067
H	-0.912562	-0.791376	-3.727029
C	-2.549660	2.755463	-3.658703
H	-2.237235	3.745245	-3.312860
H	-2.730984	2.778452	-4.737745
H	-3.462567	2.454857	-3.136683
C	0.255054	2.021520	-4.243271
H	0.502930	3.071230	-4.072633
H	1.087581	1.370106	-3.967184
H	0.013614	1.876831	-5.301306

7PR-C5-PMe₃⁺

E = -1013.833801 a.u.

C	1.75337600	3.88674500	-0.00499100
C	2.31341500	2.65921100	-0.24925800
C	1.54624700	1.44762800	-0.17388300
C	0.13692300	1.50066800	0.14094400
C	-0.37015500	2.79423000	0.44421400
C	0.39436000	3.94424800	0.37955600
C	2.19860700	0.23316800	-0.52266300
C	0.12168900	-1.08016700	-1.01289600
C	1.55829700	-0.89639800	-1.09077900
C	2.34942700	-1.80383700	-1.87909900
C	1.77976800	-2.80555300	-2.61998800
C	0.37456400	-2.96406700	-2.58427900
C	-0.40926700	-2.12739400	-1.81409100
H	2.34019300	4.79392100	-0.11212900
H	3.33994600	2.62084500	-0.59196300
H	-0.05948600	4.90328300	0.61751600
Cl	-2.69685900	-2.04306600	0.39151000
P	-2.30107400	0.81128900	-1.66395300
P	-0.10581800	-1.06944600	2.14841700
C	1.20218800	-0.09249000	3.00919800
H	1.46928600	-0.59128200	3.94731300
H	2.09396400	-0.00866000	2.38805100
H	0.82053300	0.90972900	3.22522600
C	-1.27962700	-1.43825100	3.51632200
H	-0.75349800	-2.00976000	4.28891800
H	-1.65477900	-0.50194100	3.93324500
H	-2.11895400	-2.01487900	3.12395900
C	0.68809100	-2.70354900	1.82690800
H	1.50472600	-2.60038500	1.10965600
H	1.07556400	-3.11839000	2.76381800
H	-0.06418300	-3.37972700	1.41175300
C	-3.24277800	2.36962700	-1.38255300
H	-3.81083200	2.60192700	-2.28990400
H	-3.92431700	2.23686500	-0.53982700

H	-2.56040800	3.19435200	-1.16691800
C	-3.58765100	-0.29152000	-2.38448000
H	-4.04653200	0.21714400	-3.23954900
H	-3.14982100	-1.23508300	-2.71539300
H	-4.34630500	-0.50092300	-1.62699200
C	-1.21424300	1.23240100	-3.09523200
H	-1.80969900	1.66013500	-3.90894000
H	-0.46510700	1.96152700	-2.77223400
H	-0.70633000	0.33212100	-3.45163300
H	-1.40387300	2.87568400	0.74874800
Cl	-2.70869300	1.07396300	1.79524900
Ir	-1.08147600	-0.07515300	0.20253700
H	-1.47500800	-2.30270300	-1.78482200
H	-0.09375400	-3.75572600	-3.16384500
H	3.41587800	-1.65282500	-1.97376800
H	2.39547300	-3.44869700	-3.24121100
P	4.02613500	0.08407600	-0.11133800
C	4.28091700	-1.55626000	0.65427700
H	4.06990900	-2.38238600	-0.02257200
H	5.32657900	-1.59827400	0.97525000
H	3.62902100	-1.61858800	1.53193400
C	4.54393500	1.24246500	1.21282000
H	5.35726200	0.74091700	1.74627000
H	4.91699500	2.17659500	0.79182800
H	3.72574800	1.44303700	1.90568800
C	5.14700700	0.37811300	-1.52132500
H	6.17080100	0.36125300	-1.13330000
H	5.03463000	-0.37769500	-2.30032900
H	4.92523600	1.36722200	-1.93330900

7RE-C28-PMe₃⁺

E = -1013.047631 a.u.

C	3.41258000	0.17240200	-1.54971900
C	2.49863900	-0.62743200	-2.19451500
C	1.11049400	-0.38566300	-2.00027500
C	0.69846300	0.66429900	-1.08762900
C	1.65787800	1.48195300	-0.44412400
C	2.99642000	1.23352100	-0.68335900
C	-0.07423500	-1.02728900	-2.53362400
C	-0.75990100	0.66568100	-1.06626300
C	-1.20883300	-0.31258900	-2.05070500
C	-2.60640300	-0.46745700	-2.28737700
C	-3.48754500	0.31410700	-1.58947700
C	-3.04148900	1.27950600	-0.62021700
C	-1.70070400	1.46803800	-0.36675300
H	-0.08571600	-1.83826100	-3.24859700
H	4.47071900	-0.01288400	-1.70051300
H	2.82383700	-1.42657400	-2.85196400
Cl	-2.03528600	-2.52168700	0.40890000

P	0.41263600	-1.00744500	1.99006400
C	2.22431700	-0.93220600	2.30079000
H	2.41261100	-0.63186200	3.33700700
H	2.65171600	-1.92203200	2.12131000
H	2.68860100	-0.21765800	1.61878100
C	-0.18164800	-2.28182600	3.17265700
H	0.24968200	-2.07831300	4.15877100
H	-1.27132300	-2.25726200	3.23149000
H	0.13524600	-3.26841200	2.82630700
C	-0.24947300	0.57763000	2.65338200
H	-0.01172000	0.66603600	3.71924300
H	0.19481100	1.41593200	2.10981200
H	-1.34930600	2.19590300	0.35646300
H	-1.33471300	0.59392700	2.52041200
H	1.32565200	2.28000500	0.21230900
Cl	1.21037400	-3.37009000	-0.11935900
Ir	-0.07476800	-1.32616500	-0.25451400
H	-2.95632300	-1.20215100	-3.00442300
H	-4.55045400	0.18916700	-1.76608200
P	4.24298600	2.30617600	0.10415100
C	5.87985400	1.52122300	0.04256000
H	6.19712700	1.40566100	-0.99722000
H	6.58555600	2.17404700	0.56552500
H	5.84278800	0.54664600	0.53714200
C	4.30817100	3.89768900	-0.77856900
H	3.33955100	4.39779300	-0.68956900
H	5.08917300	4.51973800	-0.32983200
H	4.53579700	3.71617500	-1.83288100
C	3.79061300	2.61535800	1.84024500
H	3.81630200	1.67705000	2.39988500
H	4.51517400	3.31893100	2.26170500
H	2.79019300	3.05365400	1.89037900
P	-4.24378900	2.29093300	0.29450000
C	-4.18472500	4.00739200	-0.31169200
H	-4.90605700	4.60864400	0.25082900
H	-3.17767400	4.41026500	-0.17161300
H	-4.44059800	4.01897300	-1.37528400
C	-3.81933200	2.27307000	2.06482200
H	-4.54532000	2.89096900	2.60256600
H	-3.85849300	1.24499500	2.43478100
H	-2.81582200	2.68501900	2.20304600
C	-5.92510800	1.64528300	0.05764800
H	-6.60972700	2.26808800	0.64173600
H	-6.19648200	1.70124600	-1.00030100
H	-5.97982000	0.61038400	0.40661200

7PR-C28-PMe₃⁺

E = -1139.414739 a.u.

C	3.68715100	-2.17255800	-1.42604400
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C	2.41604800	-2.68109700	-1.49372100
C	1.28454900	-1.93550400	-1.02305700
C	1.44103700	-0.64280100	-0.40986300
C	2.77341400	-0.14082100	-0.41020700
C	3.85060100	-0.87045100	-0.88651500
C	0.03011700	-2.52836600	-1.24549700
C	-1.42039900	-0.67848400	-0.41269000
C	-1.23945200	-1.97340600	-1.01172300
C	-2.35448500	-2.73930300	-1.48406700
H	-2.16557400	-3.72656400	-1.89686700
C	-3.63476500	-2.24409300	-1.44106400
C	-3.81672700	-0.93664600	-0.92866900
C	-2.75191900	-0.18615500	-0.45199100
H	0.04204800	-3.50624300	-1.72454600
H	4.53808100	-2.74383300	-1.78328300
H	2.24422000	-3.66549900	-1.92056300
H	-4.47028700	-2.83432500	-1.80068000
Cl	-1.74031000	1.65960500	1.87526500
P	-0.01918900	2.08737900	-1.17427300
P	-0.03879200	-1.11083600	2.36966000
C	1.16788700	-2.50575200	2.31713600
H	1.11568400	-3.06856800	3.25544700
H	0.93919600	-3.17434200	1.48427500
H	2.17810500	-2.10570700	2.18855000
C	0.30471300	-0.31956900	3.99303800
H	0.16940900	-1.06191700	4.78733400
H	1.32898100	0.05806000	4.00384000
H	-0.38268700	0.51628900	4.13646800
C	-1.66762900	-1.93758200	2.61887000
H	-1.89552900	-2.58353700	1.76674600
H	-1.64033200	-2.53911000	3.53358300
H	-2.44109200	-1.17022800	2.70698900
C	1.63408500	2.55640300	-1.84198700
H	1.50929100	3.37218900	-2.56208300
H	2.27452600	2.88873800	-1.02184600
H	2.09305500	1.69983400	-2.34203600
C	-0.72249700	3.69727000	-0.63261800
H	-0.63166800	4.42304200	-1.44820800
H	-1.77205600	3.57296600	-0.35907200
H	-0.17249100	4.04923500	0.24338100
C	-0.97066000	1.67334500	-2.69999300
H	-0.88894800	2.49302900	-3.42209500
H	-0.56760600	0.75713300	-3.14287700
H	-2.94107600	0.79738300	-0.04211200
H	-2.02337400	1.51342800	-2.45345500
H	2.94039700	0.83459900	0.02102000
Cl	1.65602800	1.86123400	1.75616600
Ir	-0.00635200	0.38233800	0.49922900
P	5.52963200	-0.16319700	-0.78909400

C	6.32802500	-0.31059000	-2.41830600
H	7.34402600	0.09038100	-2.34798000
H	6.36743500	-1.36222200	-2.71574900
H	5.75306200	0.26019200	-3.15327500
C	6.49478900	-1.09576000	0.44125700
H	7.50945000	-0.68704300	0.47772700
H	6.01665100	-0.99426700	1.41989000
H	6.53043300	-2.15012800	0.15313100
C	5.45573900	1.58744700	-0.31128600
H	4.88212700	2.14657600	-1.05558200
H	4.99561400	1.69228600	0.67453300
H	6.48166500	1.96716800	-0.27781200
P	-5.46707600	-0.16210800	-0.84785600
C	-6.74007400	-1.28877700	-1.48969900
H	-7.70968100	-0.78888100	-1.40158200
H	-6.54121900	-1.51670600	-2.54053200
H	-6.75017200	-2.20909600	-0.89908500
C	-5.83835000	0.25739000	0.88335700
H	-5.85745200	-0.66068100	1.47797900
H	-5.06541100	0.92965200	1.26605800
H	-6.81466700	0.75024400	0.92385700
C	-5.43826900	1.36296600	-1.84299200
H	-4.68572800	2.04465500	-1.43676900
H	-5.19534300	1.11265800	-2.87994700
H	-6.42533500	1.83368200	-1.79428800

7RE-C1-OMe

E = -876.502068 a.u.

C	0.054393	0.092507	-2.061324
C	-0.193161	1.387050	-1.451341
C	1.813078	0.530699	-0.582106
H	-0.480548	-0.305205	-2.914210
C	1.407241	-0.316196	-1.668970
C	2.197947	-1.414536	-2.053181
C	3.009571	0.256842	0.127708
C	3.370305	-1.644384	-1.350908
H	1.883973	-2.066500	-2.861218
C	3.779521	-0.832698	-0.268395
H	4.002138	-2.484455	-1.626851
H	4.702084	-1.071600	0.247039
C	0.800164	1.578974	-0.411380
C	0.749156	2.736840	0.415608
C	-0.229191	3.673908	0.173862
H	1.483193	2.871849	1.200897
C	-1.178932	2.387664	-1.679856
C	-1.173206	3.510075	-0.884119
H	-0.281889	4.566453	0.790782
H	-1.895440	2.268298	-2.486368
H	-1.907452	4.292553	-1.055703

Cl	-0.530636	-2.776365	-0.108976
Cl	-0.046228	-0.443059	2.472428
P	-2.581322	-0.271039	0.360669
C	-3.296683	-1.620287	1.383897
H	-4.343837	-1.379279	1.597912
H	-3.234482	-2.567126	0.845244
H	-2.732749	-1.698080	2.315948
C	-3.580380	-0.299922	-1.184037
H	-4.647399	-0.287318	-0.935019
H	-3.341172	0.571517	-1.798219
H	-3.346743	-1.210721	-1.743283
C	-3.091136	1.257137	1.244250
H	-2.746838	2.138555	0.699701
H	-4.182780	1.284994	1.333925
H	-2.637589	1.250793	2.238815
O	3.309686	1.107646	1.133992
C	4.447596	0.814006	1.952921
H	5.373015	0.855673	1.367016
H	4.462364	1.588636	2.720908
H	4.341321	-0.170982	2.420832
Ir	-0.336420	-0.364532	-0.001244

7PR-C1-OMe

E = -1002.839095 a.u.

C	-2.47418300	3.22655000	-1.71651800
C	-1.10808700	3.24959200	-1.81671100
C	-0.34096300	2.11514200	-1.38659200
C	-0.95103600	0.97130200	-0.75699500
C	-2.37795800	0.92278700	-0.89244900
C	-3.11037600	2.03998800	-1.28343200
C	1.01651400	2.11922700	-1.73945200
C	1.72473400	-0.07984100	-0.78613200
C	1.97659100	1.10524100	-1.56210100
C	3.22867500	1.30911000	-2.22681500
H	3.37517700	2.23579300	-2.77686700
C	4.22031400	0.35768100	-2.18284800
C	3.97379500	-0.82889800	-1.45760000
C	2.77451400	-1.03281200	-0.78918800
H	5.16797000	0.51052400	-2.69109500
H	4.74512800	-1.59448700	-1.40528200
H	2.65453400	-1.93817500	-0.21238700
Cl	1.29982800	-1.95052700	1.89755200
Cl	-1.79330300	-0.51623900	2.08108100
P	-0.61557500	-2.21719100	-0.89995700
P	0.74216600	1.46295100	1.82721700
C	2.31662800	2.36106700	1.45918800
H	2.22915500	2.94564600	0.54140700
H	2.54367700	3.03723700	2.29092700
H	3.13084700	1.63916700	1.34620500

C	-0.49769000	2.82346200	1.97018100
H	-0.17705800	3.53689600	2.73726400
H	-0.60262300	3.34206300	1.01437600
H	-1.46071500	2.38923900	2.24944200
C	1.00716300	0.95118700	3.57662400
H	1.87438000	0.29038400	3.63299700
H	1.17636100	1.84405600	4.18872900
H	0.12579600	0.41224400	3.92789000
C	0.67125500	-3.50437100	-1.22328200
H	0.18386500	-4.37771000	-1.67107900
H	1.42474400	-3.12341500	-1.91646800
H	1.15141600	-3.79347400	-0.28607400
C	-1.20302400	-1.88186400	-2.61944800
H	-0.42008500	-1.33819300	-3.15828500
H	-1.40203700	-2.82841800	-3.13447600
H	-2.11157700	-1.27890000	-2.59895800
C	-1.93928800	-3.21870700	-0.10416600
H	-2.76458900	-2.57428600	0.19250800
H	-2.28396600	-3.99349500	-0.79826600
H	-1.52398400	-3.68998400	0.79129100
Ir	0.08976300	-0.31730000	0.34665400
H	1.35020200	2.98941900	-2.30322100
H	-0.58611000	4.10705800	-2.23287600
H	-3.07713100	4.08055100	-2.01095700
H	-4.19389200	2.00903000	-1.27156400
O	-2.97456500	-0.26468900	-0.61733500
C	-4.39052600	-0.32876700	-0.51336000
H	-4.87562200	-0.10840400	-1.47335500
H	-4.62230900	-1.35443400	-0.22111500
H	-4.75887600	0.35985500	0.25650600

7RE-C2-OMe

E = -876.486791 a.u.

C	3.22083000	0.81863100	-1.18179100
C	2.06501000	0.98624100	-1.90621700
C	0.85932700	1.32684600	-1.23233700
C	0.88169400	1.45143900	0.21160200
C	2.08214500	1.29069300	0.93837100
C	3.23454300	0.97343400	0.24304000
C	-0.49066500	1.59753200	-1.70704800
C	-0.47208400	1.79355300	0.63236400
C	-1.26734700	1.99871500	-0.57273100
C	-2.61881200	2.43987300	-0.44785300
H	-3.22835800	2.57001000	-1.33632400
C	-3.11152600	2.70099500	0.80497100
C	-2.31821600	2.53013900	1.98817300
C	-1.02118300	2.09213800	1.91631100
H	-0.80304800	1.63241200	-2.74162800
H	4.13453000	0.56145900	-1.70370400

H	2.07009900	0.87478200	-2.98556900
H	-4.13543600	3.04835900	0.91406100
H	-2.76225300	2.75596600	2.95340100
Cl	-2.86398900	-1.03766500	-0.33654400
P	-0.00953600	-1.80374500	1.19174900
C	1.73168800	-2.38268200	1.02131700
H	1.97749900	-3.08567400	1.82495800
H	1.84741700	-2.87500400	0.05199700
H	2.41008600	-1.52701800	1.06758000
C	-0.97823500	-3.36921400	1.21668700
H	-0.52234100	-4.07010500	1.92452500
H	-2.00825500	-3.16002500	1.51273100
H	-0.97925900	-3.80300000	0.21348300
C	-0.10287500	-1.19529700	2.92925100
H	0.14858300	-2.00290300	3.62593100
H	0.60279300	-0.37067100	3.06398100
H	-0.41334100	1.97430200	2.80763600
H	-1.11677500	-0.83909800	3.13438900
H	2.10641400	1.40477700	2.01679100
Cl	-0.08349100	-1.90879500	-2.10170200
Ir	-0.58974100	-0.21682900	-0.42073100
O	4.36062500	0.80553400	0.98803800
C	5.59095700	0.47150900	0.33564900
H	6.32935500	0.39112900	1.13509600
H	5.51247600	-0.48814200	-0.18777800
H	5.89356500	1.25873100	-0.36415500

7PR-C2-OMe

E = -1002.854491 a.u.

C	-3.80320200	1.80657600	-0.74049300
C	-2.62132200	2.48654900	-0.88417300
C	-1.34904200	1.85256800	-0.69669000
C	-1.27068800	0.47245200	-0.26611800
C	-2.49798600	-0.19630100	-0.17084700
C	-3.72937100	0.43060800	-0.39773100
C	-0.23306300	2.61070600	-1.05251600
C	1.56391700	0.89631100	-0.74449900
C	1.11541500	2.20319200	-1.13964600
C	2.01075600	3.15422200	-1.72348100
H	1.62296100	4.13790000	-1.97868400
C	3.32447700	2.83387500	-1.98172600
C	3.76481700	1.53328000	-1.65958400
C	2.91436000	0.60774300	-1.06706500
H	-0.43908200	3.62765200	-1.38516400
H	-4.75306700	2.30239700	-0.89780700
H	-2.63563600	3.53501500	-1.17138800
H	4.00101700	3.55554600	-2.43034300
Cl	2.50730600	-1.70496700	1.07926500
P	0.32170500	-1.79379300	-1.68568400

P	0.50567500	0.83016600	2.27286200
C	-1.15395200	1.37380900	2.87185100
H	-1.05370900	1.88946700	3.83320900
H	-1.61424800	2.04823000	2.14519500
H	-1.79126000	0.49373600	2.99304800
C	1.20508200	-0.04281600	3.73550200
H	1.08167400	0.58265600	4.62664400
H	0.68125500	-0.99222700	3.86566900
H	2.26394200	-0.24547800	3.56356500
C	1.48096100	2.39771300	2.23218100
H	1.03320000	3.10384500	1.52924000
H	1.50138600	2.84663600	3.23143700
H	2.50361800	2.17867000	1.91046200
C	-0.94367000	-3.13346000	-1.65750600
H	-0.91167200	-3.68564400	-2.60333800
H	-0.73593800	-3.80909600	-0.82461500
H	-1.93934900	-2.70431900	-1.52119500
C	1.85528600	-2.69729100	-2.16324600
H	1.66837900	-3.27188800	-3.07721400
H	2.66757800	-1.98800200	-2.33967700
H	2.14568200	-3.36929300	-1.35268700
C	-0.10019100	-0.84380100	-3.21157000
H	-0.14754900	-1.51332800	-4.07742500
H	-1.06896500	-0.35365200	-3.07878900
H	3.31005600	-0.36475200	-0.80791300
H	0.66288400	-0.07954300	-3.38533400
H	-2.52521800	-1.23061500	0.14504100
Cl	-0.81322900	-2.17214000	1.67334700
Ir	0.44064300	-0.43637400	0.25533200
O	-4.81821100	-0.34973900	-0.25165200
C	-6.12361900	0.22040400	-0.43029100
H	-6.82288400	-0.59860300	-0.25781600
H	-6.30215600	1.01896100	0.29753900
H	-6.24523000	0.60264000	-1.44940700
H	4.79468600	1.24899700	-1.86577500

7RE-C3-OMe

E = -876.486646 a.u.

C	3.47780000	0.77221000	-0.06390500
C	2.57642700	1.15924000	-1.04008900
C	1.24823200	1.44871600	-0.65953000
C	0.84392200	1.31865900	0.73007500
C	1.80700400	0.94857800	1.70824500
C	3.09395600	0.67646200	1.31556500
C	0.07394800	1.78490900	-1.43509700
C	-0.54750400	1.75235900	0.83368300
C	-0.98537800	2.10081400	-0.50579400
C	-2.30404500	2.60363100	-0.69936200
H	-2.64755900	2.84678600	-1.69953600

C	-3.10776700	2.78616900	0.40031300
C	-2.66176300	2.47451600	1.72286500
C	-1.40527400	1.96634200	1.94941500
H	0.05077800	1.95966500	-2.50201100
H	2.88620200	1.21756500	-2.07775700
H	-4.11130100	3.18168800	0.26907900
H	-3.33442700	2.64621600	2.55827900
Cl	-2.49540700	-0.78712300	-1.58181100
P	-0.77391300	-1.87556900	1.09948800
C	0.79943000	-2.57008600	1.76339800
H	0.58674500	-3.35557700	2.49707000
H	1.37870700	-2.98806400	0.93543100
H	1.38528000	-1.77739000	2.23632600
C	-1.65568700	-3.36433800	0.46903000
H	-1.64386600	-4.14903200	1.23344000
H	-2.68662500	-3.10191900	0.22237600
H	-1.15529900	-3.71877500	-0.43533400
C	-1.72614200	-1.42450600	2.61349400
H	-1.88085000	-2.31145200	3.23797600
H	-1.17827700	-0.67098600	3.18598500
H	-1.05890500	1.74260400	2.95330800
H	-2.69600600	-1.01047100	2.32134800
H	1.52743500	0.89112000	2.75583300
Cl	0.73420300	-1.75905000	-1.81286200
Ir	-0.45431900	-0.14193500	-0.44182400
H	3.82352600	0.38194000	2.05967700
O	4.73778100	0.49439000	-0.48650500
C	5.71490400	0.03966600	0.45674100
H	6.61724600	-0.14479200	-0.12836000
H	5.92009700	0.80447500	1.21428200
H	5.39417400	-0.89131600	0.93792400

7PR-C3-OMe

E = -1002.845508 a.u.

C	-4.16228000	0.51303100	-0.38482700
C	-3.25749600	1.54864500	-0.47877500
C	-1.85009600	1.30527900	-0.41481200
C	-1.32051900	-0.01104800	-0.17739400
C	-2.29363500	-1.03807800	-0.15100800
C	-3.65944900	-0.80222100	-0.24521100
C	-1.02768200	2.40929100	-0.70219600
C	1.20761200	1.28707400	-0.67986400
C	0.36458400	2.43916600	-0.88085200
C	0.90006500	3.67977800	-1.36291900
H	0.22537700	4.52693800	-1.46222800
C	2.22348700	3.79565800	-1.71290600
C	3.04701200	2.65374500	-1.59005000
C	2.55368000	1.45392000	-1.09704500
H	-1.96863200	-2.05862600	-0.00132000

H	-4.33841200	-1.64693700	-0.19521700
H	2.62670900	4.73329600	-2.08400600
H	4.09569500	2.71783600	-1.87271700
H	3.23585600	0.62285200	-0.98361300
Cl	3.00476800	-1.05729700	0.81601600
Cl	0.00043900	-2.55403600	1.46251400
P	0.79198500	-1.56800500	-1.86900000
P	0.41522800	0.61724400	2.34256100
C	0.90476200	2.39415800	2.45570900
H	0.23445700	3.01204300	1.85431700
H	0.85867500	2.72346000	3.49958600
H	1.92645700	2.51127400	2.08182900
C	-1.29688100	0.59427600	3.03192500
H	-1.29633700	1.01160800	4.04487200
H	-1.96655000	1.18134700	2.39824000
H	-1.65070800	-0.43972700	3.06209800
C	1.41267500	-0.16098900	3.68016500
H	2.47424900	-0.04000200	3.45582300
H	1.17285100	0.31749300	4.63619000
H	1.17986000	-1.22706700	3.72231900
C	2.49201000	-1.78910400	-2.54570900
H	2.43684200	-2.35626200	-3.48146900
H	2.94764000	-0.81508000	-2.73991000
H	3.10383900	-2.32710400	-1.81832700
C	-0.10341500	-0.73636700	-3.25270000
H	0.28291200	0.28021200	-3.37282200
H	0.03790800	-1.29119300	-4.18670500
H	-1.17050300	-0.68430800	-3.01931500
C	0.12520600	-3.28519900	-1.89451900
H	-0.93349700	-3.28229900	-1.62511200
H	0.24570500	-3.70485400	-2.89949300
H	0.67012300	-3.89414000	-1.16948900
Ir	0.60612200	-0.40720700	0.19544800
H	-1.54887600	3.34520600	-0.89958100
H	-3.61623000	2.56327300	-0.63006300
O	-5.49100500	0.82609900	-0.45310900
C	-6.44288300	-0.23597000	-0.35831500
H	-6.35590200	-0.76274800	0.59972400
H	-7.42244100	0.24101200	-0.42374200
H	-6.32767700	-0.94753700	-1.18508800

7RE-C4-OMe

E = -876.489670 a.u.

C	3.25842000	0.38954600	1.40440800
C	2.75440000	0.92209700	0.23320600
C	1.37425500	1.30553600	0.19277400
C	0.54332100	1.10244200	1.36248600
C	1.09681500	0.57919400	2.56148700
C	2.43052400	0.24093300	2.55547400

C	0.58216200	1.91483200	-0.86106100
C	-0.79087900	1.58001600	1.01534000
C	-0.71464500	2.17644300	-0.31241200
C	-1.87180900	2.80079900	-0.86460900
H	-1.83303600	3.22148200	-1.86424000
C	-3.01130100	2.86035900	-0.10339400
C	-3.07600100	2.30471400	1.21715000
C	-1.99314500	1.67818900	1.77874500
H	0.94372600	2.22398600	-1.83087400
H	-3.89765000	3.34294500	-0.50636200
H	-4.00438700	2.38709400	1.77480900
Cl	-2.11689600	-0.53402500	-1.90245500
P	-0.76019600	-2.07006500	0.73912400
C	0.73942500	-2.90788900	1.40260000
H	0.45163900	-3.76566600	2.02053800
H	1.35351900	-3.24671300	0.56406300
H	1.31911700	-2.20220400	2.00332100
C	-1.61650000	-3.40751000	-0.19154800
H	-1.68072800	-4.30268400	0.43697000
H	-2.61903200	-3.07835500	-0.47258700
H	-1.04978600	-3.63265200	-1.09860100
C	-1.82562800	-1.81636300	2.22191400
H	-2.02750600	-2.77620600	2.71042100
H	-1.31936100	-1.15163500	2.92679400
H	-2.03419900	1.26747800	2.78232900
H	-2.77044500	-1.35893300	1.91372400
H	0.48157800	0.45720800	3.44626900
Cl	1.15166100	-1.43799600	-1.88768600
Ir	-0.25656000	-0.10971500	-0.41615800
H	2.88362500	-0.16382000	3.45642200
H	4.29866100	0.09412800	1.47277000
O	3.44489600	1.16112900	-0.89897300
C	4.80232500	0.71088800	-0.96869400
H	4.85637500	-0.37143300	-0.80545400
H	5.13981000	0.95091400	-1.97787700
H	5.42552900	1.23409600	-0.23412400

7PR-C4-OMe

E = -1002.850194 a.u.

C	-3.85833800	-1.69749000	-0.72928700
C	-3.61872000	-0.36518200	-0.44830100
C	-2.25717400	0.13025400	-0.32687500
C	-1.13670300	-0.78284000	-0.35531400
C	-1.44333100	-2.11926300	-0.69218700
C	-2.74998300	-2.55253000	-0.87262800
C	-2.09379200	1.51607300	-0.31482400
C	0.40695700	1.66615700	-0.28284800
C	-0.89764100	2.26384300	-0.34708800
C	-1.06127500	3.67611600	-0.51553300

H	-2.07117800	4.07949300	-0.53099400
C	0.02435200	4.50750000	-0.67020000
C	1.31081300	3.92795200	-0.66356100
C	1.48794600	2.56264100	-0.47885600
H	-4.86284900	-2.08556800	-0.84084700
H	-0.64284900	-2.84265000	-0.75491500
H	-2.93160800	-3.59977400	-1.10522300
H	-0.10275300	5.57812300	-0.80194700
H	2.18551300	4.56227900	-0.79172800
H	2.49551700	2.17168100	-0.44490700
Cl	3.15078500	0.18035800	0.84957100
Cl	1.28907900	-2.66889300	0.84463200
P	1.45106300	-0.64262300	-2.10048800
P	0.07378700	-0.01281700	2.41213900
C	-0.42685200	1.68131300	2.95040900
H	-1.32869400	1.99739800	2.42136200
H	-0.62303900	1.68108000	4.02833800
H	0.38050600	2.38531000	2.72731400
C	-1.36709700	-1.06153100	2.89267300
H	-1.56323400	-0.95779000	3.96547200
H	-2.25554400	-0.76106600	2.33136800
H	-1.13519800	-2.10437100	2.66090700
C	1.35334400	-0.46903400	3.65493200
H	2.18904800	0.23035500	3.58719200
H	0.91423200	-0.43372600	4.65813500
H	1.71681500	-1.47540800	3.43672100
C	2.97408300	0.24490600	-2.63963000
H	3.21593600	-0.04570900	-3.66783500
H	2.81076700	1.32460700	-2.59885300
H	3.80003900	-0.01444800	-1.97378300
C	0.20660400	-0.12611200	-3.36264800
H	-0.02738600	0.93371300	-3.22296000
H	0.60099300	-0.28073200	-4.37293400
H	-0.70897100	-0.71041300	-3.23663100
C	1.82576800	-2.39003000	-2.54858900
H	0.94879900	-3.01909500	-2.37971500
H	2.11439700	-2.43971000	-3.60450400
H	2.64440500	-2.75456300	-1.92340500
Ir	0.73088400	-0.26741600	0.13277400
H	-3.00731300	2.10057000	-0.37359400
O	-4.59652400	0.55342700	-0.28107700
C	-5.96119400	0.14937700	-0.44782500
H	-6.23419600	-0.61010700	0.29303700
H	-6.55290600	1.05162100	-0.28717600
H	-6.13214200	-0.23354100	-1.45999200

7RE-C5-OMe

E = -876.477194 a.u.

C	-0.22383900	3.61405300	1.00350900
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C	-0.96091400	2.90921200	0.08065000
C	-1.21088300	1.53041700	0.32649900
C	-0.64427800	0.88815400	1.49438700
C	0.10554900	1.65251300	2.43035800
C	0.29532800	2.99180500	2.18014000
C	-1.97520900	0.52724200	-0.41305400
C	-1.06543900	-0.50983800	1.47672700
C	-1.99098600	-0.67612800	0.36574500
C	-2.64837600	-1.92466800	0.16920100
H	-3.31432700	-2.05985300	-0.67661400
C	-2.41865400	-2.92729600	1.07601700
C	-1.52837800	-2.76092100	2.19041500
C	-0.86357200	-1.58099400	2.40092800
H	-2.92053300	-3.88328800	0.95347000
H	-1.38493400	-3.59309200	2.87343100
Cl	0.42803900	-2.25533600	-1.50160000
P	2.41368900	-0.25518700	0.25092100
C	3.18907400	1.40864900	0.39235800
H	4.21105700	1.31811000	0.77683900
H	3.20721400	1.87177000	-0.59789200
H	2.59941500	2.03658400	1.06517800
C	3.55755900	-1.16352700	-0.86895600
H	4.58716600	-1.03292800	-0.51777700
H	3.30021200	-2.22458400	-0.87760000
H	3.45854100	-0.76580000	-1.88203900
C	2.69786400	-1.03484900	1.89694500
H	3.77029400	-1.06905600	2.11956700
H	2.18661700	-0.45507100	2.67026200
H	-0.19446100	-1.45000500	3.24536600
H	2.29577200	-2.05237400	1.88630200
H	0.50152600	1.18131000	3.32442900
Cl	0.88651100	0.98769500	-2.41495200
Ir	0.16451900	-0.14056700	-0.37562500
H	0.85832000	3.59542800	2.88645400
H	-0.02935400	4.67040800	0.84121900
H	-1.35955500	3.38224500	-0.81051500
O	-2.73686800	0.76984100	-1.51430900
C	-4.00325500	1.38358300	-1.20220300
H	-4.51178600	1.53200400	-2.15705100
H	-4.60103400	0.72613900	-0.55942900
H	-3.85541800	2.35024100	-0.70644100

7PR-C5-OMe

E = -1002.843363 a.u.

C	2.39738900	-3.61685600	0.69800800
C	2.88202500	-2.39958400	0.28439800
C	2.02464500	-1.25515500	0.17684800
C	0.60780400	-1.37817500	0.38576300
C	0.17848300	-2.63635500	0.88753000

C	1.03035900	-3.71752400	1.03849800
C	2.65274100	0.00049900	-0.04831700
C	0.61773900	1.46596600	0.02526400
C	2.03712600	1.28188700	-0.11579000
C	2.91074100	2.40804800	-0.26812900
H	3.96270500	2.22876500	-0.45295600
C	2.43775400	3.69582000	-0.19070200
C	1.06207800	3.89308800	0.05552300
C	0.19640400	2.81656300	0.15879300
H	3.05315800	-4.47944800	0.77243600
H	3.93000300	-2.29034800	0.03318500
H	3.10817800	4.54181500	-0.31129600
Cl	-2.62491500	1.63579000	-0.71571900
P	-1.26911600	0.29916900	2.23364800
P	-0.35924200	-0.35373100	-2.39637800
C	0.22751600	-2.05815100	-2.79142700
H	0.31551800	-2.18070800	-3.87649900
H	1.20014000	-2.23826200	-2.32648500
H	-0.49439800	-2.77865900	-2.39798100
C	-1.83427500	-0.15575000	-3.47987200
H	-1.57817000	-0.46251600	-4.50003400
H	-2.64537700	-0.77491600	-3.09124200
H	-2.15213100	0.88865200	-3.47108200
C	0.89176500	0.73349600	-3.21170500
H	1.88601600	0.54659900	-2.79991600
H	0.90498300	0.53177700	-4.28851300
H	0.62785300	1.78160500	-3.04115900
C	-2.42948600	-0.93351100	2.95972600
H	-2.57673800	-0.70971400	4.02218500
H	-3.38532400	-0.88143100	2.43315800
H	-2.02433100	-1.94227900	2.85250300
C	-2.03910800	1.90288300	2.71598000
H	-2.27078300	1.88336500	3.78646100
H	-1.34999100	2.72590200	2.51180200
H	-2.95366000	2.05386900	2.13835100
C	0.21117800	0.20395800	3.33255600
H	-0.07452100	0.38585700	4.37434200
H	0.66661100	-0.78666000	3.24914000
H	-0.85826000	3.01346500	0.28850900
H	0.94034500	0.95729700	3.01951500
H	-0.87246400	-2.77347600	1.10048800
Cl	-2.59353500	-1.74611700	-0.38385200
Ir	-0.74736300	0.01091000	-0.06764600
H	0.66764900	4.90346700	0.13980500
H	0.63217400	-4.66386000	1.39800700
O	4.01134700	-0.02018000	-0.16244800
C	4.77300800	0.10442800	1.05917800
H	4.54736600	-0.72589100	1.73604300
H	5.82127200	0.07039300	0.75905600

H	4.55210100	1.05721200	1.55143100
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7RE-C28-OMe

E = -991.017897 a.u.

C	3.420253	0.510444	-1.649841
C	2.228337	0.927234	-2.192381
C	1.195342	1.396945	-1.334616
C	1.415232	1.376489	0.098747
C	2.651281	0.957893	0.637573
C	3.639396	0.535996	-0.233905
C	-0.127058	1.951710	-1.599133
C	0.205118	1.894348	0.726745
C	-0.674663	2.354188	-0.340843
C	-1.895253	3.002188	0.011044
H	-2.576899	3.333051	-0.765787
C	-2.188093	3.206967	1.332997
C	-1.301627	2.773415	2.382204
C	-0.111915	2.148346	2.090134
H	-0.550189	2.144267	-2.575322
H	4.203340	0.155592	-2.308737
H	2.076857	0.915192	-3.266948
H	-3.114703	3.705694	1.591440
Cl	-2.733920	-0.349837	0.035015
P	0.136923	-1.769128	0.865121
C	1.714658	-2.572474	0.353210
H	1.951321	-3.405256	1.024875
H	1.605151	-2.943930	-0.669605
H	2.527998	-1.843463	0.380905
C	-1.054152	-3.172884	0.905413
H	-0.619391	-4.006936	1.467198
H	-1.984992	-2.852060	1.377512
H	-1.266581	-3.487075	-0.119828
C	0.397958	-1.358157	2.642744
H	0.642937	-2.263674	3.209342
H	1.217948	-0.640803	2.735601
H	0.554829	1.836998	2.886918
H	-0.515368	-0.911031	3.046623
H	2.832490	0.967190	1.706991
Cl	-0.577089	-1.466712	-2.391403
Ir	-0.409200	0.060549	-0.470732
O	4.810144	0.135804	0.331068
C	5.891366	-0.273816	-0.514039
H	6.710868	-0.519378	0.163293
H	5.621693	-1.160497	-1.098931
H	6.198912	0.538586	-1.182459
O	-1.585380	2.967311	3.703058
C	-2.847929	3.528826	4.073673
H	-3.677459	2.911223	3.709875
H	-2.851838	3.537446	5.165104

H -2.953342 4.554794 3.701868

7PR-C28-OMe

E = -1117.393488 a.u.

C	3.67805400	2.60960700	-0.00470800
C	2.39424000	3.02382000	-0.26721000
C	1.27978700	2.12938200	-0.22437800
C	1.47507800	0.72288400	0.04201900
C	2.79340900	0.34623600	0.33438700
C	3.86849600	1.24386300	0.31908300
C	0.01746000	2.71845600	-0.38575900
C	-1.44227200	0.73094300	0.05306900
C	-1.24713300	2.13238000	-0.23430300
C	-2.36118100	3.02847800	-0.27405900
H	-2.17717700	4.07026500	-0.52673300
C	-3.63953800	2.62068700	0.02246800
C	-3.82475400	1.26256100	0.38219200
C	-2.75177800	0.36281200	0.39028100
H	0.01920900	3.79096500	-0.57785400
H	4.50357200	3.30995300	-0.03614800
H	2.20779200	4.06963100	-0.50070400
H	-4.46532700	3.32082500	-0.00426700
Cl	-1.70698900	-2.53804900	-0.36775900
P	0.01423100	-0.84948100	2.28847000
P	-0.05659900	-0.53898300	-2.44748700
C	1.13635600	0.61591200	-3.25741800
H	1.06503000	0.51928900	-4.34645400
H	0.91609600	1.64708000	-2.97161300
H	2.15298200	0.36909100	-2.93652600
C	0.26376400	-2.12609900	-3.32521100
H	0.09594000	-1.99191300	-4.39964900
H	1.29447900	-2.43718400	-3.14295900
H	-0.40914900	-2.89007200	-2.93006600
C	-1.68838700	-0.00713400	-3.12796900
H	-1.91952000	1.00821000	-2.79506600
H	-1.66584600	-0.03462600	-4.22299700
H	-2.46243300	-0.68586700	-2.75988600
C	1.52673300	-1.57079900	3.05660100
H	1.40293400	-1.60389700	4.14471100
H	1.68503700	-2.57886500	2.66740200
H	2.39694200	-0.95765200	2.80878500
C	-1.33848800	-1.86519000	3.01929300
H	-1.25631100	-1.85518100	4.11192600
H	-2.30977600	-1.46205500	2.72205600
H	-1.25810000	-2.89064000	2.65058600
C	-0.15256300	0.77191600	3.15714200
H	-0.11836300	0.62808600	4.24263800
H	0.66656400	1.43042500	2.85300900
H	-2.97762800	-0.66875900	0.62563900

H	-1.10275800	1.23875100	2.88343100
H	3.02150500	-0.69042800	0.54382000
Cl	1.69274400	-2.58282200	-0.26030200
Ir	0.01010800	-0.65473500	-0.07139700
O	5.07562900	0.71482400	0.61658300
C	6.23566300	1.55747100	0.59172700
H	7.07161100	0.90882200	0.85716000
H	6.39481900	1.97327100	-0.40926800
H	6.14777300	2.36591200	1.32610000
O	-5.02506400	0.74393700	0.72079000
C	-6.18408200	1.58858300	0.70778400
H	-6.36295900	1.99134500	-0.29511000
H	-7.01535000	0.94488000	0.99877400
H	-6.07987500	2.40597300	1.42995700

TS1-C2-PMe₃⁺

E = -1013.766358 a.u.

C	-2.62678000	-2.05110100	-1.33700800
C	-1.41734700	-2.66989600	-1.35823000
C	-0.41281200	-2.27233900	-0.39198200
C	-0.52908400	-0.89044400	0.13896500
C	-1.90428100	-0.53607700	0.46901400
C	-2.90059600	-1.04056800	-0.31969300
C	0.51928500	-3.04534200	0.21812900
C	0.87258300	-0.98360300	1.47148300
C	1.12976100	-2.38161300	1.35918800
C	1.79901100	-3.06169900	2.38107700
H	1.99635400	-4.12537000	2.27330400
C	2.16705000	-2.38862100	3.55031600
C	1.84265500	-1.03867600	3.70655600
C	1.19110900	-0.34520600	2.67925800
H	0.73317700	-4.07611600	-0.04562700
H	-3.41865400	-2.36530400	-2.00963600
H	-1.23281500	-3.52388200	-2.00436100
H	2.68162100	-2.92280400	4.34435000
Cl	2.94520200	1.60348500	0.54544500
P	-0.42197100	2.27599500	0.81857000
P	2.31580100	-0.85000400	-1.59791000
C	1.61974000	-1.91176200	-2.94441600
H	2.42289000	-2.16741200	-3.64441900
H	1.19257200	-2.83026100	-2.54147500
H	0.84316100	-1.35442700	-3.47652700
C	3.45180300	0.23730600	-2.57139800
H	4.21169000	-0.39576100	-3.04214300
H	2.88912600	0.76982800	-3.33911200
H	3.92632600	0.96125600	-1.90730500
C	3.53215200	-1.94545100	-0.74015500
H	3.05503000	-2.84295000	-0.34741200
H	4.30433400	-2.23873800	-1.45945400

H	3.99232500	-1.39128100	0.08222800
C	-1.91374000	2.78993100	-0.15438100
H	-2.54104800	3.45322900	0.45007400
H	-1.57145600	3.32577100	-1.04215300
H	-2.48966100	1.92508700	-0.48169000
C	0.52737200	3.85475700	0.88565200
H	-0.14667500	4.65472100	1.21269400
H	1.35793900	3.75788200	1.58639600
H	0.92311400	4.08282300	-0.10562600
C	-1.04282400	2.18557800	2.57060900
H	-1.81089600	2.95401800	2.70740500
H	-1.45635400	1.20989100	2.83476700
H	1.01402000	0.71078100	2.80910700
H	-0.21517800	2.40336400	3.25176300
H	-2.11794500	0.19534400	1.23354300
Cl	0.73090500	1.97578800	-2.12880700
Ir	0.81692600	0.46175700	-0.22450300
P	-4.59497000	-0.43221900	-0.13003100
C	-5.73626300	-1.84329900	0.02828900
H	-6.75519700	-1.45959400	0.13830600
H	-5.67714600	-2.46879000	-0.86706700
H	-5.46167600	-2.43060800	0.90905100
C	-5.07401200	0.53544500	-1.59796300
H	-6.10976600	0.86943500	-1.48035700
H	-4.41131800	1.39926000	-1.69760500
H	-4.99099600	-0.09567000	-2.48763700
C	-4.73064800	0.60208300	1.35880100
H	-4.45608800	0.01549500	2.23992400
H	-4.08703700	1.48032700	1.27495600
H	-5.77268400	0.92490200	1.44717200
H	2.11410000	-0.51032700	4.61633300

IN1-C2-PMe₃⁺

E = -1013.813046 a.u.

C	-2.38025300	-2.04910100	-1.29170200
C	-1.19600500	-2.72008700	-1.26965400
C	-0.25209000	-2.43917600	-0.22412100
C	-0.39521300	-1.17336100	0.55954900
C	-1.76198000	-0.68835300	0.66105900
C	-2.70420900	-1.08662300	-0.24774500
C	0.75172900	-3.21292200	0.30391600
C	0.56739800	-1.32723200	1.68050200
C	1.29369200	-2.54659700	1.46945800
C	2.33999600	-2.89298100	2.32646600
H	2.89881600	-3.81250300	2.17113300
C	2.67550200	-2.03100800	3.38175600
C	1.97060300	-0.84143700	3.59083800
C	0.90727000	-0.48164100	2.74373500
H	1.09745900	-4.16560100	-0.08231700

H	-3.12137200	-2.27935600	-2.05204700
H	-0.99495700	-3.51131800	-1.98703300
H	3.49251300	-2.29494300	4.04808100
Cl	2.70516100	2.24009100	-0.14906300
P	-0.53627600	2.35788300	0.76268100
P	2.39099600	-0.70772300	-1.51571100
C	1.78394800	-2.03867200	-2.65029700
H	2.54800400	-2.20287900	-3.41727200
H	1.60847200	-2.97046100	-2.11638900
H	0.85854800	-1.71136800	-3.12984200
C	3.20074500	0.39900800	-2.75920000
H	3.82648600	1.13583800	-2.25723200
H	3.81120800	-0.21858600	-3.42658700
H	2.43335200	0.91720900	-3.33918200
C	3.84394300	-1.46410700	-0.66619200
H	3.53379300	-2.32202900	-0.06838700
H	4.57623500	-1.78792800	-1.41409700
H	4.30124600	-0.71830500	-0.00934500
C	-2.07524400	2.67635500	-0.21645200
H	-2.75468300	3.30645500	0.36668600
H	-1.80289300	3.19672000	-1.13717900
H	-2.55967600	1.74171000	-0.48676200
C	0.23280400	4.03656300	0.69733300
H	-0.52756400	4.77010300	0.98898100
H	1.08319800	4.09478400	1.37884900
H	0.57805700	4.24685000	-0.31680900
C	-1.14099000	2.37302500	2.52101400
H	-1.77360700	3.25656700	2.66061300
H	-1.71831700	1.48348700	2.78264400
H	0.34169500	0.41638400	2.94835000
H	-0.28345500	2.45061300	3.19622100
H	-2.01387700	-0.01434600	1.46838600
Cl	-0.20981100	0.96506900	-2.20690400
Ir	0.85746000	0.55970800	-0.14458800
P	-4.42896900	-0.57869100	-0.09307100
C	-5.46202800	-2.06889300	0.10845200
H	-6.51080600	-1.76863800	0.19602300
H	-5.33955200	-2.72085700	-0.76112900
H	-5.14882300	-2.60087100	1.01157900
C	-5.00285500	0.28943300	-1.59130800
H	-6.07047400	0.50736100	-1.48723800
H	-4.44505900	1.22010000	-1.72238800
H	-4.84540400	-0.35580200	-2.46054100
C	-4.68054700	0.48352000	1.36393100
H	-4.38945300	-0.05855400	2.26778600
H	-4.10355200	1.40578100	1.27470100
H	-5.74631700	0.72730600	1.41650500
H	2.23183100	-0.19445700	4.42342400

TS2-C2-PMe₃⁺

E = -887.439391 a.u.

C	2.77142200	1.09846200	-1.72585700
C	1.62711000	1.61998100	-2.24766200
C	0.45205700	1.70307700	-1.41119400
C	0.42504800	0.78913800	-0.24567200
C	1.68355900	0.57414500	0.42803300
C	2.81608600	0.65935300	-0.33728600
C	-0.60059400	2.57254500	-1.49026500
C	-1.20625000	1.52251700	0.61792500
C	-1.40112600	2.61941900	-0.26924100
C	-2.18247800	3.70700700	0.12606800
H	-2.36166700	4.52523400	-0.56675600
C	-2.68852200	3.75586200	1.43212200
C	-2.40268900	2.73172700	2.33912800
C	-1.66536300	1.60964600	1.93193800
H	-0.74561800	3.27008500	-2.30936100
H	3.67936000	1.07821200	-2.31990700
H	1.61393300	2.06790000	-3.23759700
H	-3.28522200	4.60803800	1.74554800
H	-2.77760800	2.78456900	3.35739200
Cl	-3.56910300	-0.59747900	-0.24682000
P	-0.55292300	-1.92065900	1.07024200
C	0.98529900	-2.82283600	0.61764700
H	1.21078200	-3.56098500	1.39491200
H	0.83706300	-3.32523700	-0.34052400
H	1.81566200	-2.11871000	0.52585300
C	-1.83467500	-3.22067900	1.25300500
H	-1.46574100	-3.96874500	1.96373600
H	-2.75425100	-2.76831700	1.62891100
H	-2.03002100	-3.68498900	0.28499100
C	-0.26519500	-1.39813500	2.81396600
H	0.17554900	-2.25204300	3.34056200
H	0.41127800	-0.54477300	2.88924600
H	-1.51413200	0.79933000	2.63062500
H	-1.21968600	-1.15161400	3.28585100
H	1.71324800	0.24351500	1.45769600
Cl	-1.19837700	-2.15868500	-2.08956000
Ir	-1.09454900	-0.36100000	-0.48000400
P	4.41415800	0.16548600	0.36246300
C	5.68912200	1.35935300	-0.15285600
H	6.63728700	1.08295300	0.31849100
H	5.80216300	1.33362400	-1.24001100
H	5.39322900	2.36295000	0.16623500
C	4.87490200	-1.48940400	-0.24432500
H	5.86278000	-1.74918700	0.14922200
H	4.13386100	-2.21792800	0.09579600
H	4.90338900	-1.47714800	-1.33798300
C	4.32483900	0.14520300	2.17855000

H	4.05954300	1.14304700	2.53962400
H	3.58708500	-0.58539700	2.51974800
H	5.31131400	-0.13329200	2.56176800

IN2-C2-PMe₃⁺

E = -887.519742 a.u.

C	2.99379000	2.39925800	-0.21182900
C	1.74804300	2.96095500	-0.39094200
C	0.56460200	2.16318800	-0.37029500
C	0.63461200	0.73749500	-0.23875000
C	1.92979400	0.20498000	-0.04022400
C	3.07084200	1.00184000	-0.02092300
C	-0.66542800	2.86800500	-0.38299200
C	-2.23411300	0.97570900	0.07390800
C	-1.95399400	2.37757000	-0.13932100
C	-2.97734800	3.37071700	0.04191400
H	-2.73403000	4.40804400	-0.17384800
C	-4.22010600	3.02348900	0.50927200
C	-4.47512200	1.66321900	0.80346600
C	-3.51660100	0.68210500	0.59079300
H	-0.58067700	3.94852000	-0.48256000
H	3.88351900	3.01914200	-0.21537400
H	1.65217300	4.03477900	-0.53099800
H	-4.99083200	3.77297400	0.66080700
H	-5.45236800	1.37500600	1.18338600
Cl	-2.90010600	-1.81067000	-1.35411300
P	-0.82261500	-1.35927800	1.49803800
C	0.72993600	-2.28833700	1.83441600
H	0.56707100	-2.88066600	2.74131200
H	0.95798800	-2.95022100	0.99663800
H	1.55817800	-1.59935700	2.00602000
C	-2.12631500	-2.60828400	1.82989800
H	-1.98723200	-2.97092900	2.85452000
H	-3.12207100	-2.17713500	1.72482300
H	-2.01746500	-3.43388000	1.12316000
C	-0.92455800	-0.15426300	2.87983000
H	-0.75545900	-0.68187400	3.82481000
H	-0.15854300	0.61446700	2.74521300
H	-3.78602500	-0.34735200	0.78341400
H	-1.91022800	0.31572000	2.89454000
H	2.03772700	-0.86682900	0.04356000
Cl	0.50402900	-2.05073400	-1.76178600
Ir	-0.95570800	-0.42215400	-0.54351500
P	4.68016800	0.16860800	0.18255200
C	5.98069900	1.37782700	0.57155400
H	6.91860900	0.83206000	0.71389300
H	6.09484900	2.08383100	-0.25585200
H	5.72465100	1.91353400	1.49002100
C	5.10132800	-0.69889700	-1.36222800

H	6.06187500	-1.20732000	-1.23370300
H	4.31927600	-1.42957500	-1.58762500
H	5.16883200	0.02956400	-2.17560500
C	4.56596700	-1.04538000	1.53501500
H	4.28647200	-0.53173100	2.45936900
H	3.82247700	-1.80801200	1.29065200
H	5.54461500	-1.52018700	1.65612900

TS1-C28-PMe₃⁺

E = -1139.316024 a.u.

C	-3.53705400	-0.11714300	-2.00122200
C	-2.58303300	0.61585600	-2.63171700
C	-1.19649800	0.41527400	-2.25792100
C	-0.96798400	-0.08043900	-0.87972700
C	-1.87192400	-1.16561000	-0.51845500
C	-3.14588600	-1.11475500	-1.00931300
C	-0.09506800	0.45726100	-3.05128500
C	0.94314700	-0.35173500	-1.00183800
C	1.06961600	-0.11710200	-2.40476400
C	2.21002400	-0.54955800	-3.09082500
H	2.30448800	-0.34793000	-4.15423600
C	3.20464500	-1.26485400	-2.42543500
C	3.03965300	-1.58506000	-1.06996200
C	1.89945900	-1.15039500	-0.37127100
H	-0.09025000	0.79366600	-4.08248000
H	-4.57832900	-0.04174600	-2.29925700
H	-2.82670900	1.25275000	-3.47735400
H	4.08573500	-1.58877000	-2.96942400
Cl	2.16208400	1.55624000	1.53684200
P	-0.46079500	-0.50741400	2.31019800
P	0.39212400	2.97965900	-0.89438600
C	-0.96824500	3.68252800	-1.93017800
H	-0.70745800	4.71008600	-2.20614600
H	-1.11412100	3.09570700	-2.83732400
H	-1.89520700	3.69085600	-1.34945700
C	0.81023600	4.42622900	0.17769700
H	1.15104600	5.24127600	-0.46964900
H	-0.07059700	4.74365200	0.73639900
H	1.59987100	4.14986400	0.87813100
C	1.85668700	2.95086200	-2.02157000
H	1.65550400	2.37868600	-2.92667100
H	2.09598200	3.98214600	-2.30183700
H	2.70754300	2.51224000	-1.49376400
C	-2.24042800	-0.60753300	2.80142700
H	-2.36018800	-1.35088700	3.59654700
H	-2.54539100	0.37361200	3.17201600
H	-2.87251900	-0.86733600	1.95320900
C	0.31996100	0.07314900	3.87599500
H	-0.03193200	-0.56152000	4.69693100

H	1.40594800	0.01145600	3.79526000
H	0.03709000	1.11072900	4.06078100
C	0.10260800	-2.27937100	2.29503400
H	-0.38712600	-2.80671000	3.12058800
H	-0.11995600	-2.79606700	1.35851000
H	1.81094500	-1.37663500	0.68053100
H	1.18299800	-2.30587300	2.46549400
H	-1.56865700	-1.92539500	0.18573100
Cl	-1.17133900	2.55251600	1.93895200
Ir	-0.05237100	1.00480800	0.44512100
P	-4.40639300	-2.27885900	-0.42974900
C	-5.20488300	-3.05621500	-1.86890200
H	-6.00438500	-3.71547500	-1.51715700
H	-5.62489000	-2.28209100	-2.51707800
H	-4.45865500	-3.63505000	-2.42098200
C	-5.65641100	-1.37893300	0.54107900
H	-6.41189900	-2.08793200	0.89414200
H	-5.16441500	-0.90104000	1.39343300
H	-6.12878400	-0.61823900	-0.08688100
C	-3.65691700	-3.56617300	0.61243000
H	-2.88724600	-4.10067800	0.04882600
H	-3.22696900	-3.11688800	1.51099300
H	-4.44863100	-4.26498900	0.89969800
P	4.32039900	-2.48103500	-0.15182400
C	5.63278700	-3.04110100	-1.27654500
H	6.38140700	-3.57332400	-0.68172100
H	5.21486600	-3.71666800	-2.02809200
H	6.10039900	-2.17959200	-1.76124200
C	5.04024400	-1.38417100	1.11176900
H	5.49632800	-0.52214600	0.61635800
H	4.25390500	-1.03841600	1.78809500
H	5.79983300	-1.93880000	1.67191100
C	3.57378300	-3.92286500	0.67365700
H	2.75022900	-3.58684900	1.31103300
H	3.19475500	-4.61476700	-0.08421000
H	4.33419400	-4.41812700	1.28498100

IN1-C28-PMe₃⁺

E = -1139.367471 a.u.

C	-3.68139100	0.24697500	-2.16411000
C	-2.69838800	0.95900200	-2.84629300
C	-1.34439900	0.69344700	-2.58419400
C	-0.99856700	-0.28192100	-1.58438900
C	-1.99056300	-0.99648400	-0.90798600
C	-3.34049200	-0.74432800	-1.21610600
C	-0.13988400	1.23667300	-3.14593400
C	0.47145600	-0.24912900	-1.43100400
C	0.94450400	0.66432300	-2.50408800
C	2.34661400	0.75511300	-2.75999700

H	2.72485400	1.49880000	-3.45523200
C	3.20024300	-0.14292800	-2.18176200
C	2.70645400	-1.22556900	-1.36210100
C	1.36889400	-1.30896800	-1.04734400
H	-0.09997900	1.97598500	-3.93744400
H	-4.72441200	0.45821300	-2.38071100
H	-2.98285000	1.70881200	-3.57913300
H	4.26235200	-0.07477700	-2.39349900
Cl	2.42364500	1.01219000	1.27629200
P	-0.02991100	-1.15469300	2.08936000
P	0.41279000	3.07984200	-0.18221800
C	-1.15686800	3.82826200	-0.80256000
H	-1.00893800	4.90040700	-0.97319800
H	-1.45803400	3.35147500	-1.73756500
H	-1.94343100	3.68617900	-0.05568500
C	0.89097400	4.20981800	1.20086500
H	1.02685600	5.21569000	0.79026800
H	0.11908600	4.22416400	1.96893800
H	1.82969400	3.86533000	1.64200800
C	1.67187600	3.58755300	-1.43713700
H	1.36834100	3.30245600	-2.44236000
H	1.76762800	4.67740300	-1.38886100
H	2.63554500	3.13223300	-1.19867800
C	-1.74157600	-1.30630700	2.78182900
H	-1.84654100	-2.26822000	3.29401000
H	-1.91100400	-0.49576800	3.49165300
H	-2.48724600	-1.22953400	1.98806700
C	1.00683600	-0.93492300	3.59851200
H	0.71875200	-1.68573900	4.34215500
H	2.06246600	-1.05452000	3.34463000
H	0.85022700	0.06661400	4.00400100
C	0.34154900	-2.92021600	1.66148000
H	0.15110500	-3.52895900	2.55194600
H	-0.29819500	-3.27727400	0.84882200
H	0.97526000	-2.15366700	-0.50455800
H	1.38983100	-3.02993600	1.37911000
H	-1.72155600	-1.77462200	-0.20493800
Cl	-0.91370700	1.87861900	2.52611600
Ir	0.19223500	0.79186100	0.60919000
P	-4.65364900	-1.69695800	-0.41599600
C	-5.95756700	-2.10160300	-1.62332400
H	-6.72985500	-2.68683600	-1.11418700
H	-6.40264800	-1.18697600	-2.02412100
H	-5.52290700	-2.68839100	-2.43753800
C	-5.40912500	-0.75338400	0.94948500
H	-6.22298200	-1.34207500	1.38469800
H	-4.65116700	-0.54818800	1.71042700
H	-5.80248800	0.18918700	0.55753900
C	-3.99559500	-3.26457600	0.23602200

H	-3.54559600	-3.83682100	-0.58030300
H	-3.25591100	-3.07907700	1.01692600
H	-4.83169500	-3.82882800	0.66085400
P	3.85920700	-2.45321800	-0.70786400
C	5.39827800	-2.45609100	-1.68181400
H	6.03211500	-3.26553400	-1.30674500
H	5.16831100	-2.62827300	-2.73702200
H	5.92266800	-1.50441200	-1.56282100
C	4.29546000	-2.09847400	1.02726300
H	4.84448700	-1.15407100	1.06545900
H	3.38692600	-2.00886600	1.62573500
H	4.92286200	-2.90982200	1.40981900
C	3.14055400	-4.12549500	-0.81547200
H	2.20130300	-4.17571800	-0.26040500
H	2.95955300	-4.36350500	-1.86776500
H	3.85393700	-4.83884500	-0.39113300

TS2-C28-PM₃⁺

E = -1012.985983 a.u.

C	3.27793600	1.26431000	-1.87620300
C	2.37810300	0.71973500	-2.74210500
C	1.03326100	0.45889700	-2.28794800
C	0.85008800	0.39862500	-0.82176000
C	1.66711000	1.25887500	-0.00736700
C	2.89512000	1.59663000	-0.51292500
C	-0.11596000	0.33218900	-3.02981700
C	-1.13178500	0.33846500	-0.82181900
C	-1.32254800	0.48816000	-2.22853300
C	-2.55903300	0.91827900	-2.71798700
H	-2.73099400	0.97917600	-3.78883100
C	-3.55078300	1.33309100	-1.82540900
C	-3.30625200	1.32456200	-0.44338000
C	-2.09546800	0.80907700	0.05999800
H	-0.13361700	0.30389600	-4.11434800
H	4.27693100	1.51687500	-2.21895900
H	2.62364100	0.57529100	-3.79049500
H	-4.49687800	1.69129800	-2.21780500
Cl	-1.89637500	-2.76028000	-0.28592500
P	0.50459000	-1.37386900	1.83594000
C	2.28616200	-1.22783000	2.26716800
H	2.39059400	-1.24000700	3.35720400
H	2.82047900	-2.07724500	1.83549200
H	2.70309000	-0.30250500	1.86666700
C	-0.03793800	-2.93720300	2.62786500
H	0.21055400	-2.87979900	3.69353300
H	-1.11512800	-3.05452400	2.49930400
H	0.47454000	-3.78266500	2.16736200
C	-0.34946600	-0.09996900	2.85356800
H	0.03398600	-0.18591700	3.87624500

H	-0.17276700	0.91362200	2.48897700
H	-1.94316200	0.73635100	1.12636300
H	-1.42256600	-0.30846600	2.86349300
H	1.38177900	1.49241600	1.00963800
Cl	1.46581500	-3.38796000	-0.45189500
Ir	0.16569300	-1.35281900	-0.41385200
P	4.14342000	2.37031200	0.55163000
C	4.75339900	3.88383400	-0.25399500
H	5.56447400	4.30611500	0.34730600
H	5.12530100	3.63597700	-1.25260700
H	3.93339600	4.60323200	-0.33529600
C	5.53122100	1.21270700	0.77845600
H	6.29378500	1.69521900	1.39794100
H	5.16945400	0.30532000	1.27040400
H	5.95593400	0.95854400	-0.19662700
C	3.43901400	2.78656400	2.17359400
H	2.58240000	3.45446400	2.04729000
H	3.14072600	1.87471100	2.69804700
H	4.21638600	3.29685900	2.75102400
P	-4.56541600	1.90916300	0.72330400
C	-5.69985600	3.06547200	-0.10299800
H	-6.24794300	2.55340000	-0.89828100
H	-6.41014700	3.43687500	0.64193000
H	-5.12966300	3.90084200	-0.51901500
C	-5.50947800	0.49887200	1.38682500
H	-6.24381800	0.86774800	2.10954500
H	-6.01848800	-0.00990900	0.56294400
H	-4.82023600	-0.19556500	1.87615400
C	-3.75027100	2.77534200	2.10158000
H	-3.09500100	2.08766500	2.64312600
H	-3.16828300	3.61273400	1.70612400
H	-4.52197200	3.14888100	2.78176700

IN2-C28-PMe₃⁺

E = -1013.064825 a.u.

C	3.66307900	2.54283500	-0.20734100
C	2.40617300	2.99422000	-0.52577000
C	1.28092100	2.10797800	-0.53254000
C	1.44473100	0.70138900	-0.28403200
C	2.74943200	0.29140200	0.09075700
C	3.82186000	1.17253400	0.12069700
C	0.01681400	2.71235800	-0.68058900
C	-1.44690200	0.72347200	-0.28088200
C	-1.25752900	2.13049200	-0.51154200
C	-2.36263300	3.03747900	-0.47961900
H	-2.18323400	4.08672800	-0.69864200
C	-3.62991400	2.60832000	-0.15977600
C	-3.81733500	1.23653500	0.12860900
C	-2.75967600	0.33347900	0.07355000

H	0.02558500	3.78917100	-0.83842200
H	4.50981400	3.22165900	-0.19948800
H	2.24567400	4.04289600	-0.76201600
H	-4.45582200	3.31030300	-0.13114300
Cl	-1.72934300	-2.19113200	-1.57894500
P	-0.01396400	-1.40856500	1.41905100
C	1.33786400	-2.59847800	1.77727400
H	1.22932800	-2.91142700	2.82156100
H	1.23946400	-3.46226800	1.11683700
H	2.31834500	-2.14471100	1.63540700
C	-1.50886800	-2.36662600	1.89379800
H	-1.31060600	-2.80564100	2.87765700
H	-2.38516900	-1.72190500	1.96557000
H	-1.68759900	-3.15631700	1.16229500
C	0.12673000	-0.09588500	2.69528800
H	0.09084800	-0.55439700	3.68936000
H	1.07122600	0.43958100	2.57152100
H	-2.95431700	-0.71780100	0.23562200
H	-0.70386500	0.60674800	2.58403900
H	2.92091300	-0.75516900	0.29252800
Cl	1.69686300	-2.20006800	-1.59335400
Ir	-0.00853900	-0.59099900	-0.68642200
P	5.49699100	0.55272700	0.50177300
C	6.29457300	1.67874200	1.68889300
H	7.30291200	1.30683400	1.89596100
H	6.35541400	2.68292200	1.26039500
H	5.71001300	1.70219200	2.61302900
C	6.46469900	0.51135100	-1.03927000
H	7.47168300	0.14535400	-0.81492200
H	5.97269300	-0.15997700	-1.74911900
H	6.52105400	1.51970700	-1.45917400
C	5.41631800	-1.11836300	1.21134400
H	4.83052800	-1.10093900	2.13439900
H	4.97345800	-1.81100500	0.49088600
H	6.44053800	-1.43362400	1.43401000
P	-5.48228000	0.57252400	0.49076200
C	-6.66030200	1.91847800	0.81272000
H	-6.75578700	2.55292000	-0.07263800
H	-7.63025600	1.46647700	1.04217300
H	-6.32035000	2.51064300	1.66704900
C	-6.03714600	-0.39910500	-0.94430600
H	-7.02789800	-0.81221000	-0.73005200
H	-6.08560500	0.25377000	-1.82079700
H	-5.32657200	-1.20999100	-1.12711500
C	-5.38889800	-0.50744800	1.95344600
H	-4.71755500	-1.34439800	1.74365800
H	-5.01818900	0.06803000	2.80645600
H	-6.39211700	-0.88805400	2.16860000

TS1-C2-OMe

E = -1002.743110 a.u.

C	-3.15240500	-2.00347100	-1.22189600
C	-1.93407800	-2.58460600	-1.36281400
C	-0.88240200	-2.21614300	-0.43356300
C	-0.97160100	-0.86071400	0.17502200
C	-2.32858500	-0.56033600	0.60575800
C	-3.36804700	-1.04682200	-0.13895000
C	0.03765500	-3.03312100	0.13419500
C	0.40175700	-1.02679800	1.45001200
C	0.66733200	-2.41943100	1.29610900
C	1.34274900	-3.12748600	2.29124600
H	1.53989300	-4.18810600	2.15539700
C	1.72062600	-2.48283500	3.47564800
C	1.39123600	-1.14044300	3.67355400
C	0.72421300	-0.42170900	2.67202100
H	0.22369200	-4.05968400	-0.16589600
H	-3.97947400	-2.30634100	-1.85209500
H	-1.77804500	-3.40191200	-2.06170800
H	2.24353000	-3.03716100	4.25047400
Cl	2.59080800	1.65430000	0.58483100
P	-0.83114400	2.28929200	0.80227000
P	1.89005100	-0.83617900	-1.58355800
C	1.16877700	-1.80258400	-2.98951300
H	1.96764700	-2.07870800	-3.68685300
H	0.67821400	-2.70818900	-2.63106800
H	0.43518400	-1.18016200	-3.51040800
C	3.09099300	0.24150900	-2.48982900
H	3.78876600	-0.39919100	-3.04000600
H	2.55629300	0.89019200	-3.18450400
H	3.63260100	0.85881800	-1.77121500
C	3.05997000	-2.02883400	-0.78580600
H	2.54986100	-2.93710600	-0.46584500
H	3.83695500	-2.29548500	-1.51050000
H	3.52249500	-1.55067400	0.08189200
C	-2.40659200	2.70715800	-0.07749300
H	-2.79506300	3.65587700	0.30890900
H	-2.19302100	2.80662500	-1.14419200
H	-3.15602600	1.92603100	0.06201500
C	0.07966300	3.89203400	0.71115800
H	-0.56631800	4.69115400	1.09151500
H	0.99049300	3.82672300	1.30834200
H	0.35247200	4.09453100	-0.32621000
C	-1.34156100	2.30224700	2.58904500
H	-2.04171800	3.13085700	2.74313800
H	-1.82108100	1.37044800	2.89729000
H	0.52371900	0.62555200	2.83703900
H	-0.46133300	2.47033300	3.21657300
H	-2.53393200	0.17316900	1.37111600

Cl	0.29097100	1.94104500	-2.15075800
Ir	0.40894400	0.47190500	-0.20074300
O	-4.61032800	-0.56963100	0.15558700
C	-5.72940400	-0.94712700	-0.65506000
H	-6.58389100	-0.41787000	-0.22982400
H	-5.58874700	-0.63432200	-1.69567200
H	-5.91002900	-2.02679800	-0.60590500
H	1.66514600	-0.63871300	4.59770500

IN1-C2-OMe

E = -1002.783946 a.u.

C	-3.11161200	-2.37335400	-0.66661300
C	-1.92096500	-3.04471700	-0.62311000
C	-0.86697400	-2.55623800	0.21455300
C	-0.98485300	-1.18171400	0.76276000
C	-2.32621600	-0.66824300	0.90907500
C	-3.33934200	-1.21501700	0.17438300
C	0.25508600	-3.17982200	0.72443400
C	0.18314700	-1.01375700	1.61062900
C	0.95046900	-2.25033400	1.57921200
C	2.14841700	-2.32296900	2.26366500
H	2.72169000	-3.24638100	2.27777300
C	2.67043700	-1.16404600	2.89596500
C	1.98177100	0.03170500	2.88086500
C	0.69629300	0.13937500	2.25691300
H	0.59661000	-4.18059100	0.48358400
H	-3.91472100	-2.75121100	-1.28856600
H	-1.79206200	-3.97082200	-1.17764000
H	3.63024100	-1.22723400	3.40153200
Cl	2.29251700	2.17474000	-0.13510400
P	-1.04937700	2.31675300	0.40469700
P	2.01511600	-0.92130600	-1.31752900
C	1.28070700	-2.25141700	-2.37363600
H	2.04392400	-2.61049500	-3.07303700
H	0.93407300	-3.08272100	-1.76053900
H	0.43769600	-1.83895300	-2.93279100
C	2.88842700	0.10063600	-2.59243400
H	3.40797500	-0.57515200	-3.28056800
H	2.17049200	0.71013700	-3.14171800
H	3.60966100	0.75419800	-2.09996200
C	3.47596900	-1.76888300	-0.55784200
H	3.18498000	-2.69736000	-0.06799400
H	4.18907900	-1.99768300	-1.35766500
H	3.95253900	-1.10754400	0.17028600
C	-2.76954900	2.24267500	-0.28940700
H	-3.12945400	3.26830100	-0.42489500
H	-2.75279000	1.73359600	-1.25434700
H	-3.44962600	1.71546700	0.37935700
C	-0.43703400	3.87987700	-0.36906400

H	-1.19595900	4.65821200	-0.23488600
H	0.50031000	4.18587800	0.09561900
H	-0.26495900	3.71154900	-1.43451100
C	-1.35580200	2.87685000	2.14502100
H	-2.00829600	3.75678300	2.12318400
H	-1.84430800	2.09324600	2.73203500
H	0.05351300	0.94270400	2.58229900
H	-0.40870600	3.14983800	2.62122600
H	-2.52403000	0.16155000	1.57479000
Cl	-0.38936700	0.87236000	-2.33494700
Ir	0.45233800	0.46016900	-0.08493400
O	-4.57539300	-0.62429400	0.28036100
C	-5.68931200	-1.21268100	-0.39079800
H	-6.55051100	-0.59739900	-0.12202100
H	-5.55827900	-1.19219600	-1.47956600
H	-5.86109300	-2.24319000	-0.05621800
H	2.38113900	0.89885000	3.39820600

TS2-C2-OMe

E = -876.419741 a.u.

C	3.58379300	0.86324500	-1.03851400
C	2.56631000	1.39158800	-1.77244100
C	1.26562300	1.53527400	-1.16352400
C	0.98837600	0.68185300	0.01892300
C	2.09957300	0.39431100	0.88286700
C	3.35691000	0.42334600	0.33148400
C	0.29518000	2.46334400	-1.44677500
C	-0.61341400	1.55927800	0.60099200
C	-0.64598200	2.63085400	-0.33948600
C	-1.38376400	3.78127000	-0.06661400
H	-1.43769300	4.58255000	-0.79926700
C	-2.00808900	3.91594300	1.18365200
C	-1.87751100	2.91836500	2.15288600
C	-1.18380300	1.73315300	1.86076500
H	0.32625200	3.13235800	-2.30115300
H	4.58162300	0.82088300	-1.45719300
H	2.75072300	1.82362200	-2.75232100
H	-2.57082900	4.81828200	1.40736500
H	-2.33645700	3.04431200	3.12961500
Cl	-3.14950600	-0.23869200	-0.65391700
P	-0.44553300	-1.93344800	1.10210700
C	1.05270900	-2.98359000	0.90114600
H	1.05532100	-3.76541600	1.66855900
H	1.03613100	-3.43783400	-0.09215300
H	1.95153600	-2.36935200	0.99909100
C	-1.85847500	-3.10747600	1.03501100
H	-1.70158400	-3.89148200	1.78447400
H	-2.78258600	-2.56572900	1.24750600
H	-1.92273400	-3.54652200	0.03810400

C	-0.42233400	-1.46014900	2.88327100
H	-0.22079500	-2.36800800	3.46292700
H	0.34992500	-0.72079200	3.10327000
H	-1.14128200	0.94938000	2.60423800
H	-1.40150200	-1.06830700	3.17021000
H	1.96248600	-0.02321100	1.87203000
Cl	-0.66486400	-2.10788400	-2.11484000
Ir	-0.59076900	-0.32571600	-0.47108100
O	4.37529200	-0.02656900	1.11226100
C	5.68998100	-0.17049700	0.55897700
H	6.29772800	-0.58127500	1.36676200
H	5.68824300	-0.86612300	-0.28740900
H	6.09915100	0.79819100	0.25204600

IN2-C2-OMe

E = -876.508338 a.u.

C	3.74392800	1.93316100	-0.14311200
C	2.57501400	2.61435000	-0.37278700
C	1.30086700	1.95875900	-0.36516000
C	1.22185500	0.52371000	-0.20129900
C	2.42765400	-0.13161900	0.05939500
C	3.65982800	0.53696300	0.09796800
C	0.17655000	2.78884700	-0.40122800
C	-1.64137600	1.10024600	-0.01881200
C	-1.18317800	2.45255000	-0.19244200
C	-2.08126900	3.55705900	-0.06351300
H	-1.69685400	4.55915600	-0.23825300
C	-3.39818000	3.36672100	0.29608200
C	-3.84555400	2.05032900	0.52546200
C	-2.99423000	0.96144300	0.36886700
H	0.37985700	3.85402100	-0.50581600
H	4.69524300	2.45041800	-0.14172300
H	2.60350700	3.68709200	-0.54595300
H	-4.07605300	4.20875100	0.40130300
H	-4.88154000	1.87696300	0.80829400
Cl	-2.54392500	-1.75067200	-1.29887600
P	-0.50582400	-1.22416700	1.57480600
C	0.52973600	-2.72144400	1.83031200
H	0.46647300	-2.99985100	2.88837300
H	0.14633600	-3.53380100	1.20903300
H	1.57001700	-2.52700700	1.56654800
C	-2.14329400	-1.75303200	2.22559000
H	-1.97228100	-2.25515600	3.18412400
H	-2.78889800	-0.88825800	2.38629800
H	-2.61639600	-2.44049400	1.52221400
C	0.08770200	-0.00936300	2.82119400
H	-0.01962000	-0.44086000	3.82235300
H	1.13662100	0.23336100	2.63746300
H	-3.40293100	-0.03143600	0.49552500

H	-0.51307100	0.90144900	2.74965100
H	2.45405400	-1.20640200	0.17933400
Cl	0.79743700	-2.31951300	-1.62577900
Ir	-0.49466100	-0.45367000	-0.53234700
O	4.73322500	-0.23419100	0.35078600
C	6.04447300	0.35227500	0.33985200
H	6.72938900	-0.46946600	0.55177000
H	6.26923400	0.77825700	-0.64347700
H	6.13453000	1.11930500	1.11623000

TS1-C28-OMe

E = -1117.276113 a.u.

C	3.26819900	1.45411200	-2.00506900
C	2.28133500	0.86839900	-2.73183900
C	0.94644000	0.81376400	-2.17096600
C	0.83840800	0.83282600	-0.68499200
C	1.73644700	1.81595000	-0.10064700
C	2.94662000	2.03070600	-0.70336500
C	-0.22654700	0.99941400	-2.82656600
C	-1.01358500	1.06674700	-0.53843500
C	-1.32588100	1.27738400	-1.91491300
C	-2.53779100	1.86112800	-2.26846200
H	-2.77228500	2.02252600	-3.31787200
C	-3.44905200	2.28390100	-1.28785500
C	-3.11057000	2.14885000	0.06075500
C	-1.88528600	1.55633000	0.42967200
H	-0.33000900	1.03572400	-3.90680800
H	4.26167500	1.57010400	-2.42033200
H	2.44795100	0.56463400	-3.76192900
H	-4.38734800	2.73430400	-1.58958300
Cl	-1.99338500	-1.78780100	1.41612000
P	0.75660500	0.10176400	2.45015400
P	-0.50027100	-2.11052800	-1.59499000
C	0.74189900	-2.38507800	-2.94222700
H	0.45789400	-3.27169100	-3.52019400
H	0.79212400	-1.52390000	-3.60945700
H	1.72606100	-2.54827300	-2.49311500
C	-0.80003200	-3.85314800	-1.04828300
H	-1.16807500	-4.43084400	-1.90306300
H	0.12838000	-4.28985200	-0.67852100
H	-1.53915100	-3.85460000	-0.24536800
C	-2.07342500	-1.78071600	-2.51329400
H	-1.97628800	-0.92346400	-3.17889600
H	-2.32541300	-2.66601500	-3.10744300
H	-2.87293600	-1.58736900	-1.79279100
C	2.58959800	0.22002700	2.69229900
H	2.80593400	0.33922800	3.75958300
H	3.05146200	-0.69982100	2.32635000
H	3.00443100	1.06804900	2.14420600

C	0.27575200	-1.06415600	3.79794900
H	0.67252000	-0.69400200	4.74979300
H	-0.81203900	-1.13443000	3.84399000
H	0.68349300	-2.05374300	3.58323900
C	0.14755800	1.70263100	3.16943900
H	0.73166300	1.92056100	4.07053100
H	0.24255100	2.54013200	2.47464500
H	-1.69471800	1.43524300	1.48431300
H	-0.90364900	1.59736700	3.45438300
H	1.56048300	2.23521100	0.87889400
Cl	1.49357200	-2.59102300	0.93269300
Ir	0.09256700	-0.70408800	0.27205000
O	3.84962200	2.78104700	-0.01100500
C	5.16320200	2.98600200	-0.54375500
H	5.68235900	3.59578500	0.19775900
H	5.69359900	2.03544200	-0.66881700
H	5.12553800	3.52570500	-1.49660800
O	-3.89715300	2.54467000	1.10204500
C	-5.16530400	3.13087600	0.80385100
H	-5.80363200	2.42819800	0.25448200
H	-5.61987900	3.35902300	1.76952200
H	-5.04618700	4.05556300	0.22583600

IN1-C28-OMe

E = -1117.333408 a.u.

C	4.63843500	-1.68928900	0.58528000
C	3.61964100	-2.59698800	0.87396800
C	2.32493400	-2.36937800	0.38588200
C	2.03339500	-1.17139700	-0.35237500
C	3.06259100	-0.30773300	-0.68987500
C	4.36213800	-0.56396700	-0.21933400
C	1.16339500	-3.21136400	0.36144000
C	0.59191400	-1.18409700	-0.66863700
C	0.15791600	-2.55915800	-0.33437100
C	-1.01832400	-3.10010500	-0.90897600
H	-1.30479000	-4.12298900	-0.67796700
C	-1.77813200	-2.36414800	-1.78870400
C	-1.36109900	-1.05191900	-2.17288900
C	-0.15155500	-0.46698500	-1.69488500
H	1.10772700	-4.21804600	0.76312200
H	5.63897300	-1.87070400	0.95918700
H	3.84052400	-3.48883300	1.45515900
H	-2.67166000	-2.79287000	-2.22351500
Cl	-2.65097500	2.02634800	-0.01857100
P	0.69760400	2.31523900	-0.36825800
P	-2.35626100	-0.89436000	1.31018200
C	-1.92268200	-2.47497100	2.18329000
H	-2.70119400	-2.69260900	2.92323400
H	-1.85061000	-3.31493800	1.49250900

H	-0.96421100	-2.35011500	2.69531700
C	-3.05373900	0.05287500	2.74483500
H	-3.93261600	-0.48010200	3.12459000
H	-2.30131000	0.13348700	3.52988000
H	-3.33669700	1.05430500	2.41729100
C	-3.93258900	-1.31892800	0.42961500
H	-3.77091300	-2.07785300	-0.33450400
H	-4.66081800	-1.69343400	1.15762500
H	-4.32046600	-0.40862700	-0.03478100
C	2.29641200	2.51875500	0.56132200
H	2.09578200	3.11154800	1.45677700
H	2.70693500	1.55934900	0.86939700
H	3.02327900	3.04705300	-0.06536200
C	-0.09204900	3.94043900	0.02575500
H	0.66420300	4.72563900	-0.09053000
H	-0.93181000	4.12942200	-0.64358300
H	-0.45528500	3.92763600	1.05554100
C	1.15222600	2.61474600	-2.14385200
H	1.63463900	3.59455000	-2.22857700
H	1.83326900	1.85629000	-2.53750300
H	0.32983600	0.23483100	-2.36484400
H	0.23751600	2.61506400	-2.74590800
H	2.90555600	0.56112600	-1.31446400
Cl	0.02625700	1.06007200	2.51281700
Ir	-0.67806300	0.44513400	0.18970200
O	5.30250600	0.34535800	-0.59953700
C	6.65532400	0.15303800	-0.17927800
H	7.21576900	0.98824300	-0.60298000
H	6.73543600	0.17460400	0.91396300
H	7.05682500	-0.79202900	-0.56391000
O	-2.00749900	-0.33465000	-3.09586000
C	-3.33164000	-0.71504600	-3.51160500
H	-3.99291000	-0.80711200	-2.64559100
H	-3.67271800	0.09747700	-4.15383700
H	-3.30648500	-1.64994300	-4.08031700

TS2-C28-OMe

E = -990.952447 a.u.

C	3.03538000	2.43922900	-0.91969300
C	2.17556800	2.08594400	-1.91458700
C	0.87916300	1.56474800	-1.56209000
C	0.72694900	0.99920900	-0.19451000
C	1.49749600	1.62881600	0.84329200
C	2.65604900	2.27005800	0.47573500
C	-0.29519200	1.67598700	-2.26164700
C	-1.14912000	0.87126000	-0.16138800
C	-1.46764100	1.48093500	-1.41153900
C	-2.74288800	1.99124400	-1.61951400
H	-3.00892000	2.43090200	-2.57736200

C	-3.68591100	1.98947900	-0.57525500
C	-3.32965800	1.49497500	0.68350600
C	-2.05312000	0.93218100	0.88956800
H	-0.36025500	2.03919600	-3.28290300
H	3.98252300	2.90217000	-1.16671700
H	2.39906300	2.31288400	-2.95362300
H	-4.67238200	2.40147900	-0.75234300
Cl	-1.86139300	-2.22056100	-1.23371700
P	0.62106700	-1.65607300	1.54544300
C	2.42387800	-1.63525000	1.92072600
H	2.59991000	-2.09381100	2.89994800
H	2.95420500	-2.19484600	1.14711900
H	2.78616700	-0.60369400	1.92741600
C	0.12217800	-3.42029300	1.69873000
H	0.40738900	-3.78730500	2.69115600
H	-0.96029600	-3.49691100	1.57033300
H	0.61671300	-4.00758100	0.92329100
C	-0.14528900	-0.91291700	3.04823000
H	0.31178900	-1.39435900	3.92009900
H	0.02315400	0.16351000	3.11054000
H	-1.83637100	0.50949600	1.85993700
H	-1.21859400	-1.11988200	3.05438500
H	1.30266800	1.44900200	1.89299500
Cl	1.54462300	-2.60331400	-1.37079200
Ir	0.14396900	-0.82646100	-0.49407600
O	3.46264000	2.69520900	1.48552100
C	4.72246400	3.30726800	1.18077300
H	5.16713400	3.54690000	2.14799400
H	5.37790700	2.61642000	0.63908200
H	4.58530900	4.22888200	0.60434700
O	-4.14792400	1.48613500	1.77414200
C	-5.46699000	2.01834600	1.63610200
H	-6.04130500	1.45692200	0.88931900
H	-5.93364000	1.90723000	2.61636300
H	-5.43628400	3.07978900	1.36157300

IN2-C28-OMe

E = -991.047517 a.u.

C	3.65348400	2.55700300	-0.09827200
C	2.38095900	2.97933800	-0.40453800
C	1.26779800	2.08323900	-0.42371000
C	1.46668200	0.67144500	-0.19590200
C	2.76653600	0.28278200	0.14171300
C	3.83847500	1.18501200	0.19967200
C	-0.00027500	2.67216200	-0.56534300
C	-1.47055500	0.66894800	-0.20176200
C	-1.26812900	2.08285300	-0.41970100
C	-2.37972000	2.98051800	-0.39799300
H	-2.20013000	4.03245300	-0.60721400

C	-3.65464200	2.55905700	-0.09984600
C	-3.84533000	1.18410300	0.17796300
C	-2.77576200	0.27888600	0.11292900
H	-0.00073000	3.75095500	-0.71601700
H	4.47892000	3.25789400	-0.08215100
H	2.20397800	4.02999400	-0.62236000
H	-4.47757600	3.26278800	-0.07864800
Cl	-1.68655500	-2.32110100	-1.41220500
P	-0.00451900	-1.27768400	1.59154900
C	1.32158500	-2.47141000	2.03626100
H	1.23669200	-2.68782500	3.10730700
H	1.18644900	-3.38966900	1.46033000
H	2.30808500	-2.05652600	1.82649100
C	-1.52558800	-2.13815400	2.16766800
H	-1.33055300	-2.52274500	3.17496000
H	-2.36743100	-1.44516800	2.20766500
H	-1.76171800	-2.96333100	1.49308000
C	0.19037500	0.11252800	2.78036100
H	0.11071800	-0.27281900	3.80266400
H	1.16521400	0.58570800	2.64174500
H	-3.01270200	-0.76629300	0.25815800
H	-0.59801000	0.84953100	2.60557400
H	2.99916100	-0.76018300	0.31087000
Cl	1.71174900	-2.27912000	-1.44991900
Ir	0.00011200	-0.65134700	-0.55826000
O	5.03279300	0.65180900	0.52967100
C	6.19554200	1.49235900	0.55061000
H	7.02185200	0.83685700	0.82865100
H	6.38182400	1.92233600	-0.43948500
H	6.08839900	2.28897200	1.29503700
O	-5.04270900	0.65040900	0.49625700
C	-6.19890900	1.49892700	0.54254600
H	-6.38840900	1.95229100	-0.43642500
H	-7.02856000	0.84397900	0.81176500
H	-6.08042200	2.27816600	1.30359400

TS1-C5-OMe

E = -1002.740863 a.u.

C	1.50286500	-2.35263400	-2.91825700
C	2.19580700	-1.29123100	-2.42437600
C	1.90949500	-0.87211900	-1.06638700
C	0.55367900	-1.17541000	-0.54260900
C	0.14191000	-2.54052600	-0.87872900
C	0.54254000	-3.04944400	-2.07599400
C	2.77687200	-0.42276300	-0.12310000
C	0.80939900	-0.65824000	1.27645700
C	2.21356100	-0.43380800	1.22581200
C	2.97535900	-0.38847100	2.39317300
H	4.04258500	-0.19630800	2.33193200

C	2.36546300	-0.62973800	3.63002200
C	1.00589500	-0.94359700	3.68733700
C	0.23551300	-0.96701600	2.51650800
H	1.72021400	-2.74584500	-3.90736000
H	3.02161600	-0.83956200	-2.96652100
H	2.95847300	-0.59984300	4.54013900
Cl	-1.68239100	1.80156700	1.70791200
P	-2.58430400	-1.21132600	0.22958200
P	0.72943800	2.15894700	-0.58624800
C	1.72857100	2.17955500	-2.14561800
H	2.01553000	3.21294100	-2.37065500
H	2.63085600	1.57562500	-2.04112300
H	1.12332600	1.78675900	-2.96771100
C	-0.26904100	3.70264200	-0.79265200
H	0.41641300	4.55414900	-0.86342800
H	-0.86948600	3.63575100	-1.70077500
H	-0.93177800	3.82324900	0.06582700
C	1.93856200	2.69815900	0.70799000
H	2.82656500	2.06633500	0.71482700
H	2.24359000	3.72826400	0.49387000
H	1.45832800	2.65872100	1.68912200
C	-3.14118600	-2.10027900	-1.29706300
H	-4.16345500	-2.46395500	-1.14653400
H	-3.12040000	-1.40638600	-2.14030800
H	-2.48847300	-2.94708800	-1.51652400
C	-4.10447700	-0.27281800	0.69375000
H	-4.95047300	-0.96752800	0.73900400
H	-3.95553100	0.20354500	1.66376000
H	-4.29494900	0.50086400	-0.05231000
C	-2.61958100	-2.55638900	1.51110100
H	-3.49018000	-3.19324000	1.31816400
H	-1.71810000	-3.17340300	1.49641400
H	-0.82305500	-1.15723100	2.60078800
H	-2.72958000	-2.11311000	2.50510500
H	-0.56945300	-3.07103100	-0.26176100
Cl	-2.17891600	1.23400400	-1.76116700
Ir	-0.68435400	0.25734200	-0.10425500
H	0.53022500	-1.14899800	4.64247200
H	0.12463700	-3.98936200	-2.42771600
O	4.06692400	-0.03091300	-0.35250100
C	5.03275300	-1.10129000	-0.39570800
H	4.82365400	-1.77370600	-1.23473400
H	6.00649100	-0.62633200	-0.53310900
H	5.02375100	-1.66784100	0.54219400

IN1-C5-OMe

E = -1002.782968 a.u.

C	1.21057200	-3.65435200	-1.20207000
C	2.13818500	-2.65100500	-1.16001600

C	1.98389900	-1.61668400	-0.17932500
C	0.67876700	-1.46830900	0.51921600
C	-0.10766800	-2.68590200	0.61717300
C	0.12127200	-3.71117000	-0.24871500
C	2.89125300	-0.72514600	0.34997900
C	0.90300600	-0.43457400	1.53149400
C	2.25537700	0.05949900	1.39159300
C	2.67667000	1.14606800	2.13978200
H	3.68671700	1.53265100	2.04089300
C	1.76053600	1.79215900	3.00094500
C	0.45676500	1.33854900	3.13435900
C	0.00418900	0.20028400	2.41411100
H	1.32091000	-4.46659600	-1.91624000
H	3.01122100	-2.66160400	-1.80676000
H	2.09027200	2.65743500	3.56960500
Cl	-1.82362700	2.49383000	0.05914400
P	-2.77539400	-0.68674700	0.60733500
P	0.95650800	1.50150700	-1.42632100
C	2.02957900	0.54730700	-2.59625700
H	2.36653800	1.22444200	-3.38902300
H	2.90153800	0.13851800	-2.08660100
H	1.44996400	-0.26575400	-3.03913100
C	0.06005000	2.60730500	-2.61137700
H	0.79007800	3.02701200	-3.31193200
H	-0.69001400	2.03374500	-3.15824700
H	-0.43441800	3.40938600	-2.06293500
C	2.13674500	2.70723800	-0.66874200
H	3.00145700	2.19437100	-0.24814600
H	2.47752300	3.39571400	-1.45016200
H	1.63221500	3.27445700	0.11791900
C	-3.21865900	-2.39745600	0.03411100
H	-4.30914700	-2.46511600	-0.03970300
H	-2.77614400	-2.58896200	-0.94484400
H	-2.87135700	-3.15110100	0.74299600
C	-4.17506500	0.28062000	-0.11663400
H	-5.11183000	-0.24445400	0.09844600
H	-4.19818500	1.28167400	0.31354200
H	-4.03678600	0.36220400	-1.19706600
C	-3.26933800	-0.74946700	2.39263900
H	-4.31379700	-1.07366800	2.46004700
H	-2.64792200	-1.45886000	2.94761300
H	-0.93177800	-0.25561700	2.69320100
H	-3.17529300	0.24497500	2.83997600
H	-0.89063500	-2.74549900	1.36303400
Cl	-1.42786300	-0.43055300	-2.25443200
Ir	-0.64071000	0.27000400	-0.09340900
H	-0.22358000	1.82663800	3.82588400
H	-0.51092600	-4.59492700	-0.22914000
O	4.15201700	-0.50627500	-0.13962900

C	5.22355200	-0.87822900	0.74459600
H	5.18331000	-1.95368800	0.95670900
H	6.15043300	-0.63785300	0.21866300
H	5.17866900	-0.31714600	1.68445900

TS2-C5-OMe

E = -876.414858 a.u.

C	3.621774	0.891945	-0.996211
C	2.612022	1.426659	-1.742476
C	1.307361	1.539501	-1.138906
C	1.020729	0.684651	0.034897
C	2.136408	0.405388	0.910044
C	3.388302	0.448009	0.362754
C	0.329719	2.477977	-1.396755
C	-0.618241	1.543835	0.613187
C	-0.648564	2.622829	-0.310324
C	-1.432527	3.745420	-0.057864
H	-1.506602	4.542535	-0.791322
C	-2.093242	3.851153	1.177078
C	-1.952656	2.854156	2.144710
C	-1.218483	1.690887	1.861583
H	-2.695334	4.730469	1.388770
H	-2.439268	2.958555	3.110556
Cl	-3.014221	-0.026398	-0.944771
P	-0.447256	-1.934231	1.123468
C	1.010136	-3.039671	0.914257
H	0.981728	-3.830796	1.671395
H	0.983531	-3.478638	-0.085235
H	1.929855	-2.458550	1.024317
C	-1.910013	-3.046777	1.059233
H	-1.800614	-3.823507	1.824503
H	-2.812556	-2.461026	1.251204
H	-1.980885	-3.500664	0.069536
C	-0.394175	-1.473104	2.908086
H	-0.169583	-2.383656	3.474742
H	0.370554	-0.724759	3.122193
H	-1.177702	0.899508	2.596271
H	-1.372930	-1.099315	3.219568
H	1.979970	0.023747	1.911612
Cl	-0.659129	-2.160331	-2.048489
Ir	-0.545256	-0.324370	-0.460519
H	4.236311	0.102276	0.948228
H	4.631767	0.849034	-1.393450
H	2.792277	1.865264	-2.719505
O	0.329626	3.312709	-2.467954
C	1.080140	4.539560	-2.310762
H	0.887062	5.124667	-3.211623
H	0.742909	5.091567	-1.427728
H	2.149901	4.321914	-2.226162

IN2-C5-OMe

E = -876.496666 a.u.

C	4.160846	0.864392	-1.256738
C	3.085502	1.721630	-1.269212
C	1.778758	1.274122	-0.888660
C	1.539632	-0.112979	-0.602998
C	2.690387	-0.938200	-0.547818
C	3.959179	-0.473910	-0.856411
C	0.782534	2.274748	-0.689897
C	-1.083414	0.821690	0.169195
C	-0.545586	2.106048	-0.192066
C	-1.306905	3.298059	0.030847
H	-0.916930	4.242424	-0.328560
C	-2.517216	3.260246	0.684195
C	-3.009055	2.016335	1.129261
C	-2.313625	0.844635	0.870400
H	-3.084699	4.171398	0.849557
H	-3.962540	1.966836	1.650126
Cl	-2.592675	-1.893470	-0.763362
P	0.045795	-1.682399	1.565618
C	0.788634	-3.363436	1.581503
H	0.951103	-3.652538	2.625845

H	0.095941	-4.061425	1.105655
H	1.736970	-3.379626	1.043624
C	-1.455454	-1.896857	2.606641
H	-1.163202	-2.484215	3.484034
H	-1.834489	-0.928349	2.936829
H	-2.226511	-2.426434	2.044292
C	1.146891	-0.644069	2.608785
H	1.181325	-1.065577	3.619256
H	2.153966	-0.619162	2.187456
H	-2.766725	-0.093393	1.156311
H	0.745384	0.372486	2.649571
H	2.571971	-1.987390	-0.313390
Cl	0.507779	-2.907415	-1.806775
Ir	-0.291861	-0.877940	-0.504041
H	4.802254	-1.160067	-0.822602
H	5.148549	1.212055	-1.545014
H	3.218840	2.754139	-1.568532
O	1.170417	3.555299	-0.930511
C	1.759738	4.286996	0.169502
H	1.995818	5.275094	-0.227153
H	1.046480	4.371461	0.995635
H	2.672367	3.788354	0.511255