DFT supporting information for:

DFT Investigation of the Mechanism of Phosphine-Thioether Isomerization in the Triosmium Cluster $Os_3(CO)_{10}(Ph_2PCH_2CH_2SMe)$: Migratory Preference for the Formation of an Edge-Bridged Thioether Versus Phosphine Moiety

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1) B3LYP geometries and energies for all optimized minima and transition structures (S2-S20)
2) The complete list of authors for ref. 9 (S21)

1) B3LYP geometries and energies for all optimized minima and transition structures (S2-S44)

Species A1
HF energy = -2727.2145652
No imaginary frequency
Zero-point correction = 0.367820 (Hartree/Particle)
Thermal correction to Energy = 0.412748
Thermal correction to Enthalpy = 0.413692
Thermal correction to Gibbs Free Energy = 0.284575
Sum of electronic and zero-point Energies = -2726.846745
Sum of electronic and thermal Energies = 2726.801817
Sum of electronic and thermal Enthalpies = -2726.800873
Sum of electronic and thermal Free Energies = -2726.929990

Coordinates: **A1**

Os	-1.14977300	2.64316700	8.49558300
Os	-3.92057200	3.55412500	9.02094200
Os	-3.39654100	0.69269900	8.74567500
P	0.79160800	1.24912100	8.43344300
S	-2.18484200	-1.29169300	7.94867600
C	-4.12844000	0.95802300	6.94306500
O	-4.61268400	1.02623900	5.90053800
C	-2.59962200	0.48217600	10.51725600
O	-2.15328200	0.21786600	11.55055200
C	-3.81096100	3.90192100	7.08105100
O	-3.81022600	4.19413200	5.96968700
C	-3.91061400	3.06696300	10.93280500
O	-3.98770400	2.84544100	12.05746700
C	-3.55314100	5.41605900	9.40285600
O	-3.35527500	6.51869200	9.66906500
C	-0.36305100	4.34499000	8.12904300
O	0.08821800	5.38142400	7.88024800
C	-1.00771300	2.91947300	10.43275000
O	-0.85330800	3.12275100	11.55719100
C	-1.50332400	2.20295600	6.62425000
O	-1.60469500	1.95567200	5.49793200
C	-5.05971500	-0.01715600	9.34075300
O	-6.05898800	-0.43798900	9.74827300
C	-5.85443500	3.52072500	8.99411300
O	-7.00467100	3.53193600	8.94394000
C	-2.89655300	-2.76177400	8.78242600
H	-3.93712000	-2.83483900	8.45493200
H	-2.86497400	-2.64361500	9.87010700
H	-2.34854700	-3.65897700	8.47362000
C	-0.48556400	-1.39047400	8.67058500
H	-0.54512800	-1.14448900	9.73490500
H	-0.20194900	-2.44692700	8.58049100

C	0.54321900	-0.53393400	7.91355200
H	0.29133500	-0.49321200	6.84585700
H	1.52241800	-1.02742500	7.96889900
C	1.73851300	1.14316000	10.01449500
C	2.21205400	2.34530500	10.57137000
H	2.00515400	3.29108000	10.07465000
C	2.94690400	2.34061500	11.75592500
H	3.30484200	3.28078500	12.16966900
C	3.21462400	1.13521200	12.41228000
H	3.78078800	1.13241900	13.34109900
C	2.75147100	-0.06364100	11.87001300
H	2.95598400	-1.00712900	12.37177200
C	2.02265100	-0.06159500	10.67583300
H	1.68738900	-1.01237200	10.27152200
C	2.13215700	1.68917100	7.22651100
C	1.89212500	2.55477300	6.14953600
H	0.91942200	3.01871500	6.02684100
C	2.90211300	2.83510100	5.22415300
H	2.69714500	3.51139800	4.39716000
C	4.16453700	2.25765900	5.36544800
H	4.95131800	2.48090200	4.64791600
C	4.41662300	1.39634300	6.43767100
H	5.40045800	0.94784700	6.55992700
C	3.40943400	1.11426700	7.36085100
H	3.62681200	0.45624200	8.19943000

Species TSA1A2
HF energy = -2727.1971416
One imaginary frequency: 80*i*
Zero-point correction = 0.366669 (Hartree/Particle)
Thermal correction to Energy = 0.410806
Thermal correction to Enthalpy = 0.411750
Thermal correction to Gibbs Free Energy = 0.285964
Sum of electronic and zero-point Energies = -2726.830472
Sum of electronic and thermal Energies = -2726.786336
Sum of electronic and thermal Enthalpies = -2726.785391
Sum of electronic and thermal Free Energies = -2726.911177

Coordinates: **TSA1A2**

Os	-1.15346900	2.63797600	8.41368000
Os	-3.96326800	3.45196900	8.58333000
Os	-3.26473400	0.78589900	9.40160800
P	0.80695100	1.25518900	8.44905900
S	-2.23829700	-0.97768300	7.97002000
C	-4.32420400	1.35759400	7.69651100

O	-4.86780700	0.97237500	6.73197400
C	-2.09695000	0.36482000	10.90377200
O	-1.44484000	0.04015400	11.79861600
C	-3.84153300	4.09509100	6.73562600
O	-3.80603100	4.53889700	5.67510100
C	-3.95065300	2.48717300	10.50479100
O	-4.21492500	2.71433900	11.62961900
C	-3.40937800	5.10956400	9.41406600
O	-3.11463700	6.11660000	9.88647400
C	-0.37016900	4.27568600	7.81300500
O	0.07385900	5.28368700	7.46096300
C	-1.02182400	3.17343500	10.29921300
O	-0.92167900	3.51910200	11.39229500
C	-1.60980600	2.03129500	6.61116200
O	-1.84299600	1.68431800	5.53562700
C	-4.76419700	-0.23495800	10.03057600
O	-5.65686100	-0.84656400	10.43461500
C	-5.87091200	3.72936300	8.74440200
O	-7.00208100	3.92420900	8.83375000
C	-3.03683000	-2.57165200	8.39537700
H	-4.09073600	-2.47674100	8.11960600
H	-2.95592100	-2.77814400	9.46736200
H	-2.57808600	-3.37588700	7.80997600
C	-0.53056100	-1.38346100	8.54742700
H	-0.50794600	-1.34404800	9.64039300
H	-0.36993500	-2.42493800	8.24169400
C	0.56115100	-0.52080700	7.89952300
H	0.38817800	-0.46097900	6.81736500
H	1.52481500	-1.03391200	8.02122900
C	1.70369400	1.14645200	10.05522900
C	2.14452000	2.34914200	10.63732500
H	1.94769400	3.29676500	10.13997700
C	2.83923900	2.34162100	11.84600600
H	3.17297100	3.28154500	12.27988700
C	3.09816800	1.13282000	12.49971900
H	3.63228200	1.12758800	13.44727300
C	2.66777700	-0.06638600	11.93141600
H	2.86543200	-1.01186800	12.43195400
C	1.97936000	-0.06155900	10.71398000
H	1.66638200	-1.01175600	10.29067000
C	2.16859100	1.69288600	7.26594100
C	1.88481300	2.37645200	6.07346300
H	0.87228000	2.70403700	5.85943000
C	2.89865000	2.65044500	5.15177100
H	2.65944600	3.18576000	4.23550100
C	4.21048700	2.24971600	5.41209300
H	5.00124200	2.47086100	4.69835200

C	4.50447800	1.56801600	6.59609700
H	5.52485500	1.25542600	6.80846100
C	3.49191600	1.28889500	7.51598400
H	3.73823200	0.76468100	8.43606600

Species A2
HF energy = -2727.2133354
No imaginary frequency
Zero-point correction = 0.367622 (Hartree/Particle)
Thermal correction to Energy = 0.412507
Thermal correction to Enthalpy = 0.413451
Thermal correction to Gibbs Free Energy = 0.285099
Sum of electronic and zero-point Energies = -2726.845713
Sum of electronic and thermal Energies = -2726.800829
Sum of electronic and thermal Enthalpies = -2726.799885
Sum of electronic and thermal Free Energies = -2726.928237

Coordinates: **A2**

Os	-1.14553300	2.66052400	8.31516000
Os	-4.05289500	3.12521100	8.13388800
Os	-3.01154400	0.95034200	9.88033400
P	0.80857900	1.30285700	8.44701800
S	-2.30951400	-0.68821900	8.09772400
C	-4.45481300	1.49794000	7.11096500
O	-4.78247300	0.58435900	6.48751400
C	-1.87786500	0.07040800	11.15406600
O	-1.28189600	-0.42860800	12.01298900
C	-4.08057900	4.28788800	6.58575900
O	-4.13453100	4.93897100	5.63737600
C	-3.50064800	2.30035500	11.13969100
O	-3.80733200	3.02756300	11.98189800
C	-3.46525800	4.61477800	9.29529400
O	-3.20508400	5.54058900	9.92551500
C	-0.44183200	4.26485800	7.54648700
O	-0.03162200	5.26888500	7.14359800
C	-0.93993500	3.35165900	10.13918100
O	-0.74786000	3.80287500	11.18383000
C	-1.58328000	1.93451600	6.54793700
O	-1.75160100	1.56733100	5.46420900
C	-4.67934800	0.02610900	10.16926400
O	-5.66610900	-0.54438000	10.35540600
C	-5.88218200	3.22921400	8.74942800
O	-6.96616600	3.34050200	9.12359500
C	-3.19404800	-2.26709300	8.40821600
H	-4.25425900	-2.07841100	8.21918600

H	-3.05694900	-2.59685500	9.44333300
H	-2.83265300	-3.02776700	7.70808200
C	-0.60340200	-1.30013200	8.47301500
H	-0.50309700	-1.41794400	9.55510300
H	-0.56044700	-2.29731500	8.01713000
C	0.52214600	-0.45582800	7.86587900
H	0.36316300	-0.36199500	6.78404700
H	1.46580700	-1.00524200	7.98843400
C	1.67174800	1.16791500	10.06743400
C	2.13653200	2.35663000	10.65931400
H	1.97443900	3.31051400	10.16211600
C	2.81365900	2.32670200	11.87771800
H	3.16500300	3.25621900	12.32005700
C	3.03324700	1.10907000	12.52930600
H	3.55427700	1.08630900	13.48391600
C	2.58107000	-0.07683200	11.94960100
H	2.74823500	-1.02915300	12.44820100
C	1.90849800	-0.04939000	10.72395400
H	1.57673000	-0.98918300	10.29210400
C	2.20803700	1.71528300	7.29612100
C	1.94967100	2.33677100	6.06429100
H	0.93754800	2.63156100	5.80450800
C	2.98638500	2.58892700	5.16241900
H	2.76608400	3.07602300	4.21497700
C	4.29717400	2.22857200	5.48176900
H	5.10603800	2.43319100	4.78350300
C	4.56579700	1.60790500	6.70438400
H	5.58458900	1.32596900	6.96263900
C	3.52984400	1.34940500	7.60459900
H	3.75655700	0.86994600	8.55331700

Species TSA2A3
HF energy = -2727.1799239
Imaginary frequency: 82*i*
Zero-point correction = 0.366354 (Hartree/Particle)
Thermal correction to Energy = 0.410866
Thermal correction to Enthalpy = 0.411810
Thermal correction to Gibbs Free Energy = 0.283704
Sum of electronic and zero-point Energies = -2726.813570
Sum of electronic and thermal Energies = -2726.769058
Sum of electronic and thermal Enthalpies = -2726.768114
Sum of electronic and thermal Free Energies = -2726.896220

Coordinates: **TSA2A3**

Os	2.19139500	14.69261700	5.76204800

Os	1.49183600	13.18573900	3.23493900
Os	-0.58350700	15.19025100	4.83056600
S	0.32241100	15.15075500	2.20072300
P	0.34368500	11.97511100	1.53718500
O	2.11358600	16.43175600	8.31163400
C	2.10876300	15.78013900	7.36135300
C	4.01355400	14.02334700	5.78795700
O	5.10369700	13.65423500	5.83756300
C	2.63256800	16.20852100	4.62391500
O	2.92505300	17.12006900	3.97536900
C	1.48505400	13.10001200	6.71298100
O	1.10833700	12.19380700	7.30640400
C	2.12827800	11.63812500	4.11204700
O	2.51457500	10.67237800	4.61432400
C	3.25660100	13.61219600	2.52475600
O	4.32357600	13.87298100	2.15690200
C	-1.07741700	14.83787900	6.60453100
O	-1.42399500	14.64540100	7.68914100
C	-2.38998500	15.22237900	4.19139900
O	-3.49153200	15.23051100	3.83765300
C	-0.33936000	17.18371600	4.99380100
O	-0.32300400	18.30830000	5.23851900
C	-0.36993100	13.09803200	4.42739400
O	-1.01157700	12.13938800	4.75802300
C	-0.29002000	10.29910800	1.93262700
C	0.58323700	9.20740500	1.77401100
H	1.58291600	9.36106000	1.37246600
C	0.17470300	7.91968100	2.11982400
H	0.86089700	7.08523000	1.99274200
C	-1.11020600	7.70482900	2.62719500
H	-1.42905600	6.70039200	2.89731700
C	-1.98081900	8.78340600	2.79090700
H	-2.97941600	8.62551600	3.19218400
C	-1.57422100	10.07648000	2.45229100
H	-2.26093600	10.90087900	2.61222700
C	1.06634900	11.73666000	-0.15234400
C	2.33514900	12.22928200	-0.48485400
H	2.93424500	12.72796900	0.26932100
C	2.84508600	12.06914700	-1.77828800
H	3.83569000	12.45105100	-2.01603800
C	2.08995100	11.41586300	-2.75255500
H	2.48591700	11.28982600	-3.75805400
C	0.82387900	10.91411400	-2.43018300
H	0.23369900	10.39531700	-3.18277600
C	0.31727400	11.06890600	-1.14022500
H	-0.65797800	10.65222600	-0.89630600
C	-1.16803400	13.00754900	1.14151100

H	-1.69691200	12.60636700	0.26759500
H	-1.84856700	12.96751100	1.99819700
C	-0.75927300	14.45033400	0.85271900
H	-1.63003500	15.10817300	0.76163700
H	-0.16664000	14.51186900	-0.06736100
C	1.37140600	16.28443200	1.22020500
H	2.01013400	16.82912200	1.91678100
H	0.72418400	16.98489600	0.68354700
H	1.98133400	15.69985700	0.52455300

Species A3
HF energy = -2727.1846741
No imaginary frequency
Zero-point correction = 0.367241 (Hartree/Particle)
Thermal correction to Energy = 0.412142
Thermal correction to Enthalpy = 0.413086
Thermal correction to Gibbs Free Energy = 0.284317
Sum of electronic and zero-point Energies = -2726.817433
Sum of electronic and thermal Energies = -2726.772532
Sum of electronic and thermal Enthalpies = -2726.771588
Sum of electronic and thermal Free Energies = -2726.900357

Coordinates: **Species A3**

Os	2.11154700	14.86094700	5.66095000
Os	1.46179600	13.08674500	3.31745400
Os	-0.71436500	15.36545800	4.68271300
S	0.16786100	14.98180800	2.37014500
P	0.35113600	11.84450300	1.62362700
O	2.05334100	16.86686400	8.01025000
C	2.03465700	16.12138800	7.13148300
C	3.90850800	14.14061300	5.74669100
O	4.99103700	13.75429100	5.82717900
C	2.61831600	16.24636700	4.39308100
O	2.96154400	17.08773800	3.67740000
C	1.39590000	13.38631400	6.78126300
O	1.02830000	12.54806200	7.47179000
C	2.13091000	11.60406300	4.26778500
O	2.53505300	10.68251300	4.83775700
C	3.18412000	13.47191000	2.45773900
O	4.20930200	13.71556400	1.98311700
C	-1.11299100	15.19769200	6.53228300
O	-1.39862700	15.09455300	7.64390300
C	-2.54727600	15.21810200	4.14468700
O	-3.66409600	15.13085100	3.85622800
C	-0.51240600	17.34943900	4.73820200

O	-0.46042100	18.49636300	4.82271700
C	-0.35513600	13.18157600	4.51719600
O	-1.00469000	12.31122900	5.04593400
C	-0.20128600	10.11330900	1.91388300
C	-0.21376400	9.16168200	0.87911200
H	0.11928100	9.42906800	-0.11995100
C	-0.64596200	7.85766400	1.12962800
H	-0.64636900	7.12789200	0.32250900
C	-1.06952500	7.49157000	2.40956200
H	-1.40227000	6.47375400	2.60290500
C	-1.06060900	8.43429400	3.44057300
H	-1.38688800	8.15699600	4.44057700
C	-0.62482700	9.73960200	3.20192600
H	-0.63118400	10.46537000	4.01191100
C	1.17816600	11.77188500	-0.02558300
C	2.52359200	11.36455700	-0.07046500
H	3.04322300	11.11611700	0.85210900
C	3.20150400	11.27515300	-1.28635500
H	4.24136900	10.95628800	-1.29959600
C	2.55041900	11.60372600	-2.47946800
H	3.08191900	11.54395800	-3.42671400
C	1.21453100	12.00736700	-2.44959500
H	0.69755600	12.25845700	-3.37354200
C	0.53001300	12.08376400	-1.23207300
H	-0.51649200	12.37818100	-1.24135800
C	-1.24925300	12.77604100	1.32655500
H	-1.80080100	12.37192900	0.46846800
H	-1.85992000	12.58727700	2.21648300
C	-1.03428500	14.27618500	1.12597600
H	-1.96751800	14.84115400	1.22235300
H	-0.59031100	14.48567600	0.14656100
C	0.85287500	16.33984500	1.36039500
H	1.54428500	16.91191900	1.97836800
H	0.02552300	16.97664400	1.03176200
H	1.38028400	15.90982300	0.50351000

Species TSA3A4
HF energy = -2727.1813889
One imaginary frequency: 77*i*
Zero-point correction = 0.366770 (Hartree/Particle)
Thermal correction to Energy = 0.411079
Thermal correction to Enthalpy = 0.412023
Thermal correction to Gibbs Free Energy = 0.285085
Sum of electronic and zero-point Energies = -2726.814619
Sum of electronic and thermal Energies = -2726.770310

Sum of electronic and thermal Enthalpies = -2726.769366
Sum of electronic and thermal Free Energies = -2726.896304

Coordinates: **TSA3A4**

Os	2.12815500	14.89322200	5.69675500
Os	1.31564900	13.19336000	3.33187900
Os	-0.68954600	15.29432500	4.88219800
S	0.06736500	15.05950400	2.20751700
P	0.26884300	11.89127800	1.63185500
O	2.17479700	16.82270100	8.10739300
C	2.12576600	16.09998400	7.21148000
C	3.95794300	14.24561100	5.67580800
O	5.05327800	13.88877800	5.69179700
C	2.47906700	16.31398600	4.41262500
O	2.71528100	17.16848900	3.67034100
C	1.48690100	13.36975300	6.79256200
O	1.14665800	12.50284200	7.46254200
C	2.02763500	11.72542200	4.28241600
O	2.46497600	10.80581100	4.82976700
C	3.02510100	13.59174000	2.48485400
O	4.05314400	13.83817500	2.01628000
C	-1.09795600	15.07423400	6.69883800
O	-1.39166000	14.96115000	7.80985700
C	-2.52527500	15.27412500	4.32721100
O	-3.64199900	15.25644000	4.02670600
C	-0.46043200	17.29845000	4.88130600
O	-0.44110300	18.43880300	5.03365000
C	-0.48937300	13.18801100	4.61579400
O	-1.11508600	12.25981300	5.05742800
C	-0.23417300	10.14266000	1.91238900
C	-0.23335800	9.20442000	0.86479500
H	0.08589800	9.49260100	-0.13299700
C	-0.63407100	7.88789900	1.10029400
H	-0.62482800	7.16953800	0.28306800
C	-1.03874800	7.49456200	2.37850700
H	-1.34670000	6.46686900	2.56029900
C	-1.04296800	8.42305100	3.42194000
H	-1.35502200	8.12516700	4.42055700
C	-0.63931300	9.74139200	3.19743400
H	-0.66022800	10.45642900	4.01588800
C	1.15265100	11.82921500	0.01147600
C	2.49940200	11.42350700	0.00941300
H	2.98855000	11.17032200	0.94720000
C	3.21732200	11.33975000	-1.18362400
H	4.25736000	11.02185700	-1.16376100
C	2.60541800	11.67172100	-2.39653900
H	3.16790300	11.61569300	-3.32593000

C	1.26855400	12.07278100	-2.40946000
H	0.78162200	12.32531700	-3.34918800
C	0.54403400	12.14362500	-1.21478000
H	-0.50253100	12.43480700	-1.25713600
C	-1.34223600	12.77005500	1.27409900
H	-1.86927700	12.32397900	0.42081500
H	-1.96216500	12.59354900	2.16055600
C	-1.15881600	14.26970300	1.03465200
H	-2.10077700	14.81337900	1.15913100
H	-0.76855100	14.47031400	0.03196400
C	1.09273000	16.02818800	1.03666300
H	1.81605800	16.59098600	1.62889200
H	0.44535800	16.71955400	0.48879300
H	1.60947700	15.34330000	0.35743000

Species A4
HF energy = -2727.2186058
No imaginary
Zero-point correction = 0.367813 (Hartree/Particle)
Thermal correction to Energy = 0.412746
Thermal correction to Enthalpy = 0.413690
Thermal correction to Gibbs Free Energy = 0.284877
Sum of electronic and zero-point Energies = -2726.850792
Sum of electronic and thermal Energies = -2726.805860
Sum of electronic and thermal Enthalpies = -2726.804915
Sum of electronic and thermal Free Energies = -2726.933729

Coordinates: **A4**

Os	2.16364100	15.06397600	5.47662200
Os	1.51723800	13.48524200	3.07811800
Os	-0.13986100	13.18938100	5.58386900
S	0.59489300	15.62458300	2.04568400
P	0.24580000	12.42864000	1.34644700
O	2.32472400	15.71425300	8.49650600
C	2.23669100	15.47668100	7.37369900
C	3.47080800	16.29382600	4.78375800
O	4.22315700	17.07652500	4.38862800
C	0.65288900	16.29541600	5.19240500
O	-0.18394600	17.07957600	5.08581800
C	3.52272700	13.63651700	5.57933700
O	4.37518000	12.87043700	5.66776400
C	2.05980700	11.81517800	3.77402500
O	2.43946900	10.75999100	4.07482400
C	3.16575300	13.81959900	2.21520500
O	4.21872100	13.98385300	1.75052200

C	-0.93511200	13.98190800	7.15832200
O	-1.47013000	14.46084100	8.05947100
C	-1.24401100	11.61631500	5.40534700
O	-1.89499800	10.66542800	5.38558600
C	-1.21980700	14.14056900	4.26212700
O	-1.99531800	14.64323400	3.55986700
C	1.19749900	12.15613700	6.61412000
O	1.89768700	11.51889000	7.26768700
C	-0.96223200	11.09675000	1.75538400
C	-0.45175200	9.82357000	2.06928400
H	0.62155100	9.64738800	2.05923800
C	-1.31147800	8.77477500	2.39283900
H	-0.89895300	7.79811400	2.63626500
C	-2.69485700	8.97786100	2.40565500
H	-3.36506900	8.15948000	2.65899000
C	-3.21099000	10.23709900	2.09745800
H	-4.28577300	10.40579400	2.10688200
C	-2.35202500	11.29282100	1.77629200
H	-2.78349100	12.26257900	1.54634300
C	1.13595200	11.65700700	-0.08355200
C	2.51977800	11.43889500	-0.05209200
H	3.09466000	11.73434300	0.81856900
C	3.17035900	10.83720900	-1.13474500
H	4.24519300	10.67562600	-1.09114100
C	2.44435100	10.44836000	-2.26057600
H	2.95040200	9.98382100	-3.10426500
C	1.05998700	10.64904700	-2.29777500
H	0.48512000	10.33645600	-3.16710800
C	0.41001000	11.24074900	-1.21552800
H	-0.67157200	11.35767400	-1.24786400
C	-0.77731200	13.76683200	0.53462300
H	-1.14298400	13.43210400	-0.44284000
H	-1.64428500	13.97245500	1.17105600
C	0.04539100	15.04217100	0.37776700
H	-0.55209900	15.84368800	-0.07208700
H	0.93691600	14.87519300	-0.23965000
C	1.93643400	16.74362000	1.50736100
H	2.36795600	17.19852200	2.40106300
H	1.49987400	17.52521400	0.87691500
H	2.71433500	16.20008500	0.96338200

Species A4_isomer
HF energy = -2727.2082532
No imaginary frequency
Zero-point correction = 0.367690 (Hartree/Particle)

Thermal correction to Energy = 0.412610
Thermal correction to Enthalpy = 0.413554
Thermal correction to Gibbs Free Energy = 0.284328
Sum of electronic and zero-point Energies = -2726.840563
Sum of electronic and thermal Energies = -2726.795644
Sum of electronic and thermal Enthalpies = -2726.794699
Sum of electronic and thermal Free Energies = -2726.923925

Coordinates: **A4_isomer**

Os	-1.88578700	3.98097200	8.83671800
Os	-4.32702400	2.25088400	8.89697100
Os	-1.61500600	1.05544200	8.44291000
P	0.69383000	0.61632400	8.41449600
S	-1.92128700	-1.29848600	7.93748600
C	-1.68267100	1.35500500	6.51621400
O	-1.68906500	1.41873300	5.36250500
C	-1.71325100	0.66145400	10.34492300
O	-1.75162500	0.28587300	11.43936700
C	-4.42854200	2.12093800	6.93290500
O	-4.61653200	2.03101200	5.80208400
C	-4.05727100	2.35339000	10.84606400
O	-4.01075400	2.41374400	11.99348800
C	-2.83109500	5.58807100	9.37042200
O	-3.36383500	6.55216900	9.70569500
C	-0.11389500	4.66255300	8.53916500
O	0.93234500	5.12203100	8.36649400
C	-1.37749700	3.50836500	10.68089000
O	-1.02161200	3.33708100	11.76084000
C	-2.36678400	4.20394200	6.94061700
O	-2.60317900	4.42969700	5.83744400
C	-5.36904700	0.64427200	9.06561100
O	-6.01908100	-0.30417400	9.18779400
C	-5.66259000	3.65425100	8.95075400
O	-6.49605400	4.44910000	8.96010200
C	-3.01083000	-2.20541400	9.09752000
H	-4.03837000	-1.90586800	8.88257700
H	-2.76597700	-1.96427500	10.13622300
H	-2.89659900	-3.27954300	8.91471600
C	-0.30501000	-2.06267100	8.45914700
H	-0.32342100	-2.14951000	9.55179600
H	-0.26671000	-3.07065800	8.02914000
C	0.86938400	-1.21538600	7.97452300
H	0.92871800	-1.25109000	6.87891000
H	1.80876400	-1.62422000	8.36619400
C	1.62666000	0.80996700	9.99381500
C	2.20564300	2.05538200	10.29613000
H	2.15233800	2.87045400	9.57842100

C	2.86572900	2.25474500	11.50910000
H	3.30975300	3.22430400	11.72463200
C	2.95792400	1.21624900	12.44032800
H	3.47085900	1.37412200	13.38651800
C	2.38941200	-0.02471100	12.14910300
H	2.45811800	-0.84054700	12.86564700
C	1.72751900	-0.22675100	10.93470700
H	1.29288100	-1.20279500	10.73411300
C	1.85938000	1.36944900	7.19445300
C	1.46399900	2.40520800	6.33852200
H	0.45873100	2.80542200	6.40682100
C	2.35963800	2.93666300	5.40486700
H	2.03480400	3.74089200	4.74841400
C	3.66085200	2.44086000	5.32095300
H	4.35762600	2.85527000	4.59534000
C	4.07011100	1.41343600	6.17800000
H	5.08607000	1.02770400	6.12347300
C	3.17815600	0.88354800	7.10957400
H	3.51685900	0.09712200	7.78106800

Species TSA1A5
HF energy = -2727.153926
One imaginary frequency: 27*i*
Zero-point correction = 0.365894 (Hartree/Particle)
Thermal correction to Energy = 0.410909
Thermal correction to Enthalpy = 0.411854
Thermal correction to Gibbs Free Energy = 0.280308
Sum of electronic and zero-point Energies = -2726.788032
Sum of electronic and thermal Energies = -2726.743017
Sum of electronic and thermal Enthalpies = -2726.742072
Sum of electronic and thermal Free Energies = -2726.873618

Coordinates: **TSA1A5**

Os	-1.52079900	3.20565800	9.40288000
Os	-4.33864300	3.53777100	9.81954700
Os	-3.40847700	0.94983200	8.87428800
P	1.20897300	0.89039000	7.66323500
S	-1.95415000	-0.66943100	7.66116300
C	-3.98671700	1.59430100	7.11452600
O	-4.35033000	1.87706200	6.05725100
C	-2.63655900	0.40200900	10.58206500
O	-2.18278100	-0.05916600	11.54204300
C	-4.26669500	4.37956500	8.03086700
O	-4.26842600	4.93984900	7.03146600
C	-4.31160200	2.55497700	11.53499900

O	-4.38368900	2.03903500	12.55649200
C	-4.33875600	5.27680800	10.68988900
O	-4.35439500	6.28384200	11.24310700
C	-0.95378400	5.00397000	9.54697000
O	-0.67418700	6.12738200	9.61429600
C	-1.33255500	2.93515900	11.32159600
O	-1.13273900	2.81055200	12.45033800
C	-1.58649300	3.26583300	7.43031800
O	-1.50819500	3.34470900	6.28413200
C	-4.99249300	-0.08172800	9.13569400
O	-5.94950400	-0.69749700	9.35185900
C	-6.24205500	3.24168900	9.68039500
O	-7.37369700	3.07266800	9.56328800
C	-2.86770500	-2.25999500	7.59296400
H	-3.78094300	-2.07496900	7.02075500
H	-3.13051300	-2.60101700	8.59900100
H	-2.25647200	-3.00706700	7.07471800
C	-0.47350700	-1.23383300	8.64097200
H	-0.51379200	-0.76632500	9.62662400
H	-0.59590500	-2.31434700	8.77820200
C	0.84582500	-0.93565800	7.92119700
H	0.83084100	-1.37441600	6.91516700
H	1.66490400	-1.43058600	8.46259600
C	1.73086900	1.46338300	9.34607200
C	1.87022300	2.85761000	9.50955800
H	1.68978200	3.51832200	8.66327700
C	2.27996300	3.40284700	10.73097100
H	2.38967600	4.48086500	10.82883900
C	2.53046400	2.56684200	11.82057400
H	2.83474200	2.98863800	12.77586800
C	2.38243000	1.18374600	11.67914600
H	2.57317700	0.52609400	12.52488700
C	1.99425900	0.63681100	10.45270700
H	1.90140400	-0.44348000	10.37072700
C	2.82155500	0.73188000	6.76468900
C	2.80730900	0.94844200	5.37666600
H	1.87677800	1.23138600	4.88672700
C	3.97579700	0.81086000	4.62213200
H	3.94916900	0.98050800	3.54758300
C	5.17581300	0.46886500	5.24952500
H	6.08827200	0.36915600	4.66502900
C	5.20425600	0.26369500	6.63266100
H	6.13907100	0.00411900	7.12606800
C	4.03556200	0.39282800	7.38556100
H	4.07134100	0.23995800	8.46243500

Species A5
HF energy = -2727.1571953
No imaginary frequency
Zero-point correction = 0.366387 (Hartree/Particle)
Thermal correction to Energy = 0.412025
Thermal correction to Enthalpy = 0.412970
Thermal correction to Gibbs Free Energy = 0.280221
Sum of electronic and zero-point Energies = -2726.790809
Sum of electronic and thermal Energies = -2726.745170
Sum of electronic and thermal Enthalpies = -2726.744226
Sum of electronic and thermal Free Energies = -2726.876974

Coordinates: **A5**

Os	-1.76257200	3.62804500	10.18260400
Os	-4.55323900	3.28001400	10.79230700
Os	-3.31053800	1.32138500	9.03881200
P	1.72681300	0.51751700	6.69362900
S	-1.66378900	0.56700700	7.34062100
C	-4.24374200	2.31106400	7.62837500
O	-4.81211200	2.80525200	6.75409500
C	-2.30461000	0.48208000	10.49332300
O	-1.72357700	-0.12926300	11.28527600
C	-4.76080200	4.62373900	9.35720400
O	-4.92812000	5.45257700	8.58340400
C	-4.21690500	1.86814500	12.13480000
O	-4.11327200	1.07641100	12.95769200
C	-4.77356400	4.64816500	12.15447200
O	-4.91870200	5.42243300	12.99143200
C	-1.56917700	5.40358500	10.81190100
O	-1.53397100	6.50306100	11.17792800
C	-1.38418500	2.86938300	11.93803500
O	-1.08829300	2.47006600	12.97933400
C	-2.02689900	4.14340800	8.30283200
O	-2.03172100	4.49335800	7.20172600
C	-4.59574500	-0.08430000	9.00675400
O	-5.36007200	-0.95450200	9.04174300
C	-6.38104600	2.67652500	10.61286000
O	-7.47064000	2.33486300	10.47557100
C	-2.52540100	-0.53658700	6.16027000
H	-3.27792000	0.06907100	5.64763300
H	-3.01587500	-1.35727500	6.69314300
H	-1.80869800	-0.91749500	5.42546700
C	-0.50826100	-0.65096700	8.11209900
H	-0.20883700	-0.18854300	9.05432500
H	-1.08832400	-1.55071900	8.35185300
C	0.72834700	-0.98917200	7.27568700

H	0.44678900	-1.55676900	6.37916800
H	1.35996700	-1.65132400	7.88424500
C	1.72339500	1.55013400	8.23666100
C	1.14273700	2.82331500	8.15431200
H	0.76163900	3.17833300	7.19914100
C	1.07053200	3.65827700	9.28463800
H	0.73355700	4.68618500	9.17901200
C	1.56749000	3.20479400	10.51756300
H	1.53206900	3.85657600	11.38712800
C	2.14420000	1.93293700	10.61082700
H	2.53743700	1.58274600	11.56273200
C	2.23185400	1.12078600	9.47863700
H	2.71000500	0.14599000	9.55685300
C	3.43694200	-0.18829100	6.69713100
C	3.68592400	-1.51368300	6.29964300
H	2.86040000	-2.18312100	6.06664000
C	4.99336400	-1.99545100	6.19131400
H	5.16242200	-3.02681400	5.88761800
C	6.07682000	-1.16061000	6.47161100
H	7.09434400	-1.53648100	6.38863500
C	5.84385100	0.16334300	6.85446900
H	6.68069400	0.82413500	7.07240800
C	4.53865600	0.64647900	6.96012700
H	4.37636300	1.68028300	7.25887800

Species TSA1A6
HF energy = -2727.1744517
One imaginary frequency: 105*i*
Zero-point correction = 0.366120 (Hartree/Particle)
Thermal correction to Energy = 0.411404
Thermal correction to Enthalpy = 0.412348
Thermal correction to Gibbs Free Energy = 0.279502
Sum of electronic and zero-point Energies = -2726.808332
Sum of electronic and thermal Energies = -2726.763048
Sum of electronic and thermal Enthalpies = -2726.762104
Sum of electronic and thermal Free Energies = -2726.894950

Coordinates: **TSA1A6**

Os	-1.17676500	2.69341400	8.56534800
Os	-3.91905000	3.70657900	8.99680700
Os	-3.52037600	0.86911900	8.89462900
P	0.76152900	1.26427700	8.45073200
S	-1.55541600	-2.37751000	7.47779800
C	-4.05244800	0.83496800	7.01305800
O	-4.41188400	0.70499500	5.92786400

C	-2.86083900	0.67730500	10.73510000
O	-2.50270400	0.40543500	11.79644100
C	-3.85787700	3.86002900	7.02578900
O	-3.89593900	4.03969500	5.89417600
C	-3.82922100	3.47068600	10.95786000
O	-3.86279700	3.38629400	12.09988300
C	-3.50809800	5.58463400	9.15256400
O	-3.25422400	6.70011800	9.26955900
C	-0.33412000	4.37634700	8.20287100
O	0.14464400	5.40311900	7.96900300
C	-0.98859100	2.88957600	10.50531500
O	-0.80837900	3.03889400	11.63496400
C	-1.52630800	2.23402200	6.69909000
O	-1.61482200	1.96954600	5.57586600
C	-5.23766000	0.25406700	9.39641500
O	-6.29896700	-0.06151100	9.73839000
C	-5.86143600	3.79679200	9.04301000
O	-7.00738200	3.87428100	9.03963800
C	-2.46266800	-3.40053400	8.69074800
H	-3.09905700	-4.08029000	8.11498800
H	-3.10037800	-2.78457900	9.33474600
H	-1.77344600	-3.99352800	9.30305200
C	-0.58173800	-1.31711500	8.62526600
H	-1.27404800	-0.67185600	9.17954500
H	-0.07464800	-1.96285900	9.35119000
C	0.42456100	-0.47318700	7.82881000
H	0.04529000	-0.28954200	6.81459200
H	1.37719900	-1.00318700	7.70873700
C	1.72021400	1.08794800	10.01383700
C	2.21448100	2.25692100	10.62107200
H	2.01288000	3.22818800	10.17393700
C	2.96593800	2.18576800	11.79303800
H	3.33933200	3.10037000	12.24839100
C	3.23205000	0.94605500	12.38295800
H	3.81240500	0.89138300	13.30140400
C	2.75098300	-0.22023000	11.78739900
H	2.95655900	-1.18976600	12.23620900
C	2.00371200	-0.15138200	10.60691500
H	1.65386600	-1.07374900	10.15420100
C	2.09236000	1.74712700	7.25085200
C	1.84605400	2.62784500	6.18730200
H	0.87036700	3.08630500	6.06874100
C	2.85379800	2.93033800	5.26666000
H	2.64347900	3.61781200	4.45028700
C	4.12049700	2.36006200	5.39832600
H	4.90532700	2.60030400	4.68418600
C	4.37820900	1.48238000	6.45555200

H	5.36435000	1.03685900	6.56943500
C	3.37334000	1.17785300	7.37402200
H	3.59376100	0.50381400	8.19852900

Species A6
HF energy = -2727.1814694
No imaginary frequency
Zero-point correction = 0.365722 (Hartree/Particle)
Thermal correction to Energy = 0.411503
Thermal correction to Enthalpy = 0.412447
Thermal correction to Gibbs Free Energy = 0.279249
Sum of electronic and zero-point Energies= -2726.815748
Sum of electronic and thermal Energies = -2726.769966
Sum of electronic and thermal Enthalpies = -2726.769022
Sum of electronic and thermal Free Energies = -2726.902220

Coordinates: **A6**

Os	-1.15225100	2.86369500	8.48505900
Os	-3.92541200	3.68512900	9.04494300
Os	-3.29506300	0.87712000	8.95677300
P	0.70759800	1.34265100	8.40517800
S	-1.06631700	-2.76293600	7.66929000
C	-4.00556700	0.86711200	7.14029900
O	-4.46359000	0.76435500	6.08847200
C	-2.48058900	0.76301400	10.74695100
O	-2.01335200	0.55010800	11.77806000
C	-3.92983100	3.87693800	7.07567100
O	-4.01422900	4.08047300	5.95006100
C	-3.78071200	3.41194000	10.99680000
O	-3.78782300	3.29933700	12.13752100
C	-3.64008300	5.58492600	9.22294700
O	-3.45921500	6.71253300	9.35907300
C	-0.30902400	4.52386500	8.02300500
O	0.17689500	5.53000900	7.72401400
C	-0.91801300	3.21109200	10.39970100
O	-0.71489000	3.46016200	11.50729900
C	-1.54480500	2.37798000	6.63274600
O	-1.67177200	2.09697300	5.51809600
C	-4.89167100	0.06116600	9.57835100
O	-5.87656800	-0.38186500	9.99819000
C	-5.86499700	3.61753600	9.13895800
O	-7.01363500	3.59886700	9.15941300
C	-2.46864600	-3.36979800	8.66868300
H	-2.74026200	-4.35342900	8.27253800
H	-3.32894500	-2.69618200	8.57380600

H	-2.19085300	-3.47244500	9.72371700
C	-0.85845000	-1.11220900	8.42767700
H	-1.80894700	-0.53496500	8.25855400
H	-0.72502100	-1.22052800	9.50822200
C	0.30837100	-0.37474100	7.76734500
H	0.09647800	-0.23526900	6.69957400
H	1.22364200	-0.97829600	7.82654400
C	1.60663600	1.07762100	9.99126600
C	2.16464100	2.20294700	10.62459800
H	2.04658600	3.18934100	10.18078400
C	2.87676100	2.06843100	11.81545700
H	3.30154400	2.95012200	12.29019900
C	3.03835900	0.80777500	12.39858100
H	3.58773700	0.70387100	13.33167400
C	2.49401200	-0.31640900	11.77689200
H	2.61937300	-1.30225000	12.21955200
C	1.78632100	-0.18509000	10.57751900
H	1.39075600	-1.08038000	10.10680300
C	2.09574400	1.75385900	7.24443900
C	1.90122900	2.61740200	6.15641800
H	0.94107200	3.09935400	6.00608500
C	2.93966900	2.87173700	5.25610000
H	2.77047100	3.54727900	4.42044600
C	4.18598400	2.26909600	5.43366100
H	4.99567600	2.47209700	4.73592300
C	4.39123500	1.40717200	6.51485400
H	5.36086400	0.93628700	6.66312500
C	3.35491800	1.14995500	7.41333900
H	3.53386000	0.48616000	8.25585500

2) Complete list of authors for reference 9 (S21)

(9) Gaussian 09, Revision A.02: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.