

Supporting Information

Probing an Origin of the Stereoselectivity and Enantioselectivity of Cobalt-Catalyzed [2+2] Cyclization of Ethylene and Enynes

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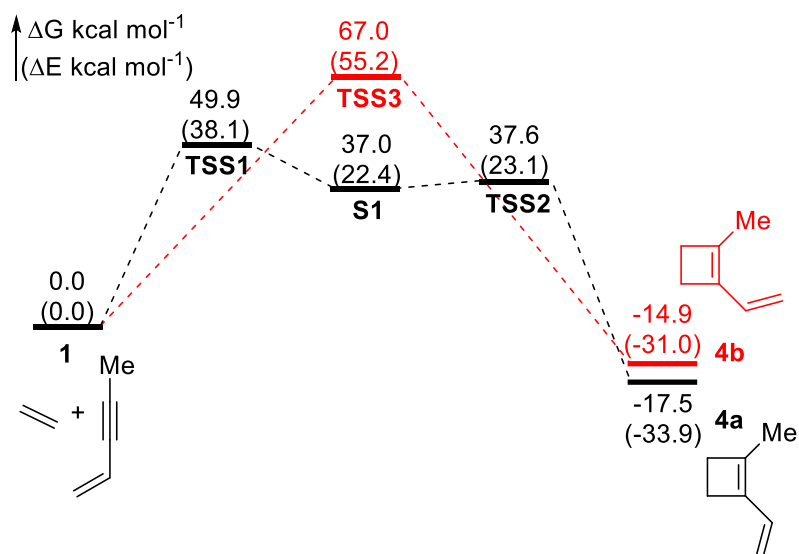


Figure S1. The free energy profiles (in kcal mol⁻¹) of the [2+2] cycloaddition between cyclobutene and ethylene in the non-metal catalytic condition (closed-shell singlet state).

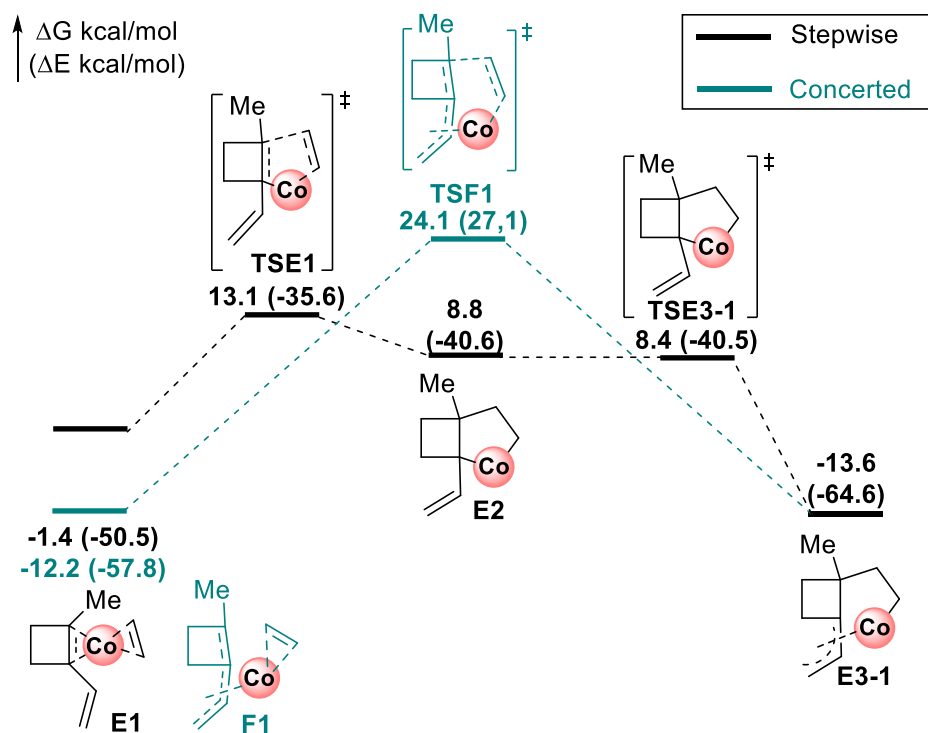


Figure S2. The Gibbs free energy profiles (in kcal mol⁻¹) for the oxidative coupling (in the closed-shell singlet state).

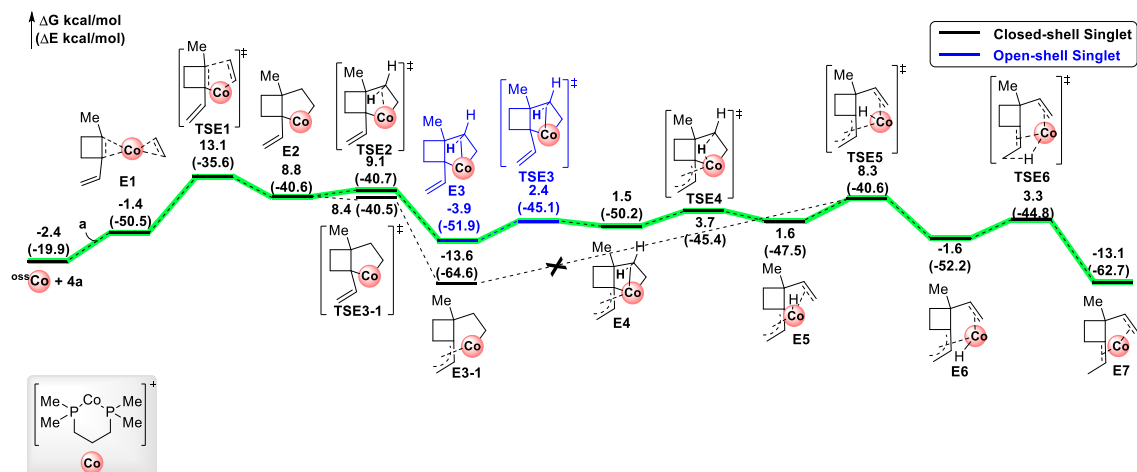


Figure S3. The Gibbs free energy profiles (in kcal mol⁻¹) for the oxidative coupling between cyclobutene and ethylene (Except **E3** and **TSE3**, the rest are performed in the closed-shell singlet state).

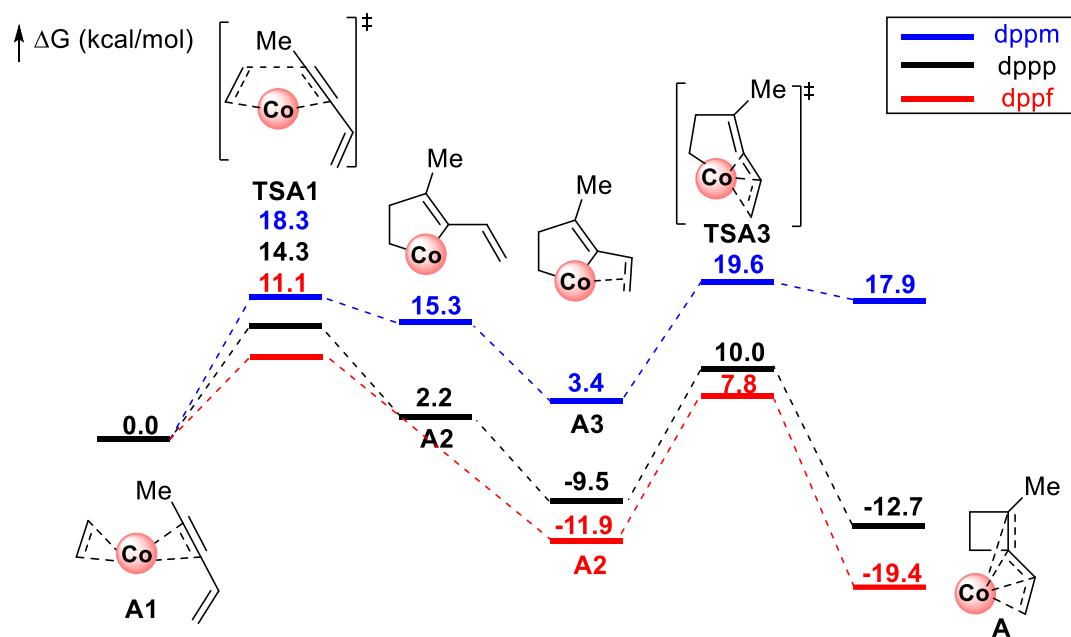


Figure S4. Ligand effects for the oxidative coupling between ethylene and enyne (in the closed-shell singlet state).

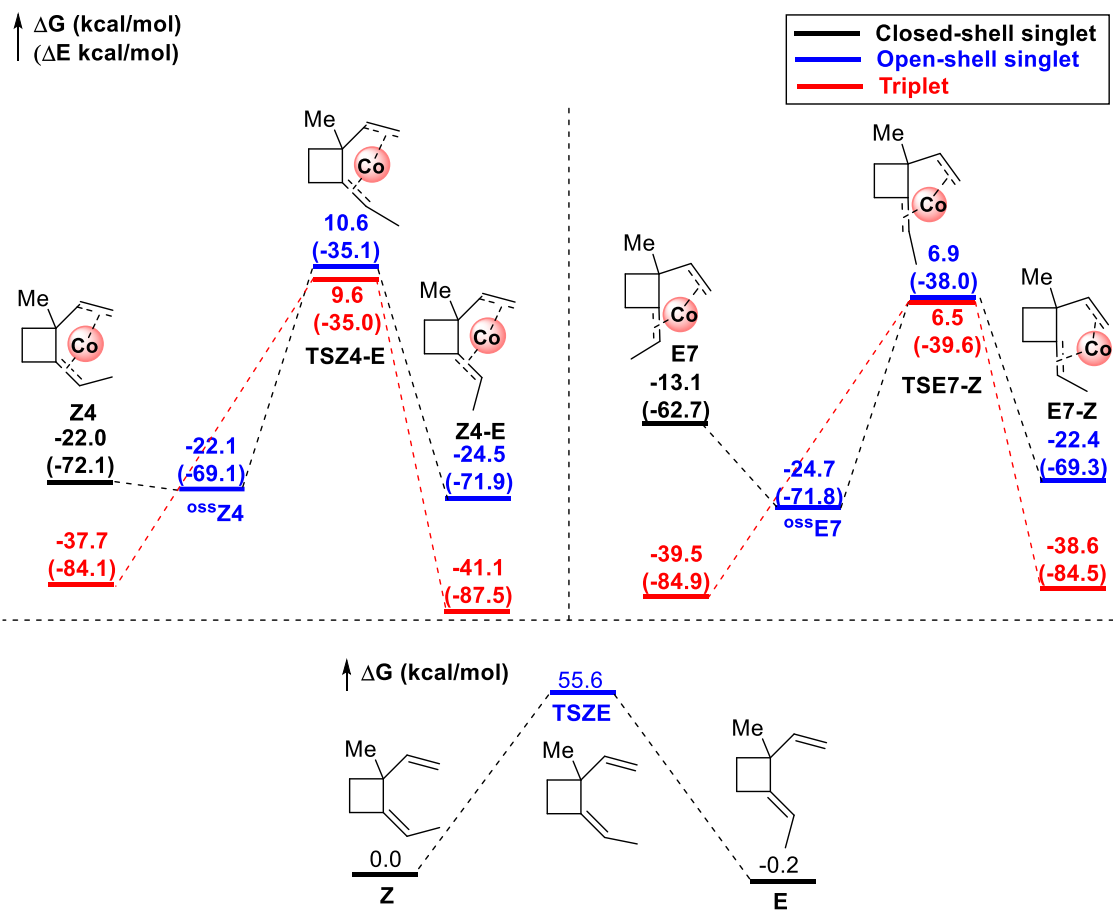


Figure S5. The Gibbs free energy profiles (in kcal mol⁻¹) for the process of tautomerization

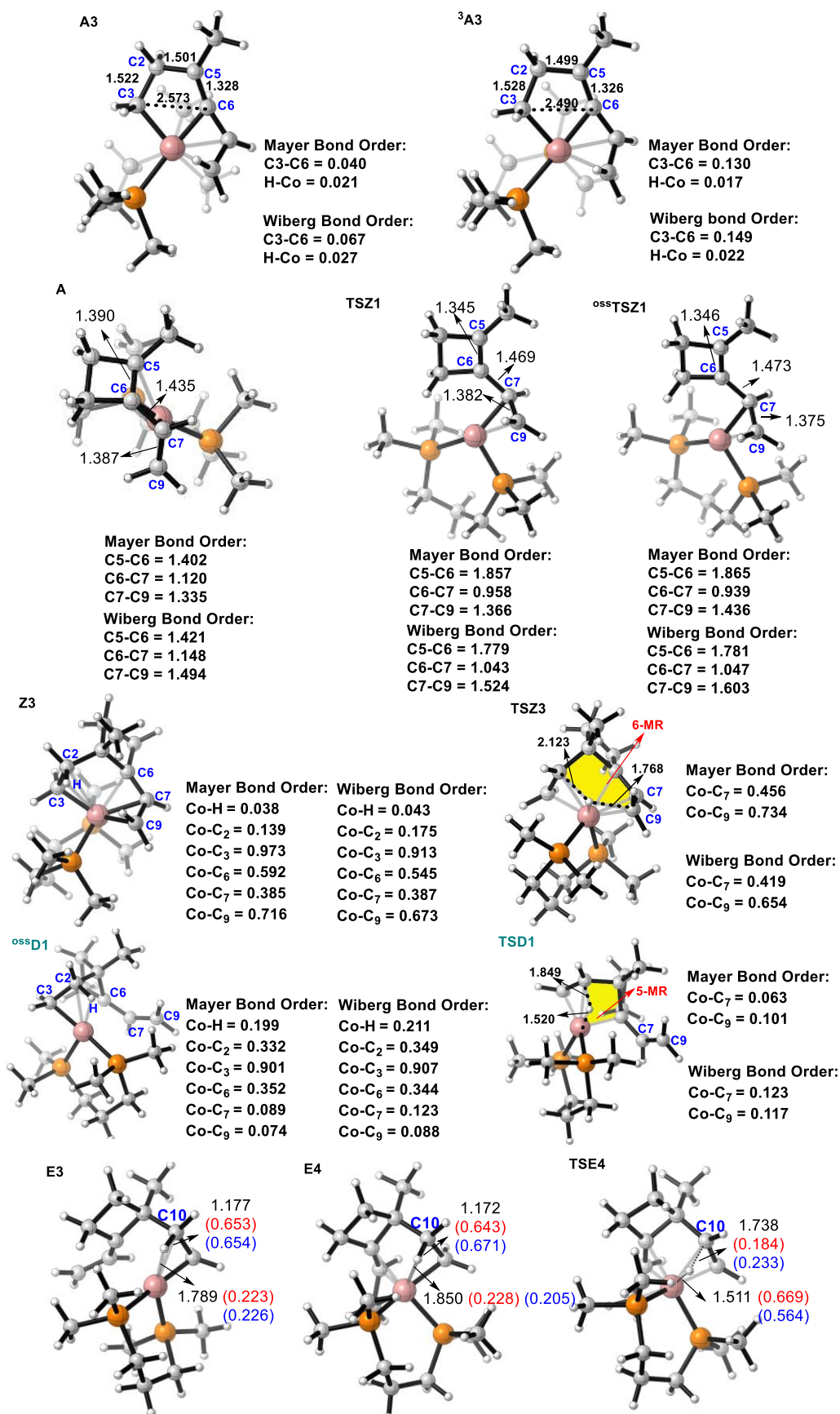


Figure S6. Mayer bond order and Wiberg bond order for selected complexes and transition states.

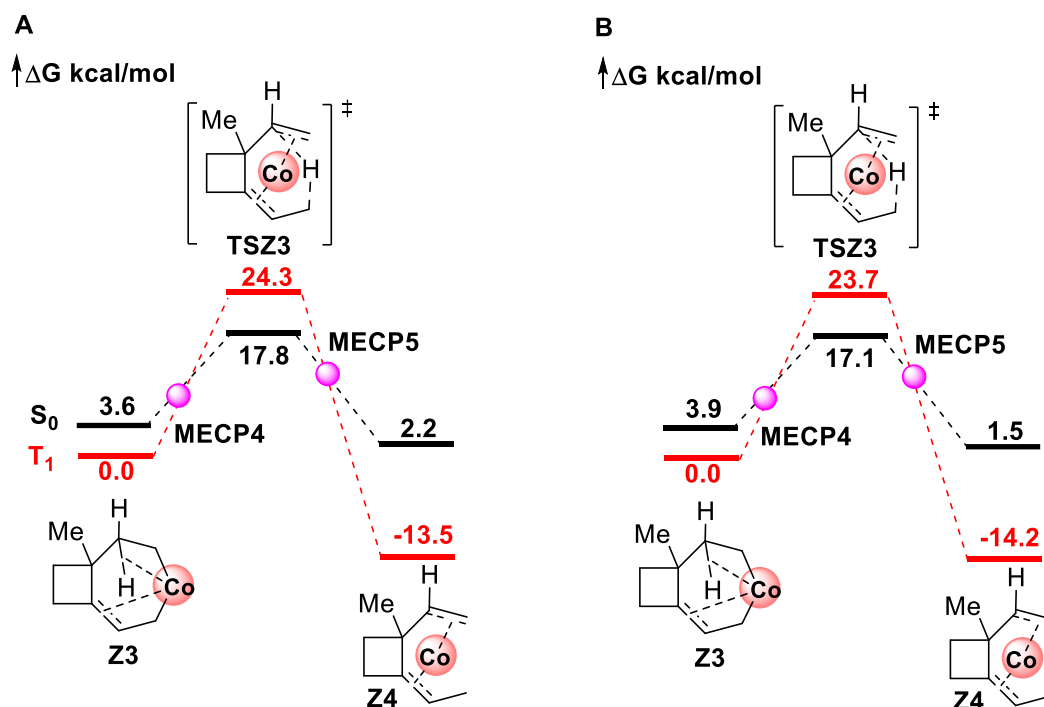


Figure S7: The Gibbs free energy (in kcal/mol) of β -H transfer in the singlet and triplet states. Optimization at M06/6-31G(d), LANL2DZ(Co) level. **(A).** Single-point solvation energy calculation (SMD, solvent = dichloromethane) at M06/6-311+G(d,p), SDD(Co) level. **(B).** Single-point solvation energy calculation (SMD, solvent = dichloromethane) at M06-GD3/6-311+G(d,p), SDD(Co) level. The Gibbs energy corrections from the frequency calculations are added to the solvation single-point energies to obtain the Gibbs free energies.

Cartesian coordinates for all the complexes including the transition states calculated in this study

A1

C 0.50437100 -0.73464600 2.62187400
C -1.90337800 0.81482300 0.44577700
C 0.19071100 -1.36322700 -2.05687900
C -1.17065300 -1.57952700 -1.96091200
C -2.48690000 -0.10284400 -0.26681800
H 0.89798900 -2.12002700 -1.71823500
H 0.58206700 -0.69337300 -2.82275200
H -1.57202900 -2.47611800 -1.48856800
H -1.85366300 -1.06521100 -2.63513300
C -3.77112800 -0.70090700 -0.67120600
H -3.77260500 -1.78935400 -0.52461300
H -4.60690900 -0.27542000 -0.10150800
H -3.96929000 -0.52754900 -1.73771600
C -2.22715700 1.91367800 1.32450200
H -3.18173900 2.40373000 1.11230500
C -1.52272600 2.31743800 2.38689800
H -0.58110500 1.84875500 2.66703900
H -1.88712600 3.10922100 3.03667300
C 2.40857400 -1.50363200 0.59972700
H 2.81440200 -2.04596500 1.46748500
H 2.54287900 -2.16342000 -0.26989200
C 3.16848400 -0.19447400 0.39030800
H 3.09235900 0.43466300 1.29141600
H 4.23672000 -0.42947600 0.29364900
C 2.72397600 0.59482200 -0.84166500
H 3.39872100 1.44703000 -1.01165200
H 2.77411100 -0.03710300 -1.74106600
P 0.59942700 -1.31691900 0.89252500
P 1.00807800 1.24798200 -0.69305300

C 0.50437100 -0.73464600 2.62187400

H -0.54656400 -0.63362000 2.91747500

H 1.00147100 -1.45000200 3.29100300

H 0.98946600 0.24263100 2.73016000

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H -0.23014100 2.70319000 -2.17353600

H 1.52761200 2.87851000 -2.43787600

H 0.65018900 1.47797600 -3.11112100

C 1.22380300 2.62974500 0.48768900

H 1.96881200 3.33631700 0.09811200

H 0.26995800 3.15165600 0.62630100

H 1.56021300 2.27604600 1.46949100

Co -0.62794300 -0.20938900 -0.46760600

TSA1

C -2.05525600 0.46512700 0.22535700

C -0.01031500 -1.30588100 -1.90866200

C -1.40425600 -1.62087000 -1.62127800

C -2.37114900 -0.72277600 -0.27350500

H 0.68517200 -2.14819400 -1.92297800

H 0.19638500 -0.58947600 -2.71050300

H -1.59263700 -2.64984300 -1.30667900

H -2.11973800 -1.28680500 -2.37846600

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H -3.69895700 1.86622200 0.43000400
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H -1.50559400 1.67590700 2.58910100
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C 2.83872300 -1.04824200 0.12556500
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H 2.95627900 -1.49792100 -0.87263000
C 3.25242100 0.42277100 0.09281300
H 3.17300700 0.85995200 1.10105800
H 4.32021200 0.47097400 -0.15886000
C 2.47357400 1.26835300 -0.91361800
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H 2.48459100 0.78580400 -1.90424300
P 1.10187100 -1.33731400 0.64403400
P 0.70573200 1.53878700 -0.46746100
C 1.05331200 -0.89972600 2.42096700
H 0.07327500 -1.18148400 2.82562300
H 1.83730400 -1.42948000 2.97967300
H 1.17591900 0.17953500 2.56457100
C 0.94975500 -3.16008300 0.69410000
H 1.70016000 -3.58442300 1.37409700
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A2
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C -0.49814400 -0.90694400 -1.63429800
C -1.65015700 -1.85521500 -1.37703300
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H -4.56831900 -1.26770800 0.49181000
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H 4.00739000 -0.85384700 -0.35657700
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C 3.70406500 -0.51575200 1.88952200
H 3.48277800 0.23516300 2.64580400
H 4.39794700 -1.30730600 2.16200900
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H -3.72835200 0.53666000 1.01481700
H -3.28441900 0.13139800 -0.64414300
C -2.73424800 -1.38030300 0.80987700
H -2.30975000 -1.43672600 1.82532900
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TSA1 (triplet state)

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H -0.32796000 0.93333700 -2.94915200
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H -2.62476700 0.27175100 -2.53391800
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H -4.45279500 -0.52743500 0.46923300
H -4.45031300 -0.51582500 -1.31165000
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H -3.36539200 2.05102200 1.59221700
C -1.73200800 1.51253100 2.80509000
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C 3.18680900 -0.52974700 0.13250500
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H 4.24412900 -0.74694600 -0.07162200

C 2.80102600 0.70236400 -0.68912900
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H 0.23652000 3.54515300 -1.12592500
H 2.01998000 3.63050100 -1.08610600
H 1.19403000 2.70514900 -2.36764700
C 1.46143100 2.17450500 1.41652200
H 2.32680900 2.85094700 1.42298800
H 0.56777600 2.72924800 1.72908400
H 1.63199600 1.37330000 2.14545000
Co -0.49723500 0.11152300 -0.42932000

A2 (triplet state)

C 1.97333900 0.59122300 0.53671700
C 0.75903200 -0.17088100 -2.12122100
C 2.25417400 0.01056400 -1.92901300
C 2.73441600 0.59177000 -0.58613700
H 0.29114700 0.68254800 -2.64237200
H 0.46547400 -1.10629900 -2.60725700
H 2.64963700 0.66964200 -2.71858100

H 2.78630800 -0.94685100 -2.05878600
C 4.12597500 1.14403400 -0.66363900
H 4.13565900 2.07567600 -1.24739600
H 4.55637100 1.36464800 0.31794300
H 4.78741000 0.43891700 -1.18913400
C 2.38840000 0.88082100 1.89252700
H 3.46003100 0.85152100 2.11681700
C 1.53912700 1.16371900 2.88955000
H 0.46125000 1.20236400 2.71587300
H 1.88365900 1.38385400 3.89697300
C -3.00804300 -0.12959200 -0.78059000
H -4.04822900 0.22745300 -0.73058600
H -2.75808500 -0.22563900 -1.85000200
C -2.88378000 -1.48647200 -0.08663800
H -2.98116600 -1.37033500 1.00485100
H -3.74632200 -2.09844500 -0.38351200
C -1.62430200 -2.28610200 -0.42399000
H -1.72208900 -3.31420200 -0.03970600
H -1.50151200 -2.36493200 -1.51496000
P -1.92041300 1.20277100 -0.10334700
P -0.04087800 -1.63399900 0.25065500
C -2.71117600 1.65404400 1.48769300
H -2.20684300 2.53008900 1.91208400
H -3.77073500 1.89806000 1.33311900
H -2.63901600 0.83758600 2.21562600
C -2.33545000 2.62474100 -1.18127300
H -3.41914300 2.80208900 -1.19305200
H -1.83212400 3.52932500 -0.82172400
H -1.99656200 2.42795100 -2.20574900
C 1.20234800 -2.88433000 -0.20796900

H 2.17334400 -2.60510800 0.21701100
H 0.90610600 -3.86369700 0.19025500
H 1.29834600 -2.95991100 -1.29648500
C -0.18758300 -1.81421100 2.05990200
H -0.39213100 -2.86069400 2.32434200
H 0.74998100 -1.49257800 2.52998000
H -0.99291600 -1.18346500 2.45416700
Co 0.27639500 0.39270000 -0.30573600
A3
C -2.19173700 -0.58037600 0.56755200
C -0.99438200 0.07276900 -1.61419300
C -2.50365000 0.26613900 -1.61884300
C -3.08356800 -0.38495200 -0.39706300
H -0.73591200 -0.94664000 -1.96544700
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H -2.94715800 -0.16956500 -2.53184700
H -2.79130500 1.32978200 -1.65215200
C -4.51773600 -0.80294500 -0.36242100
H -4.72099500 -1.55775600 -1.13446500
H -4.80207600 -1.21754000 0.60957500
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C -1.56930900 -0.96882900 1.74335000
H -1.59842600 -0.32588300 2.62836100
C -0.55132800 -1.93667400 1.61174600
H -0.71793200 -2.77879700 0.93157600
H 0.13571400 -2.12224000 2.43657800
C 2.78041200 0.14265000 -1.22603900
H 3.79724900 -0.26022500 -1.34468700
H 2.33460600 0.18415900 -2.23291100
C 2.82132100 1.53909900 -0.60955700

H 3.17666200 1.48854400 0.43269000
H 3.57037500 2.14095800 -1.14127400
C 1.48755100 2.27813400 -0.67611800
H 1.60930700 3.31548100 -0.32744200
H 1.13889400 2.33969600 -1.71807600
P 1.79047800 -1.05381800 -0.23620400
P 0.11656600 1.56906300 0.32702800
C 2.92187600 -1.49034600 1.13914700
H 2.53055300 -2.36948800 1.66455700
H 3.92362100 -1.72774900 0.75693800
H 3.00587400 -0.67324900 1.86520200
C 1.84256000 -2.56647400 -1.27081100
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H 1.36465200 -3.39924200 -0.74063200
H 1.30527800 -2.40179000 -2.21263700
C -1.19582500 2.82182600 0.11448400
H -2.10242700 2.51108800 0.64664700
H -0.85488700 3.78354900 0.51979400
H -1.43578700 2.95748000 -0.94607100
C 0.63829900 1.85213700 2.06456600
H 1.08487600 2.85001100 2.17639100
H -0.24041500 1.79054500 2.71768100
H 1.35926400 1.09440100 2.39213600
Co -0.31657900 -0.48226300 0.16092500
TSA3
C -2.06007000 -0.73610800 0.33866600
C -1.75554400 -0.26380500 -1.57629100
C -3.10454000 0.38703300 -1.27622200
C -3.28125500 -0.24898800 0.06278500
H -1.89688400 -1.25425900 -2.02338000

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H -3.88324500 0.08672800 -1.99429000
H -3.09119600 1.48434400 -1.27224900
C -4.55853200 -0.50489500 0.77311600
H -4.40489000 -1.07886000 1.69355000
H -5.06059800 0.43778200 1.03125500
H -5.25559800 -1.06324700 0.13222300
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H 4.16112000 -0.05586200 -0.46925600
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H 3.84497000 2.32015800 -0.19385000
C 1.71436400 2.43603400 -0.37482100
H 1.71072900 3.44814800 0.05789400
H 1.69656800 2.56171400 -1.46920600
P 1.94807400 -0.95095000 -0.11089200
P 0.12138000 1.63721800 0.10833300
C 2.60099200 -1.44436000 1.53105700
H 2.53604900 -0.61094800 2.24071800
H 2.02236100 -2.28030000 1.94041900
H 3.65226100 -1.75094700 1.44806800
C 2.43451900 -2.34624300 -1.19667300
H 3.52383600 -2.48389300 -1.17121800
H 1.95386800 -3.27630800 -0.87550800
H 2.12872600 -2.14015400 -2.22908100
C -1.06456600 2.94281100 -0.39779000
H -2.03865600 2.75969900 0.07007200
H -0.70244900 3.92551700 -0.06797600
H -1.18967600 2.96538900 -1.48712300

C 0.09591100 1.82392100 1.93612900	H 1.29847000 3.51179900 -0.62347300
H 0.78400300 1.11914100 2.41796500	H 1.34028100 2.29475200 -1.90206000
H 0.36354400 2.84685200 2.23524100	P 1.92146000 -0.81245100 -0.02936300
H -0.91707500 1.60207400 2.29554300	P -0.09658200 1.63830100 -0.06632600
Co -0.22930300 -0.51291700 -0.21303700	C 2.65807100 -1.07331400 1.63174800
C -1.27328700 -1.64740700 1.09443200	H 2.54077400 -0.17331000 2.24686700
H -1.05936700 -1.50935200 2.15916600	H 2.15515600 -1.89770500 2.14982500
C -0.54473100 -2.55630800 0.33414600	H 3.72841900 -1.30496400 1.54783000
H -0.90774400 -2.89989000 -0.63596500	C 2.58364900 -2.22637000 -1.00284400
H 0.19596500 -3.19366100 0.81479500	H 3.67561500 -2.13779600 -1.07201000
A	H 2.34753600 -3.19137600 -0.54501200
C -2.14607800 -1.39226700 0.00250000	H 2.16865200 -2.21177700 -2.01782400
C -2.57325600 -1.43857800 -1.45102200	C -1.35455400 2.73333300 -0.84595300
C -3.24214800 -0.06069300 -1.18551700	H -2.36250400 2.55959700 -0.45847600
C -2.70567700 -0.14554500 0.23076800	H -1.08698800 3.78140100 -0.65751200
H -3.28100300 -2.24394500 -1.68289400	H -1.36877400 2.57388700 -1.93124700
H -1.77208400 -1.44499300 -2.20167400	C -0.02010000 2.29233400 1.65222500
H -4.33997500 -0.08239800 -1.22587700	H 0.77447500 1.79382100 2.21930500
H -2.89428900 0.76907300 -1.80941100	H 0.17485100 3.37370200 1.64266700
C -3.10443600 0.57049500 1.46654000	H -0.96321400 2.11202000 2.17837300
H -2.52059300 0.24835200 2.33763900	Co -0.26399000 -0.57014700 0.07050700
H -3.03220400 1.66156600 1.37655200	C -1.25527100 -2.12356300 0.84133800
H -4.16263900 0.35156400 1.67536900	H -1.33257100 -2.04595800 1.92822200
C 3.01573500 0.49871100 -0.73621900	C -0.15359900 -2.70473300 0.24052700
H 4.04798000 0.20882800 -0.48677100	H -0.17915000 -3.00065000 -0.80986300
H 2.92714600 0.42845300 -1.83198000	H 0.58795900 -3.20799100 0.85864500
C 2.73035600 1.92164500 -0.28786100	A3 (triplet state)
H 2.77266000 2.00162100 0.81036700	C -2.34239000 -0.24317000 0.57616300
H 3.53059600 2.57689200 -0.65739700	C -1.12919700 -0.84420100 -1.51304700
C 1.39730400 2.43217100 -0.81064900	C -2.54436300 -0.32113400 -1.75508200

C -3.21913500 -0.29638300 -0.41674800
H -1.13325000 -1.94525300 -1.47864500
H -0.39527000 -0.52288800 -2.26965500
H -3.10723300 -0.92954000 -2.48355200
H -2.53125000 0.69791100 -2.17702100
C -4.70298700 -0.36797100 -0.27124400
H -5.02052400 -0.32476600 0.77523400
H -5.17874700 0.46056400 -0.81444800
H -5.08740100 -1.29636800 -0.71538800
C 2.68568300 -0.44136500 -1.28525200
H 3.63147000 -0.99865600 -1.37136200
H 2.18390800 -0.52600900 -2.26216500
C 2.97285400 1.02642000 -0.96365600
H 3.38527500 1.12083700 0.05435500
H 3.77961800 1.36356700 -1.62846300
C 1.78684200 1.97437900 -1.14783300
H 2.13075100 3.02016300 -1.14562200
H 1.31359600 1.80172000 -2.12773200
P 1.64286800 -1.33797300 -0.05632700
P 0.45980800 1.81501500 0.12204800
C 2.73639400 -1.49641500 1.40550700
H 2.82632000 -0.53907600 1.93289500
H 2.29867900 -2.22196400 2.10200300
H 3.73803400 -1.84313800 1.11754300
C 1.59390300 -3.03715300 -0.72944600
H 2.60813500 -3.44025100 -0.84882400
H 1.02901200 -3.68979700 -0.05246000
H 1.09387100 -3.03793300 -1.70544500
C -0.79746500 3.01987100 -0.43717200
H -1.62032800 3.05834800 0.28738200

H -0.36894100 4.02469300 -0.54871100
H -1.20873700 2.69793200 -1.40198200
C 1.17341100 2.60967800 1.61382300
H 1.99657100 2.01086700 2.02137600
H 1.54642000 3.61670900 1.38294100
H 0.40189200 2.69199000 2.38935000
Co -0.37700900 -0.40275100 0.29833700
C -1.77130200 -0.18660000 1.84159400
H -1.71696900 0.76730500 2.37826400
C -0.88247900 -1.22001400 2.18957000
H -1.08427200 -2.23914500 1.85061000
H -0.23013400 -1.11480700 3.05553800
TSA3 (triplet state)
C -2.28760900 -0.48807800 0.36751100
C -1.55560400 -0.92657400 -1.45683100
C -3.02206200 -0.58021800 -1.72730900
C -3.44026900 -0.43060800 -0.30620800
H -1.35994500 -2.00661700 -1.51944900
H -0.82966900 -0.37501200 -2.09113700
H -3.55647400 -1.36410900 -2.28386400
H -3.14054400 0.35174500 -2.30089300
C -4.82085400 -0.29219100 0.21921900
H -4.83477600 -0.19821000 1.31068100
H -5.31421800 0.58972900 -0.21270400
H -5.43355100 -1.16075000 -0.05859900
C 2.92964900 -0.17743800 -1.14601200
H 3.93705700 -0.62138900 -1.17079200
H 2.52347900 -0.26686300 -2.16716800
C 3.01697200 1.29679400 -0.74512300
H 3.30203800 1.38755100 0.31591700

H 3.85113200 1.74500500 -1.30192400	C -2.88985800 -1.82414300 -0.02117900
C 1.76412700 2.12777100 -1.02994100	C -3.39040500 -1.10391700 -1.30481200
H 1.99682000 3.20102700 -0.95145400	C -2.98939200 0.19293100 -0.64366900
H 1.42699000 1.95526300 -2.06549800	H -3.66697900 -2.35078300 0.54670100
P 1.88401300 -1.24346900 -0.05854000	H -2.04517200 -2.51476100 -0.17084600
P 0.32566700 1.77082700 0.07258200	H -4.46810700 -1.20357700 -1.49138600
C 2.85962400 -1.37643000 1.48656900	H -2.85904300 -1.35668700 -2.23151700
H 2.83397500 -0.43620900 2.04965700	C -3.17543300 1.59776500 -1.06491400
H 2.42467400 -2.15883000 2.12043700	H -2.78287600 2.30578500 -0.32505900
H 3.90437000 -1.63764400 1.27070100	H -2.69145700 1.79545000 -2.03122800
C 2.10124500 -2.89830100 -0.81640300	H -4.24502500 1.81185700 -1.20461900
H 3.16446100 -3.15725600 -0.90885800	C 2.71816100 -0.70778500 -1.28529000
H 1.60479700 -3.65801800 -0.20059400	H 3.58610800 -1.38180700 -1.35562200
H 1.64367100 -2.91503200 -1.81347900	H 2.28159200 -0.65217500 -2.29532800
C -0.94003200 2.95181700 -0.52817700	C 3.17119800 0.68058500 -0.83115900
H -1.83569800 2.88020700 0.10205300	H 3.48848500 0.65353000 0.22394700
H -0.57501000 3.98737100 -0.51383800	H 4.08111300 0.93308200 -1.39296500
H -1.22760400 2.69070000 -1.55476600	C 2.16581100 1.81105900 -1.05225700
C 0.83657400 2.50565500 1.67562200	H 2.66737600 2.78156700 -0.91373600
H 1.61354700 1.89743000 2.15434300	H 1.80269700 1.79320400 -2.09222300
H 1.21547700 3.52799100 1.54216000	P 1.47404200 -1.53018200 -0.19590500
H -0.02377500 2.54123200 2.35529200	P 0.67694000 1.80345600 0.04799400
Co -0.28056400 -0.48228200 0.07774500	C 2.43849600 -1.93368400 1.31207400
C -1.69126500 -0.31824100 1.65980900	H 2.66438800 -1.02989100 1.88989500
H -1.76333900 0.65710400 2.15198800	H 1.84779900 -2.60065700 1.95175900
C -0.77554600 -1.23582200 2.12243400	H 3.37962900 -2.43694100 1.05147700
H -0.79845600 -2.27245900 1.77993000	C 1.29878700 -3.17683800 -0.98675700
H -0.16908700 -1.02152200 3.00115500	H 2.27883000 -3.65489000 -1.11763100
A (triplet state)	H 0.67331200 -3.82633300 -0.36212700
C -2.56230000 -0.43256700 0.49944000	H 0.81843500 -3.07898800 -1.96747000

C -0.08298300 3.42192000 -0.37613200
H -0.91139700 3.63765600 0.31060900
H 0.65432200 4.23169900 -0.29319400
H -0.47795800 3.40807800 -1.39872500
C 1.39724900 2.17601700 1.69837900
H 1.93319300 1.30672600 2.09806100
H 2.08618800 3.03051100 1.65015200
H 0.58880400 2.41932300 2.39972600
Co -0.41293700 -0.24303500 0.13625800
C -1.85330900 0.03396500 1.67477700
H -1.93273800 1.08834300 1.95118000
C -0.99017700 -0.79229400 2.34018700
H -1.00785700 -1.87149300 2.18102400
H -0.39415600 -0.43307100 3.17670400

TSZI

C -2.62990800 -0.19959200 0.21991900
C -2.43265600 1.23276000 -0.30304300
C -3.98533700 1.26452400 -0.40885100
C -3.97004800 -0.14520600 0.12303200
H -1.91672900 1.34491900 -1.27271800
H -2.02618400 1.96566400 0.40813600
H -4.37268700 1.37790000 -1.42990100
H -4.46502200 2.01838500 0.22915600
C -5.06298800 -1.10066200 0.40326500
H -4.67563100 -2.06988200 0.73954000
H -5.73888300 -0.71365800 1.17818500
H -5.67700700 -1.26798100 -0.49225400
C 3.33177100 -0.62834400 -0.26989200
H 4.06202000 -1.37774000 0.07172100
H 3.50958900 -0.49090300 -1.34835700

C 3.53043800 0.69228300 0.45912500
H 3.24260000 0.59923300 1.51930800
H 4.60180100 0.93369300 0.46866500
C 2.77523600 1.83646700 -0.20382400
H 3.07107300 2.80600400 0.22409700
H 3.01678100 1.87781100 -1.27720900
P 1.67062800 -1.41776300 -0.09505200
P 0.94409200 1.71567200 -0.04541500
C 1.79824800 -2.27007700 1.52259600
H 1.87255600 -1.53161300 2.33051700
H 0.90615400 -2.88015500 1.70584300
H 2.68345800 -2.91945900 1.55101900
C 1.86377100 -2.76182000 -1.33107600
H 2.87339100 -3.18626000 -1.25089700
H 1.13815200 -3.56667300 -1.18331300
H 1.73122100 -2.35909600 -2.34200600
C 0.42132600 3.16733000 -1.04009600
H -0.64080200 3.38761800 -0.88934300
H 1.00571500 4.04998300 -0.74805200
H 0.58543400 2.97265800 -2.10639200
C 0.68217600 2.27551100 1.68653800
H 1.12430700 1.55516400 2.38570100
H 1.14275700 3.25971200 1.84875600
H -0.38763400 2.34524600 1.91481800
Co -0.12241500 -0.23893900 -0.22298300
C -1.66044400 -1.24828000 0.56210100
H -1.47164000 -1.48889900 1.61403500
C -1.15268700 -2.06064400 -0.43463700
H -1.53669100 -2.00606800 -1.45580600
H -0.62708900 -2.97838300 -0.17666000

TSZ1 (open-shell singlet)

C -2.77731400 -0.24670200 0.11794800
C -2.66466200 1.17386700 -0.42274000
C -4.22077500 1.16553900 -0.41920300
C -4.12326800 -0.23727500 0.12672700
H -2.20504900 1.28876000 -1.41885900
H -2.22186000 1.91712000 0.25924800
H -4.68272600 1.25630000 -1.41093800
H -4.68072500 1.90793000 0.24626600
C -5.16303500 -1.21671500 0.50883600
H -4.72313900 -2.16356500 0.84501100
H -5.79684600 -0.82650200 1.31714200
H -5.83160400 -1.43112900 -0.33618700
C 3.44246800 -0.55079400 -0.33167300
H 4.23906800 -1.22945700 0.00999700
H 3.58733900 -0.42312100 -1.41618400
C 3.55453000 0.79916200 0.36991200
H 3.29315000 0.70373600 1.43679500
H 4.60933500 1.10559300 0.36026500
C 2.73182300 1.90529900 -0.28503400
H 3.04510500 2.89167900 0.09000500
H 2.90653500 1.91378900 -1.37227000
P 1.84131200 -1.44049400 -0.09945300
P 0.90992400 1.79024300 -0.01957400
C 2.01717200 -2.18413700 1.56978000
H 2.03692800 -1.40100200 2.33771900
H 1.15920100 -2.83553900 1.77893800
H 2.93766800 -2.77862900 1.64456400
C 2.09069700 -2.87728100 -1.21331100
H 3.08166800 -3.31893900 -1.04305800

H 1.33435000 -3.65001600 -1.03813300
H 2.02121100 -2.56076800 -2.26054400
C 0.31673100 3.24912100 -0.95933200
H -0.74630500 3.42825000 -0.76255700
H 0.88344400 4.14378400 -0.66903100
H 0.44337900 3.08361800 -2.03556200
C 0.72617000 2.32882200 1.72805200
H 1.16031100 1.58484000 2.40734600
H 1.22160900 3.29481900 1.89583000
H -0.33643400 2.43064200 1.98013600
Co -0.08088200 -0.25824100 -0.21131100
C -1.76533300 -1.25657300 0.47368800
H -1.59325600 -1.47363600 1.53543200
C -1.18476000 -2.07604400 -0.46571400
H -1.48890600 -2.03279200 -1.51452600
H -0.62082600 -2.95720900 -0.16365700
Z1
C -2.28476700 -0.95079600 0.58556500
C -3.34756700 0.08608700 0.86267900
C -3.40011300 0.30580700 -0.67354000
C -2.26893600 -0.68810200 -0.80092400
H -3.03411100 0.94691100 1.46742700
H -4.27240300 -0.31843200 1.29000600
H -3.23673400 1.31777200 -1.05627900
H -4.32515600 -0.07789700 -1.12648200
C -1.75647700 -1.35275200 -2.02929300
H -0.64893200 -1.33076300 -2.07936200
H -2.04803100 -2.41222800 -2.07499300
H -2.13668700 -0.84853700 -2.92543400
C 2.89342200 0.37373400 -0.92071600

H 3.93638500 0.03319800 -0.83346200
H 2.63082900 0.31893000 -1.98962300
C 2.75127600 1.80523800 -0.42092800
H 2.92980300 1.85392100 0.66544600
H 3.54589800 2.41551000 -0.87132800
C 1.40774800 2.43560300 -0.76389200
H 1.40993800 3.50035400 -0.48567200
H 1.23788400 2.39469000 -1.85159500
P 1.84131700 -0.85990000 -0.04350200
P -0.06917200 1.67462600 0.04714500
C 2.72109500 -1.06551300 1.55250700
H 2.68057400 -0.14251800 2.14239000
H 2.25737000 -1.86208600 2.14488900
H 3.77432600 -1.32222100 1.37609300
C 2.30352500 -2.38063800 -0.96260600
H 3.39530100 -2.43701000 -1.06524300
H 1.95545800 -3.28002100 -0.44427900
H 1.85973200 -2.36487700 -1.96572400
C -1.33072200 2.91261700 -0.46120000
H -2.25732100 2.79138200 0.11031700
H -0.94405200 3.92239200 -0.27009200
H -1.55780000 2.82499000 -1.53030700
C 0.16736100 2.13517200 1.81336900
H 0.97683900 1.55276200 2.26765400
H 0.39413100 3.20562400 1.91652700
H -0.74996200 1.91393000 2.37305100
Co -0.33605800 -0.50913000 0.08121200
C -1.37627500 -1.71245600 1.35695300
H -1.32136000 -1.53901000 2.43328100
C -0.42267000 -2.49633700 0.70679100

H -0.64147000 -2.98866800 -0.24239100
H 0.33954400 -2.98845400 1.30923700
TSZ1 (triplet state)
C 2.64391900 0.23618700 -0.05089000
C 2.00568900 0.52884700 1.29944800
C 3.46353000 0.55257100 1.84411000
C 3.90117700 0.26464200 0.42791700
H 1.36842600 -0.26567300 1.72501100
H 1.47085100 1.48891200 1.38884000
H 3.69398100 -0.22701800 2.58205000
H 3.78349200 1.52004100 2.25292900
C 5.24306700 0.08919200 -0.16801900
H 5.18312200 -0.12912200 -1.24121400
H 5.85555000 0.99170500 -0.03514600
H 5.78756200 -0.73156900 0.31862100
C -1.97219000 -1.23192300 1.66529300
H -2.53593300 -2.10204200 2.03643100
H -1.16555800 -1.04978600 2.39395000
C -2.89154700 -0.01340100 1.58754100
H -3.63846700 -0.14773000 0.78809600
H -3.47658100 0.02255100 2.51678200
C -2.18519500 1.33387500 1.43356700
H -2.88387100 2.15366600 1.66258200
H -1.35926800 1.41388400 2.15869300
P -1.16783500 -1.73948700 0.07851000
P -1.47681300 1.67556600 -0.23739200
C -2.56936000 -2.43822800 -0.88134000
H -3.26701100 -1.65215000 -1.19273400
H -2.18945300 -2.92618800 -1.78659000
H -3.11616200 -3.18091900 -0.28482800

C -0.27056900 -3.25418900 0.59454600
H -0.92620100 -3.92322600 1.16760200
H 0.09002800 -3.79565800 -0.28840900
H 0.59597400 -2.99143100 1.21448800
C -0.85901400 3.39202600 -0.04926300
H -0.50731200 3.77331400 -1.01480000
H -1.65520000 4.05118300 0.32193200
H -0.01976800 3.42078600 0.65588200
C -2.96465200 1.91303300 -1.28459500
H -3.65735700 2.62384700 -0.81406900
H -2.66658200 2.30883400 -2.26241600
H -3.48871200 0.96525700 -1.45218400
Co 0.01433900 0.02791600 -0.87900200
C 2.04218200 0.02269900 -1.37875800
H 2.06296300 0.84930700 -2.10265600
C 1.57502100 -1.19789500 -1.80075900
H 1.72708000 -2.09154800 -1.19579700
H 1.24460700 -1.34875400 -2.82955800
Z1 (triplet state)
C -2.53572300 0.54201200 -0.32479900
C -3.42751300 -0.65564600 -0.08306800
C -3.16401300 -0.41694500 1.42785600
C -2.32389400 0.76581900 1.01438400
H -3.08166900 -1.61463800 -0.49268900
H -4.47302600 -0.50899800 -0.38079200
H -2.62582200 -1.22177500 1.95045300
H -4.05253800 -0.16841000 2.02455600
C -1.70675100 1.80786800 1.86767100
H -1.21096400 2.59791300 1.29340400
H -2.47926500 2.28338300 2.49034900
H -0.97881200 1.37214500 2.56862200
C 2.27217700 0.48893000 1.56281700
H 3.22192900 0.99770300 1.79067000
H 1.58324200 0.72953400 2.38848800
C 2.49651100 -1.01988100 1.49697900
H 3.18339900 -1.26676200 0.67150000
H 3.03317100 -1.31507200 2.40917500
C 1.22813300 -1.86840100 1.40543500
H 1.45490800 -2.91097200 1.67760900
H 0.47627900 -1.50796200 2.12760700
P 1.58006900 1.27093000 0.03832000
P 0.40789500 -1.90686900 -0.25066300
C 2.96112600 1.13274800 -1.16780100
H 3.08252300 0.10138500 -1.51973800
H 2.74016600 1.75785800 -2.04178900
H 3.90817600 1.47025300 -0.72515600
C 1.66850400 3.05128800 0.47537500
H 2.68710500 3.31781700 0.78713400
H 1.39814100 3.66658900 -0.39128900
H 0.98161800 3.28508900 1.29782200
C -0.83886400 -3.23235700 -0.00683000
H -1.36048700 -3.44176200 -0.94821800
H -0.35178100 -4.15474000 0.33708900
H -1.58200700 -2.92759300 0.74006200
C 1.63937900 -2.77077500 -1.30510300
H 1.99877100 -3.68336900 -0.81022400
H 1.17117200 -3.04959500 -2.25644400
H 2.49949600 -2.13082500 -1.53211600
Co -0.28963200 0.22040800 -0.85578400
C -2.01803700 1.07767900 -1.56657600

H -2.31594400 0.55183700 -2.47877500

C -1.11699700 2.11658500 -1.66279600

H -0.96728000 2.82264500 -0.84860500

H -0.74412400 2.42284600 -2.63864900

Z2

C -2.63741200 -0.35811400 0.14269000

C -0.57080100 -0.26965200 -2.03310400

C -2.32440500 0.90962200 0.69246800

C -0.61883600 1.11024500 -1.88840600

H -1.47478200 -0.86772300 -2.13809100

H 0.32394900 -0.72244800 -2.45968900

H -1.55852100 1.65443900 -1.87562300

H 0.22832100 1.70023500 -2.23226200

C 2.30515200 -1.72427500 -0.89474700

H 2.79298100 -2.68986600 -0.69152400

H 2.07002100 -1.72735200 -1.96987700

C 3.27484600 -0.58904200 -0.58118100

H 3.54593500 -0.60369700 0.48635600

H 4.21347800 -0.79279900 -1.11468200

C 2.79402200 0.80521100 -0.98346300

H 3.62641800 1.52340700 -0.92706400

H 2.44940400 0.80604000 -2.02922700

P 0.69644000 -1.75509400 0.03606800

P 1.43792700 1.45359800 0.08478700

C 1.25496300 -2.43431500 1.65223900

H 0.39448300 -2.65739100 2.29436800

H 1.81952400 -3.36332900 1.49806100

H 1.89468800 -1.72031500 2.18415500

C -0.04139100 -3.26895100 -0.70325100

H 0.71664900 -4.06154500 -0.75762700

H -0.86972300 -3.63089200 -0.08472000

H -0.41961600 -3.07640000 -1.71364200

C 1.36309000 3.23488900 -0.36411700

H 0.59240000 3.73413000 0.23600700

H 2.32977300 3.71411500 -0.16092200

H 1.11878200 3.38464500 -1.42028400

C 2.29481300 1.60996900 1.70578500

H 2.50398100 0.63904400 2.16744400

H 3.24656100 2.13916000 1.56296700

H 1.68189700 2.19672900 2.40142500

Co -0.41675900 0.20271300 -0.00642600

C -2.84639000 -1.75807900 0.61026100

H -3.86255800 -1.85335900 1.02533300

H -2.80122800 -2.44772400 -0.24442600

H -2.14702400 -2.10969100 1.37515300

C -3.58263100 0.28918900 -0.86203000

C -3.30590300 1.65153900 -0.16777100

H -4.61904800 -0.06724500 -0.78558200

H -3.28934800 0.23487600 -1.91910300

H -4.17035400 1.99429200 0.41479600

H -2.94972800 2.49498800 -0.77207800

C -1.24637000 1.23827800 1.53465400

C -0.52312900 0.12392800 2.02921000

H -0.97851500 2.27770600 1.72866600

H -1.07864400 -0.76601800 2.31837700

H 0.36911400 0.29052400 2.62857700

TSZ2

C 2.63273400 -0.54014400 -0.05016600

C 1.37985000 -1.11099000 1.63259800

C 2.10010600 0.53799800 -0.86086400

C 0.62020900 0.04631300 1.98714100
H 2.40340100 -1.20342000 1.99076000
H 0.89321600 -2.08960000 1.62457900
H 1.17724900 0.92892600 2.31855800
H -0.32890900 -0.08076100 2.50674900
C -2.32627100 1.56655400 -1.02200600
H -2.84774800 2.53589300 -1.00350400
H -1.94236100 1.43315200 -2.04611300
C -3.30721600 0.44674500 -0.67251500
H -3.63211700 0.54378200 0.37567400
H -4.21944800 0.59172100 -1.26723100
C -2.79847300 -0.96946100 -0.93483400
H -3.60228500 -1.69707700 -0.74426200
H -2.52500400 -1.08087600 -1.99447700
P -0.87269800 1.69196300 0.11479000
P -1.34313400 -1.49142800 0.07629000
C -1.67661300 2.17340900 1.69459900
H -0.91485600 2.50306700 2.41115000
H -2.37408300 3.00403500 1.52218900
H -2.22850100 1.34415700 2.15023300
C -0.15300100 3.31588800 -0.35630200
H -0.93840700 4.08282200 -0.38194500
H 0.59449100 3.61496700 0.38891100
H 0.33455000 3.28152900 -1.33695600
C -1.09100900 -3.22028300 -0.48739100
H -0.27149200 -3.68495200 0.07550000
H -2.00088000 -3.81422000 -0.32964100
H -0.83466900 -3.24781500 -1.55227200
C -2.12241000 -1.79582100 1.71635300
H -2.95206300 -2.50647300 1.60651200

H -1.39669100 -2.22404300 2.41868300
H -2.51585000 -0.87168800 2.15546400
Co 0.40060700 -0.11059900 0.01634400
C 3.14434000 -1.90168500 -0.42275600
H 3.89081400 -1.81062400 -1.22489700
H 3.64945200 -2.35931200 0.43852600
H 2.37087700 -2.60030000 -0.75872900
C 3.56110600 0.46940800 0.63890000
C 2.99237600 1.59328800 -0.26161100
H 4.61769500 0.23713000 0.45004700
H 3.43466200 0.61251500 1.71918400
H 3.72860700 2.00733700 -0.96189800
H 2.49961800 2.42576400 0.25566900
C 1.08214500 0.43655900 -1.82933700
C 0.46483300 -0.81693300 -1.97784200
H 0.70226400 1.32666800 -2.33283600
H 1.05356500 -1.73001500 -1.93392300
H -0.42024300 -0.87921700 -2.61098300
Z3
C 2.80483400 -0.62395600 0.30191200
C 1.82680400 -0.99769900 1.42953200
C 2.12447700 0.30544200 -0.73098600
C 0.84489900 0.12171000 1.69141500
H 2.38549700 -1.28113000 2.34044100
H 1.27685300 -1.92436100 1.15514700
H 1.33688200 1.07972800 1.90907400
H 0.10644600 -0.09641500 2.47213500
C -2.30738400 1.65549100 -1.01386100
H -2.70900000 2.68082000 -1.02547400
H -1.93926200 1.44429400 -2.03131300

C -3.40943400 0.67108600 -0.62664800
H -3.71767400 0.83863900 0.41776900
H -4.29906800 0.90260800 -1.22796200
C -3.05856500 -0.79821200 -0.84359800
H -3.92713700 -1.43713200 -0.62298300
H -2.79355800 -0.97059100 -1.89879000
P -0.83148300 1.67404800 0.09756300
P -1.62981600 -1.39644500 0.15317200
C -1.51588000 2.22111400 1.70470900
H -0.69957200 2.48936800 2.38504500
H -2.14880800 3.10578500 1.55321200
H -2.11318800 1.43981300 2.18558900
C 0.04291100 3.18921300 -0.43842000
H -0.66748800 4.02533300 -0.48405100
H 0.82751500 3.44695800 0.28205400
H 0.50008600 3.05604800 -1.42536200
C -1.52002100 -3.15778400 -0.34722100
H -0.70613300 -3.65458300 0.19615900
H -2.45910400 -3.67980700 -0.12130200
H -1.31841500 -3.24138900 -1.42092400
C -2.31036200 -1.57563100 1.84917000
H -3.21797200 -2.19360900 1.83623200
H -1.56528400 -2.06818100 2.48746700
H -2.55218500 -0.60781500 2.30174300
Co 0.18471700 -0.16218000 -0.12855000
C 3.53881100 -1.83382500 -0.24534000
H 4.19337100 -1.55759500 -1.08217300
H 4.16795900 -2.27274400 0.54223300
H 2.85753100 -2.62128500 -0.59622800
C 3.74236500 0.56439700 0.65086200

C 3.05702800 1.44979100 -0.41272400
H 4.79995200 0.35303200 0.45631100
H 3.65010500 0.92975800 1.68125300
H 3.69972500 1.74182000 -1.25398200
H 2.59090100 2.36234400 -0.02221500
C 1.32591100 0.03253700 -1.84491300
C 0.55640500 -1.15017300 -1.88347700
H 1.10502200 0.85073500 -2.53740200
H 0.99367400 -2.08076900 -1.51024000
H -0.18231700 -1.28587900 -2.67411200
Z2 (triplet state)
C -2.80760000 0.14457000 -0.18990700
C -1.17874900 0.37678800 2.46459000
C -2.01590500 -0.67056200 -0.97663900
C -0.34629800 -0.69798200 2.59057400
H -2.25865000 0.25487100 2.43366000
H -0.82518200 1.39194900 2.64323900
H -0.74249000 -1.71545900 2.63494000
H 0.69525000 -0.57516600 2.88381600
C 2.49906000 -0.86106200 -1.32756500
H 3.31795100 -1.57812700 -1.49426800
H 1.89840100 -0.84772900 -2.25080600
C 3.07451700 0.53033000 -1.05639400
H 3.57375800 0.55185900 -0.07400100
H 3.87878100 0.70544600 -1.78443800
C 2.08679400 1.69181600 -1.17177400
H 2.63822700 2.64498700 -1.16371800
H 1.55683400 1.64081000 -2.13589200
P 1.43180200 -1.55107800 0.01706700
P 0.79552700 1.79106700 0.15259400

C 2.65371500 -1.90730600 1.34270000
H 2.17985000 -2.50806200 2.12883400
H 3.50462900 -2.47237500 0.93906100
H 3.03132500 -0.98585400 1.80144500
C 1.09526400 -3.25097700 -0.59566800
H 2.02928100 -3.76135600 -0.86656700
H 0.59422700 -3.83280100 0.18819700
H 0.43896200 -3.22937700 -1.47402600
C 0.03875400 3.42701200 -0.20974600
H -0.71266100 3.66653800 0.55381100
H 0.79937200 4.21921400 -0.21505000
H -0.45557300 3.41523300 -1.18899400
C 1.81550400 2.21737600 1.62599000
H 2.51575300 3.03104300 1.39255600
H 1.17074400 2.54894300 2.44936900
H 2.38963100 1.35221000 1.97843600
Co -0.43371200 -0.19145400 0.45670600
C -3.16612600 1.58256300 -0.15618700
H -4.15008700 1.73440000 -0.62596200
H -3.25385300 1.95107100 0.87568800
H -2.44258100 2.21360400 -0.68356400
C -3.51296400 -1.03005200 0.45319800
C -2.59082000 -1.95106400 -0.38685700
H -4.57169700 -1.09616400 0.16670000
H -3.45729200 -1.13848700 1.54535900
H -3.11588700 -2.58866400 -1.10971900
H -1.90152200 -2.58432800 0.19266300
C -1.17581600 -0.49858200 -2.15441400
C -1.03388500 0.62568000 -2.87423600
H -0.65857400 -1.40278300 -2.48879900

H -1.57216400 1.54105300 -2.63050100
H -0.40711600 0.65163800 -3.76346700
TSZ2 (triplet state)
C 2.55421900 -0.21028100 0.22252200
C 1.81292100 -0.39866500 1.84327300
C 1.81411800 0.48528900 -0.90798800
C 0.73524300 0.53382800 2.22232300
H 2.76806200 -0.22507500 2.35242200
H 1.53594400 -1.45335800 1.96120200
H 1.03455100 1.55534400 2.48285900
H -0.06765800 0.15058800 2.85582000
C -2.51661100 1.02955900 -1.24182500
H -3.24661100 1.84011700 -1.39366100
H -1.96908900 0.91276000 -2.19088100
C -3.24457100 -0.26800300 -0.88794900
H -3.68637600 -0.19612200 0.11913100
H -4.10262400 -0.36484500 -1.56719100
C -2.40850800 -1.54114400 -1.01009400
H -3.05625800 -2.42510200 -0.90367200
H -1.95189500 -1.59859000 -2.01083100
P -1.29974900 1.63263500 0.00599900
P -1.03185300 -1.70250500 0.21089600
C -2.32730600 2.10371000 1.44570000
H -1.70371100 2.64399600 2.16830400
H -3.15824900 2.75252700 1.13766400
H -2.73472400 1.22054000 1.95075600
C -0.80414800 3.25910100 -0.67200200
H -1.68851400 3.87960200 -0.86917700
H -0.16092700 3.78469600 0.04438700
H -0.24587400 3.12503200 -1.60669800

C -0.44624600 -3.41339200 -0.11562500	H 2.21530000 2.32030800 -0.41016100
H 0.36100300 -3.67853300 0.57882400	H 1.21542300 -0.05506100 -2.12906400
H -1.26729500 -4.13078900 0.01619800	H 0.51469100 1.58781300 -2.11745700
H -0.06816400 -3.49981400 -1.14051700	C -2.84745900 -1.54651900 0.71429200
C -1.91890800 -1.95180100 1.80287100	H -3.44331500 -2.44216500 0.47927400
H -2.69068600 -2.72769600 1.70813000	H -2.66506200 -1.56821700 1.80125900
H -1.20199200 -2.26899000 2.57155400	C -3.62842900 -0.28640200 0.34600400
H -2.39001400 -1.02437800 2.14923800	H -3.79382300 -0.24368200 -0.74270600
Co 0.33549000 0.22219300 0.34141800	H -4.63250200 -0.37852700 0.78195900
C 3.24087200 -1.54049200 0.02011700	C -3.02009700 1.02666500 0.84299300
H 3.81924000 -1.53176500 -0.91334500	H -3.76396500 1.83544300 0.77222300
H 3.93648100 -1.73959700 0.84763400	H -2.74024800 0.94281800 1.90536200
H 2.53316100 -2.37847500 -0.02516100	P -1.19665100 -1.74718500 -0.09065400
C 3.43396600 1.05903300 0.31741700	P -1.52248700 1.57901300 -0.07985200
C 2.51102000 1.81070400 -0.65796200	C -1.57537500 -2.14486100 -1.83941800
H 4.42255300 0.86501100 -0.11756900	H -0.65293900 -2.46451100 -2.34118500
H 3.57124600 1.49594900 1.31547000	H -2.31536400 -2.95303800 -1.91361600
H 2.99727900 2.26248800 -1.53208200	H -1.95223400 -1.26294600 -2.37069000
H 1.89650300 2.58512200 -0.17288700	C -0.66463200 -3.36868200 0.58086200
C 1.29153500 0.00346100 -2.14966100	H -1.39871900 -4.14748400 0.33474300
C 1.14304700 -1.28412700 -2.55696100	H 0.30738500 -3.65753000 0.16371000
H 0.98911200 0.79675200 -2.84307800	H -0.56849900 -3.31428400 1.67208700
H 1.49413700 -2.12093300 -1.95703700	C -1.20522500 3.25943900 0.56672000
H 0.72333800 -1.51829100 -3.53245700	H -0.31168600 3.67429000 0.08207000
Z3 (triplet state)	H -2.05600800 3.92416500 0.36678400
C 3.12286000 0.37753700 -0.18594700	H -1.02681700 3.22140300 1.64782000
C 2.40812000 1.42546100 -1.02890000	C -2.17370000 1.92569000 -1.75854700
C 2.13979700 -0.58094800 0.51034400	H -3.14679000 2.43055000 -1.69096700
C 1.09378800 0.86421200 -1.53139100	H -1.48049800 2.58425500 -2.29427900
H 3.06027600 1.77216900 -1.85118900	H -2.28587400 1.00867100 -2.34816900

Co 0.17279900 0.16957400 0.11094400
C 4.16033000 0.97345800 0.75172200
H 4.65690600 0.19511500 1.34698700
H 4.93387600 1.49891000 0.17481900
H 3.71333100 1.69524700 1.44942500
C 3.65225100 -0.85132500 -0.97869100
C 2.72545600 -1.79148200 -0.17553900
H 4.72491800 -1.03726800 -0.85467200
H 3.43035100 -0.81656800 -2.05240000
H 3.24137400 -2.48758700 0.50116200
H 2.01835800 -2.37627100 -0.78348500
C 1.37811500 -0.46945400 1.68078600
C 0.76382100 0.74820600 2.03342700
H 1.02193200 -1.39126300 2.15101100
H 1.25085100 1.69504300 1.78384000
H 0.07313300 0.78831000 2.87530000

TSZ3

C -2.86067700 -0.60620100 -0.31813900
C -1.64256300 -1.13578000 -1.05422000
C -2.29439500 0.56281800 0.49044400
C -0.80019100 -0.31636300 -1.80426000
H -1.53680700 -2.22072400 -1.12960800
H -0.67135900 -1.52794100 0.79223900
H -1.09574300 0.69663300 -2.08119600
H -0.07657400 -0.77206900 -2.48151600
C 2.87368300 -0.90825500 -1.14010000
H 3.67932900 -1.65563100 -1.07635400
H 2.46822500 -0.96965300 -2.16238000
C 3.42098100 0.49013300 -0.87933500
H 3.81710600 0.56153200 0.14659100

H 4.28754900 0.65054600 -1.53490600
C 2.40571500 1.59930100 -1.13350700
H 2.89750900 2.58295400 -1.09529400
H 1.97456100 1.49637900 -2.14267700
P 1.54015900 -1.46417400 0.00302000
P 0.99431900 1.63662600 0.05124200
C 2.42326500 -1.82576800 1.56514400
H 1.74334500 -2.35408900 2.24473100
H 3.30304900 -2.45695900 1.38176100
H 2.74505700 -0.90321000 2.06226000
C 1.20278800 -3.14358700 -0.64278900
H 2.13440000 -3.72000900 -0.71588800
H 0.51234700 -3.66997300 0.02739400
H 0.74776300 -3.09200400 -1.63929800
C 0.15658800 3.18015100 -0.48310100
H -0.67181400 3.43073000 0.18996700
H 0.86990100 4.01513900 -0.48100500
H -0.23996600 3.06758000 -1.49968900
C 1.80105700 2.19169800 1.60712200
H 2.41153400 1.39166900 2.04255700
H 2.44082100 3.06698200 1.43016700
H 1.03897300 2.46679200 2.34693700
Co -0.23311200 -0.21697500 0.21009300
C -3.63106700 -1.69727500 0.39437600
H -4.40472400 -1.27445700 1.04695000
H -4.12722400 -2.34662800 -0.33975400
H -2.97576100 -2.33104200 1.00780800
C -3.71182100 0.42803300 -1.10830900
C -3.03012400 1.58617500 -0.34081500
H -4.78281000 0.33309500 -0.89564400

H -3.56751700 0.42165700 -2.19394100
H -3.70210800 2.23111100 0.24115600
H -2.40156500 2.24113400 -0.95868000
C -1.47954200 0.67660100 1.60243600
C -0.81448600 -0.45224100 2.18754200
H -1.22211700 1.68580200 1.93568100
H -1.41467100 -1.31397700 2.48579000
H -0.01912600 -0.23647500 2.90446200

Z4

C -2.91989200 -0.55073500 -0.25336500
C -1.70760900 -1.28017300 -0.78532300
C -2.30847200 0.72767100 0.31300300
C -0.84625100 -0.70910700 -1.72331200
H -1.61525400 -2.34317300 -0.54454600
H -0.63474200 -0.96973600 1.89690400
H -1.10039000 0.21842100 -2.24330100
H -0.15234100 -1.34143500 -2.27925000
C 2.85780300 -1.12894400 -1.10351300
H 3.59189300 -1.94291800 -1.00493400
H 2.47685700 -1.16696700 -2.13644200
C 3.51474900 0.22146600 -0.83518200
H 3.89812700 0.25983600 0.19734400
H 4.40212600 0.30798000 -1.47665300
C 2.59731400 1.40797900 -1.10794400
H 3.16719400 2.34922600 -1.08329300
H 2.16770300 1.32283200 -2.11996800
P 1.45097000 -1.52019600 0.01524700
P 1.16633200 1.58658300 0.04681400
C 2.25298300 -1.74017600 1.65253500
H 1.56212300 -2.25788100 2.32960000

H 3.16613500 -2.34405600 1.56139300
H 2.50612700 -0.77466900 2.10531900
C 1.06846900 -3.25592700 -0.43369000
H 1.97728200 -3.86946400 -0.37902300
H 0.32871500 -3.66581100 0.26496700
H 0.66201600 -3.32694100 -1.44939100
C 0.38091300 3.08312900 -0.67480700
H -0.44872900 3.43749300 -0.05204100
H 1.11615000 3.89359700 -0.77026600
H -0.01125000 2.84906400 -1.67271200
C 1.95077800 2.27969900 1.55939500
H 2.58039600 1.53314600 2.05849300
H 2.57091800 3.15292800 1.31567300
H 1.17665100 2.59268100 2.27137100
Co -0.21590200 -0.13005100 0.12299200
C -3.78328600 -1.41474900 0.64145400
H -4.54554600 -0.81765800 1.15811400
H -4.30124800 -2.17438900 0.04019200
H -3.18981200 -1.94398500 1.39969000
C -3.67867900 0.34009100 -1.28027700
C -2.95133100 1.59688800 -0.74155500
H -4.75989100 0.35246700 -1.10025200
H -3.50256400 0.09632200 -2.33346600
H -3.60026100 2.38395100 -0.33536700
H -2.26068300 2.07423600 -1.45002600
C -1.48497700 0.96856400 1.37702000
C -1.11332200 -0.07663400 2.38576800
H -1.22962000 2.00578000 1.60683200
H -1.98997300 -0.49648300 2.89714100
H -0.41343000 0.30694200 3.13496100

TSZ3 (triplet state)

C -2.96354900 -0.80704500 -0.27277700
C -1.65199600 -1.14039700 -0.96250100
C -2.82612600 0.49878000 0.49486900
C -0.91939800 -0.17131900 -1.64547000
H -1.47249000 -2.19175500 -1.20775900
H -0.72263800 -1.57670900 0.54705000
H -1.33011300 0.82902500 -1.78477600
H -0.15623100 -0.47568000 -2.36475400
C 3.20632100 -0.78874200 -1.02745800
H 4.09947000 -1.42317300 -0.91731100
H 2.88385900 -0.88203400 -2.07737300
C 3.54707100 0.66766900 -0.71580500
H 3.80328400 0.78178700 0.35034300
H 4.46778100 0.92277300 -1.25781400
C 2.47011300 1.67773600 -1.11530100
H 2.89730300 2.69203600 -1.14430700
H 2.10614400 1.46136300 -2.13308400
P 1.86430200 -1.51284300 0.00959700
P 0.98727000 1.74815200 -0.01920600
C 2.66224800 -1.82553500 1.62869800
H 1.96194300 -2.37252600 2.27206300
H 3.58158000 -2.41578700 1.51690900
H 2.90351200 -0.87927100 2.12847400
C 1.67558900 -3.18732600 -0.70392100
H 2.64020100 -3.70940300 -0.75739200
H 0.98568500 -3.77413100 -0.08543800
H 1.25696700 -3.11793500 -1.71607400
C 0.05659000 3.14704300 -0.75146500
H -0.87445200 3.31672400 -0.19754700

H 0.65712400 4.06596200 -0.72748200
H -0.19760400 2.92513200 -1.79508600
C 1.63922500 2.47444300 1.53419100
H 2.22693900 1.73742100 2.09490900
H 2.26702100 3.35214800 1.32929600
H 0.80105800 2.78609500 2.17002100
Co -0.06514600 -0.23147800 0.28471700
C -3.53590400 -1.99949900 0.47596300
H -4.43629000 -1.71415700 1.03399400
H -3.81631100 -2.79492500 -0.22853700
H -2.81551700 -2.41900600 1.19156400
C -4.00161500 -0.07381500 -1.18862200
C -3.83870100 1.21690500 -0.34963600
H -5.00101000 -0.52126000 -1.14722800
H -3.70201400 0.01320900 -2.23823000
H -4.74356600 1.53226700 0.18757000
H -3.46188600 2.09774200 -0.89254100
C -1.91065600 0.87388000 1.42937600
C -0.99444200 -0.04464900 2.07228300
H -1.83232200 1.93981500 1.67149000
H -1.40662600 -0.97720200 2.45623500
H -0.27404000 0.40296900 2.76506000
Z4 (triplet state)
C -2.88604500 -0.30289000 -0.63360900
C -1.69643700 -0.81573700 -1.40676600
C -2.39350100 -0.00151400 0.79183100
C -0.76156100 -0.08447600 -2.06327300
H -1.58221500 -1.90640400 -1.41340900
H -1.67427200 -2.66940400 0.74204700
H -0.86744500 0.98539600 -2.23555600

H 0.03627100 -0.57974800 -2.61556700
C 3.11620400 -0.55329300 -1.03254600
H 4.01562800 -1.18828700 -1.04987300
H 2.77041700 -0.47048800 -2.07551900
C 3.45351600 0.83168700 -0.47995400
H 3.64731400 0.77548300 0.60413500
H 4.40842700 1.14784600 -0.92193900
C 2.42065800 1.91749500 -0.77721200
H 2.86191200 2.91021000 -0.59613800
H 2.14589600 1.89015700 -1.84501400
P 1.81404200 -1.45621300 -0.08653300
P 0.83490700 1.84451900 0.17754000
C 2.71673400 -1.98565600 1.42465100
H 2.09850800 -2.68532300 2.00017200
H 3.65846000 -2.48731300 1.16343700
H 2.93983800 -1.12770200 2.06979400
C 1.67603600 -3.03681800 -1.01038400
H 2.65670800 -3.51702600 -1.12924800
H 1.01273200 -3.72422600 -0.46986300
H 1.24837600 -2.86101600 -2.00541800
C 0.04129500 3.38388000 -0.44644200
H -0.89057200 3.59363300 0.09138600
H 0.71535300 4.24190300 -0.32001900
H -0.19362900 3.28596600 -1.51390000
C 1.34255300 2.35461100 1.86960600
H 1.91517300 1.55668500 2.35889100
H 1.94732300 3.27154300 1.85731500
H 0.44390800 2.53444000 2.47456400
Co -0.15443700 -0.26494800 0.19151800
C -4.09767500 -1.21323200 -0.74043700

H -4.90177800 -0.86772800 -0.07736300
H -4.48516300 -1.21917000 -1.76783100
H -3.85565600 -2.24779500 -0.46232100
C -3.22251300 1.21207500 -0.75617600
C -2.91299300 1.40934000 0.74532200
H -4.25599200 1.41431300 -1.05740400
H -2.55963000 1.77401500 -1.42252300
H -3.82176800 1.51715800 1.35499800
H -2.22628100 2.21585600 1.03328600
C -1.68941000 -0.71497800 1.71064200
C -1.52881600 -2.21222000 1.72911200
H -1.42244800 -0.18967600 2.63529900
H -2.27452900 -2.65798100 2.40385900
H -0.54354600 -2.51594800 2.10742700
E1
C -2.20308300 -0.75054200 -0.71075300
C -0.80071100 1.12699100 -2.37992600
C -2.01340600 -0.72721500 0.66554200
C 0.55980700 0.81071600 -2.43907500
H -1.13789800 2.11941400 -2.08392800
H -1.51414300 0.59287300 -3.00895800
H 1.31424000 1.56132400 -2.20125700
H 0.91628700 0.03218000 -3.11840900
C -1.63085700 -1.69169900 -1.70491700
H -1.62122200 -2.73204000 -1.35294200
H -2.12295300 -1.62734200 -2.68137600
H -0.53368300 -1.48263500 -1.93833800
C -3.35780400 0.22425000 -0.67556900
C -3.09396700 0.32669500 0.85475300
H -4.32589400 -0.24501500 -0.89567700

H -3.27368500 1.14290000 -1.26863100
H -3.92903200 -0.01512100 1.48023000
H -2.78325800 1.31592600 1.21501200
C -1.48605700 -1.70514100 1.58913600
H -0.96668700 -2.55462800 1.13656300
C -1.65994500 -1.66569100 2.91578200
H -1.30090400 -2.46192700 3.56339800
H -2.18688600 -0.84295000 3.39962900
Co -0.27986400 -0.05258700 -0.77705600
C 3.10609300 -0.12553500 -0.15979300
H 3.97113200 -0.77017600 0.05660900
H 3.22742200 0.23500600 -1.19283400
C 3.06412000 1.04848100 0.81415600
H 2.88483600 0.68574600 1.83944000
H 4.05575400 1.52001900 0.84356200
C 2.04078500 2.11979300 0.45014300
H 2.12728900 2.97524900 1.13781100
H 2.24218200 2.51308800 -0.55698200
P 1.58922300 -1.17565800 -0.11235200
P 0.27079900 1.59638800 0.51676300
C 1.84298600 -2.08828900 1.46959800
H 1.20880600 -2.98216500 1.49336600
H 2.89072000 -2.40831000 1.55043200
H 1.58966800 -1.47942500 2.34467200
C 2.02548100 -2.49443300 -1.31731900
H 2.99884900 -2.93875200 -1.06993100
H 1.26764400 -3.28824400 -1.29718700
H 2.07352000 -2.08436900 -2.33341100
C -0.57399100 3.19347700 0.20648400
H -0.23506200 3.62650000 -0.74239900

H -1.66133700 3.05910600 0.16014200
H -0.33781500 3.89922100 1.01382300
C 0.00990500 1.36196100 2.31395800
H 0.55292500 2.13920100 2.86811700
H -1.05555100 1.44727200 2.55320000
H 0.34458500 0.37405000 2.64740400
TSE1
C -2.32486200 -0.77576100 -0.32991900
C -1.30172500 -1.08746500 -2.05321200
C -1.80731400 0.15845700 0.68637800
C 0.02081000 -1.61785800 -1.92539800
H -1.40926200 -0.14614900 -2.59969600
H -2.11649300 -1.77563200 -2.27984300
H 0.82145300 -1.18550100 -2.53322800
H 0.11842700 -2.69390600 -1.76498900
C -2.69738400 -2.19126300 0.02583600
H -3.33388500 -2.18935900 0.92297400
H -3.25701400 -2.68859200 -0.77729200
H -1.81487900 -2.80781200 0.25246000
C -3.37438400 0.25682800 -0.75968600
C -2.84328700 1.21973300 0.32409700
H -4.39407200 -0.09522600 -0.55770500
H -3.33629800 0.59662400 -1.80248600
H -3.56339100 1.36357600 1.14101400
H -2.50949400 2.21542300 0.00909500
C -1.43721300 -0.21008200 2.04641600
H -1.04912200 -1.22457400 2.18265900
C -1.56882500 0.57728700 3.12333500
H -1.28287400 0.23885300 4.11649600
H -1.99568700 1.57842600 3.05636100

Co -0.22392200 -0.40214800 -0.37903000
C 3.22748100 -0.39135600 -0.33346000
H 4.07491400 -0.89557700 0.15479300
H 3.28572000 -0.63242300 -1.40673900
C 3.29367100 1.11710200 -0.12413800
H 3.23529900 1.35916300 0.94935900
H 4.27869200 1.47639000 -0.45103600
C 2.21831600 1.86002600 -0.90422600
H 2.41230700 2.94346500 -0.90437600
H 2.24089700 1.53749800 -1.95825800
P 1.68460800 -1.14337000 0.32392900
P 0.47102000 1.62964200 -0.33624000
C 1.88444100 -0.93460400 2.14034500
H 1.21651000 -1.62595800 2.66752000
H 2.91882200 -1.16711100 2.42988400
H 1.63346500 0.08097000 2.46377000
C 2.02924700 -2.93452200 0.14316800
H 2.90305200 -3.20963700 0.74841300
H 1.16710200 -3.52304400 0.48123600
H 2.23307400 -3.18642800 -0.90377900
C -0.36112300 2.52715100 -1.70908400
H -0.09615100 2.03955600 -2.65616600
H -1.45082900 2.52647000 -1.61551900
H -0.01110800 3.56786900 -1.74526000
C 0.34779700 2.77032100 1.08875200
H 0.75036200 3.75544500 0.81963500
H -0.69736000 2.88642200 1.39522700
H 0.90539800 2.38074300 1.94873900
E2
C -2.45865900 -0.54970600 -0.59874300

C -1.65260900 -0.87205600 -1.93147500
C -1.72490000 0.07957800 0.64348500
C -0.39965300 -1.67633200 -1.70383100
H -1.41392000 0.06322000 -2.46375300
H -2.38084000 -1.40055200 -2.57052800
H 0.32336100 -1.65852200 -2.52645300
H -0.55765600 -2.69897500 -1.33916800
C -3.27389600 -1.77500300 -0.21780400
H -3.85181900 -1.59890700 0.69966400
H -3.98125600 -2.01445800 -1.02502000
H -2.64379300 -2.65963300 -0.05300300
C -3.28527600 0.75742100 -0.68066700
C -2.69982200 1.25024400 0.65313100
H -4.37053100 0.60171600 -0.68774600
H -3.02156100 1.37919800 -1.54588900
H -3.41159900 1.16161600 1.48649000
H -2.30043200 2.27182900 0.68155500
C -1.41513000 -0.68225300 1.85254500
H -1.11682600 -1.72783000 1.71897100
C -1.47176200 -0.18074500 3.09562700
H -1.19982200 -0.77334500 3.96625500
H -1.81544500 0.83584200 3.28956700
Co -0.16102900 -0.32267000 -0.37016500
C 3.20866800 -0.45634700 -0.58312100
H 4.08662000 -1.02076200 -0.23321900
H 3.15318700 -0.59362200 -1.67476000
C 3.35187600 1.02272900 -0.23918200
H 3.38892300 1.15866600 0.85373100
H 4.32832500 1.36803600 -0.60545700
C 2.27188700 1.90536900 -0.85223000

H 2.53874500 2.96823200 -0.74568900	H -2.07918100 -3.02970500 0.99322400
H 2.19786000 1.70753400 -1.93395200	H -0.93868600 -2.04792700 1.92549200
P 1.71797200 -1.25568900 0.14346800	C -2.71761700 -0.98420600 1.29684500
P 0.56173200 1.71041600 -0.17323700	H -3.37735600 -0.91659900 0.41648600
C 2.04819700 -1.20063500 1.94845400	H -3.36416700 -1.35070700 2.10631700
H 1.36279000 -1.88044700 2.46787800	C -2.21486400 0.40337600 1.69425200
H 3.07986400 -1.52031200 2.15162400	H -3.04625400 0.99972700 2.10117400
H 1.89222400 -0.19614100 2.35622100	H -1.46502600 0.31450900 2.49555700
C 2.01816600 -3.02468400 -0.21932800	P -0.58346800 -1.79058200 -0.44236800
H 2.98773700 -3.33544300 0.19124300	P -1.45895600 1.39951700 0.32913700
H 1.23133500 -3.64019000 0.23388500	C -1.77665500 -2.16288000 -1.79433500
H 2.01675500 -3.20509900 -1.30042600	H -1.24780600 -2.23807800 -2.75301000
C -0.30884800 2.91919300 -1.24939000	H -2.29402600 -3.11425100 -1.60998600
H -0.28727100 2.56513400 -2.28766000	H -2.52984000 -1.37049800 -1.88617000
H -1.35346400 3.05511400 -0.95210000	C 0.39743800 -3.34612900 -0.41688600
H 0.19602900 3.89358200 -1.20319300	H -0.26366400 -4.22303200 -0.42872800
C 0.64335500 2.57250700 1.44074600	H 1.06060300 -3.39444400 -1.28994900
H 1.06318000 3.57988300 1.32016300	H 1.01439900 -3.38967900 0.48913600
H -0.36089100 2.65802800 1.87168200	C -1.22097200 3.02115100 1.16584300
H 1.26284100 2.01210600 2.15077700	H -0.85527400 3.76532600 0.44719600
E1 (triplet state)	H -2.16750300 3.38068800 1.59115600
C 2.42385800 0.97446500 0.08085400	H -0.48754600 2.93763900 1.97765500
C 0.82762500 0.38733700 -2.79705900	C -2.93532800 1.77811300 -0.70206900
C 2.09741200 0.02013200 1.02423800	H -3.75870300 2.14206900 -0.07284900
C -0.35640000 1.05363100 -2.66219700	H -2.69195300 2.55607800 -1.43572400
H 0.86653000 -0.66497600 -3.08312200	H -3.28037700 0.89285500 -1.24975100
H 1.76704200 0.93778300 -2.86453800	Co 0.39687600 0.33626700 -0.68642700
H -1.31470900 0.56067500 -2.81795100	C 2.24647800 2.45224100 -0.01006100
H -0.37947800 2.14267100 -2.60108300	H 3.22206800 2.94825600 0.10281000
C -1.62715000 -2.02815800 1.06568300	H 1.85022500 2.77620500 -0.98554700

H 1.58368900 2.83942100 0.77328400	P 1.45652100 1.47708800 -0.50388600
C 3.45115700 0.07531400 -0.58718100	P 0.81950700 -1.77820400 0.17971300
C 3.06098800 -1.00341200 0.45765900	C 2.68527500 1.48125700 -1.86737200
H 4.47984100 0.44397400 -0.47308700	H 2.20590700 1.82731800 -2.79076000
H 3.30203200 -0.19002900 -1.64151400	H 3.52464500 2.14980800 -1.63225600
H 3.87266900 -1.26360500 1.14998600	H 3.07730600 0.47406600 -2.05070200
H 2.63635700 -1.93111400 0.05611500	C 1.06912300 3.25766500 -0.31232900
C 1.37769000 0.04656300 2.27780500	H 1.99246600 3.83505100 -0.17086900
H 0.88906300 0.98628300 2.55123600	H 0.54967500 3.63698700 -1.20015700
C 1.33990400 -0.99425800 3.12040800	H 0.42189400 3.40722800 0.56067700
H 0.83388500 -0.93933400 4.08150400	C 0.02300400 -3.28338700 0.86288300
H 1.84245200 -1.93312200 2.88388100	H -0.63256100 -3.73640800 0.10884300
TSE1 (triplet state)	H 0.78800200 -4.01952100 1.14449100
C -2.54563400 -0.07522600 -0.09617000	H -0.57734000 -3.04556200 1.74913600
C -2.19184400 -0.28592300 -1.85807000	C 1.89621500 -2.49843700 -1.12126200
C -1.53539100 0.67624700 0.73367400	H 2.64402400 -3.17505700 -0.68585000
C -0.99166200 -1.02365700 -2.24495000	H 1.27944100 -3.06428700 -1.82940100
H -2.23661700 0.72240300 -2.28851600	H 2.41067800 -1.71281900 -1.68752200
H -3.14431200 -0.79972200 -2.03241900	Co -0.34302200 -0.02073600 -0.67093200
H -0.39517700 -0.61730700 -3.06760200	C -3.12977800 -1.38668200 0.35971100
H -1.04426800 -2.11530300 -2.23394700	H -3.39352500 -1.34446200 1.42538900
C 2.46816600 1.15633700 1.00509800	H -4.04835500 -1.61167300 -0.19983200
H 3.28181800 1.89816200 1.01168100	H -2.43932300 -2.22684500 0.21122300
H 1.81976900 1.38173000 1.86722600	C -3.39320000 1.20767300 -0.09959300
C 3.04062800 -0.25409700 1.13817200	C -2.16493600 2.01620400 0.35018500
H 3.58881700 -0.53773500 0.22506800	H -4.12843800 1.14944600 0.71383500
H 3.80215500 -0.23073100 1.92986400	H -3.90903500 1.47644400 -1.03233900
C 2.02425100 -1.33445500 1.50792300	H -2.31920400 2.73299100 1.16546000
H 2.55021600 -2.26110000 1.78626600	H -1.66736600 2.53886300 -0.48091600
H 1.44383300 -1.01778200 2.38814300	C -1.14008900 0.32098800 2.08180800

H -1.15483400 -0.74698300 2.32268200
C -0.76815100 1.18988500 3.03626900
H -0.49529400 0.85696800 4.03463900
H -0.74969200 2.26607600 2.86034700
E2 (triplet state)
C 3.33417000 0.09256300 -0.27412800
C 2.68222600 0.09155400 -1.66672600
C 2.17388700 -0.24988500 0.64064300
C 1.30692900 0.72759600 -1.51997000
H 2.57209100 -0.94607000 -2.01870200
H 3.31075200 0.60175100 -2.41617600
H 0.65980500 0.60603100 -2.40556200
H 1.38632400 1.80257600 -1.29384600
C -3.08851600 -1.19477200 0.64266800
H -3.81787900 -1.99346800 0.43602000
H -2.89133400 -1.21967800 1.72682100
C -3.67212500 0.16142300 0.24484100
H -3.77178300 0.22746900 -0.85103100
H -4.70144800 0.20733100 0.62578300
C -2.91754800 1.37697000 0.78378000
H -3.53111400 2.28347500 0.66466600
H -2.73717400 1.25952900 1.86418500
P -1.51248600 -1.66235500 -0.19396000
P -1.28289900 1.70303900 -0.00919700
C -2.01562400 -1.98828400 -1.92803500
H -1.17994500 -2.45314500 -2.46525000
H -2.88307700 -2.66068400 -1.97206300
H -2.26283000 -1.05386200 -2.44604400
C -1.21342800 -3.34786000 0.46287400
H -2.10169800 -3.97953600 0.32809100

H -0.37007700 -3.81258100 -0.06133600
H -0.97406500 -3.30444900 1.53244500
C -0.71625000 3.21179800 0.86308800
H 0.22777000 3.56102900 0.42543100
H -1.45980800 4.01560800 0.78028100
H -0.54818800 2.99925700 1.92618200
C -1.74357300 2.36072100 -1.65832700
H -2.48955900 3.16132000 -1.56590000
H -0.85251700 2.76525300 -2.15310300
H -2.15057600 1.56998900 -2.29992800
Co 0.20293000 -0.05922800 -0.02440900
C 4.14028000 1.33681500 0.02204500
H 4.47209300 1.36046900 1.06910300
H 5.03332100 1.38219400 -0.61427100
H 3.55524300 2.24885500 -0.16859100
C 3.92342800 -1.29215500 0.10151800
C 2.52491100 -1.73265300 0.61098800
H 4.64139100 -1.21978800 0.92783200
H 4.36431100 -1.88098700 -0.71108800
H 2.46564200 -2.25804600 1.57265300
H 1.97258600 -2.31714100 -0.13927600
C 1.45418900 0.46527500 1.61058300
H 1.60225100 1.54528300 1.68885500
C 0.32123300 -0.13925700 2.16623100
H -0.35506100 0.43330600 2.80000600
H 0.30109400 -1.22147300 2.30775600
TSE2
C -2.52500900 -0.44430500 -0.56168400
C -1.74852400 -0.73763500 -1.89893100
C -1.68951100 0.06298000 0.65789200

C -0.57568700 -1.66786900 -1.71963300
H -1.40107900 0.21475500 -2.35026700
H -2.50007700 -1.11666000 -2.61224600
H 0.09757800 -1.74025100 -2.58088000
H -0.80683100 -2.65792500 -1.31008700
C -3.40707000 -1.63325400 -0.21811600
H -3.95385200 -1.46096600 0.71892100
H -4.14373400 -1.79007200 -1.01920600
H -2.83405600 -2.56320600 -0.10565200
C -3.26402800 0.91586300 -0.54813800
C -2.57992500 1.29708400 0.77672400
H -4.35677300 0.83881200 -0.50778600
H -2.99621000 1.56121000 -1.39501400
H -3.25473900 1.21156400 1.64079300
H -2.11339200 2.28839000 0.83323100
C -1.36706600 -0.77379700 1.80997700
H -1.15283800 -1.82910100 1.60941900
C -1.32172000 -0.32912100 3.07481700
H -1.05423400 -0.98063000 3.90390900
H -1.57119700 0.70147800 3.32952200
Co -0.16188800 -0.26832900 -0.47361800
C 3.15296000 -0.57617100 -0.62629600
H 4.00877100 -1.18982600 -0.30509700
H 3.07232600 -0.68594800 -1.71934200
C 3.37834700 0.88641900 -0.25294200
H 3.43388700 0.99460700 0.84228100
H 4.36976800 1.18355900 -0.62141200
C 2.34823600 1.84896600 -0.83313000
H 2.68004900 2.89014600 -0.69825200
H 2.25540900 1.68799800 -1.91950200

P 1.63628800 -1.32106800 0.11182000
P 0.63658000 1.73000200 -0.14019900
C 1.99605700 -1.30940100 1.91162800
H 1.33110900 -2.01725800 2.41996800
H 3.03587000 -1.61918100 2.08631500
H 1.82826800 -0.32209100 2.35417000
C 1.84923100 -3.09716200 -0.27556500
H 2.80247400 -3.46303800 0.12809800
H 1.03270600 -3.67827500 0.17089400
H 1.83508900 -3.26086200 -1.35921700
C -0.18030300 3.04880200 -1.12642700
H -0.20135100 2.75487500 -2.18341000
H -1.21034500 3.22180100 -0.79658900
H 0.37691700 3.99109000 -1.03707100
C 0.79807700 2.50170600 1.51452500
H 1.24347900 3.50174900 1.42928000
H -0.18652100 2.59500900 1.98733700
H 1.42709400 1.89049500 2.17206500
E3 (open-shell singlet)
C -2.88494200 -0.18794200 -0.49152000
C -1.96143700 -0.39243400 -1.68911600
C -2.03212800 0.03570300 0.76234400
C -1.06483800 -1.56734500 -1.55579900
H -1.29914400 0.58002700 -1.72230100
H -2.45645000 -0.27027200 -2.66646400
H -0.58028800 -1.91276400 -2.47614300
H -1.42815100 -2.40042800 -0.94906200
C -3.97146400 -1.24248700 -0.39228900
H -4.58431900 -1.08390400 0.50482400
H -4.63362200 -1.18757200 -1.26762100

H -3.56686800 -2.26159600 -0.34444500
C -3.38284200 1.27662300 -0.33916900
C -2.50204500 1.46384700 0.91735200
H -4.45841500 1.35458900 -0.14686900
H -3.13780500 1.93418900 -1.18391400
H -3.05818900 1.63979300 1.85001800
H -1.73924300 2.25133300 0.84465100
C -1.57351400 -0.85892900 1.74690300
H -1.56118500 -1.92454500 1.49635400
C -1.17188300 -0.46637900 2.99540900
H -0.84744600 -1.18263300 3.74675500
H -1.20019000 0.58194700 3.29349700
Co -0.08214900 -0.17300100 -0.64898400
C 3.15214400 -0.89129700 -0.60466700
H 3.91125200 -1.63256900 -0.31022600
H 3.10408300 -0.91156500 -1.70522500
C 3.56149000 0.49912700 -0.11970600
H 3.54336500 0.53878200 0.98149700
H 4.61418700 0.65301700 -0.39375000
C 2.74931600 1.65256000 -0.70499400
H 3.23003400 2.61378300 -0.46656800
H 2.72867500 1.57675300 -1.80434100
P 1.52695000 -1.49936800 0.03038600
P 0.99069200 1.74469000 -0.13958600
C 1.82335200 -1.67531500 1.83060600
H 1.04185400 -2.30873300 2.26572500
H 2.79808400 -2.15230800 2.00263000
H 1.79511400 -0.70891900 2.34541700
C 1.52922100 -3.24763300 -0.50905200
H 2.42255400 -3.76588500 -0.13651100

H 0.63866900 -3.75825800 -0.12264000
H 1.51123900 -3.31000600 -1.60323400
C 0.43429400 3.27675500 -0.98735900
H 0.45344500 3.12494900 -2.07364400
H -0.59463000 3.52477800 -0.69811600
H 1.08345100 4.12674300 -0.73778700
C 1.15725400 2.31598400 1.59901500
H 1.85476100 3.16242800 1.66009700
H 0.18185100 2.64394000 1.97858600
H 1.51486500 1.51107900 2.25163600
TSE3
C -2.90083200 -0.49787300 -0.50470500
C -1.85152100 -0.92291500 -1.52698200
C -2.15946000 0.02372200 0.72381400
C -0.91526500 -1.96065900 -1.01243500
H -2.25169100 -1.10876100 -2.53811500
H -0.32613000 -2.46868700 -1.78121600
H -1.31532800 -2.67044300 -0.28230700
C 3.38268100 -0.50176100 -0.53655100
H 4.23769000 -1.06792800 -0.13494800
H 3.43984200 -0.58208800 -1.63335300
C 3.46795900 0.96228300 -0.11455800
H 3.35878100 1.05223900 0.97897500
H 4.48554600 1.31557100 -0.32994000
C 2.47799900 1.88003100 -0.82895700
H 2.79439100 2.92991900 -0.73316200
H 2.46579000 1.65426200 -1.90742400
P 1.85498200 -1.38804900 -0.00692100
P 0.73063900 1.77604500 -0.23098200
C 2.10542400 -1.62340200 1.79606300

H 1.33816900 -2.30456300 2.18407900
H 3.09537100 -2.05733800 1.99303900
H 2.01398400 -0.67027000 2.33009900
C 2.14949600 -3.06975800 -0.66310300
H 3.13173100 -3.43715100 -0.33788900
H 1.37558500 -3.75576400 -0.29957100
H 2.12021300 -3.06598800 -1.75898100
C -0.05667000 3.00766900 -1.34714600
H -1.09878700 3.19009100 -1.05868000
H 0.48497600 3.96273900 -1.31916100
H -0.04953900 2.62923900 -2.37705400
C 0.82747200 2.70827600 1.35136100
H 1.35328100 3.66179400 1.20675300
H -0.18036400 2.92293800 1.72698400
H 1.35276900 2.12322300 2.11617200
Co -0.10930900 -0.32434700 -0.30897700
C -3.96796700 -1.54787400 -0.25622900
H -4.66002100 -1.21975900 0.53093500
H -4.55376500 -1.71834400 -1.17020900
H -3.54265700 -2.51133100 0.05329700
C -3.45304500 0.94325800 -0.70407000
C -2.79306700 1.38811300 0.62234000
H -4.54598200 1.01248600 -0.72349300
H -3.06135100 1.44933400 -1.59625300
H -3.51340600 1.56717100 1.43558600
H -2.13442700 2.26661700 0.58196800
C -1.52260600 -0.63787500 1.78896600
H -1.44438200 -1.72646900 1.74478700
C -1.01168200 0.01114200 2.88837500
H -0.54249900 -0.53139200 3.70602200

H -1.10778000 1.09129000 2.99898000
H -1.22646000 0.03051600 -1.75206700
E4
C -2.91155400 -0.44844400 -0.34416300
C -1.80438600 -1.07721400 -1.19779600
C -2.11085500 0.18411200 0.79909400
C -0.99992000 -2.07448700 -0.44618100
H -2.11265300 -1.37785300 -2.21378400
H -0.36249900 -2.69877600 -1.07817100
H -1.52678100 -2.69161200 0.28309900
C 3.27467500 -0.51781300 0.48979900
H 3.50859500 -0.99641100 1.45136000
H 4.08667800 -0.79960700 -0.19872600
C 3.23303500 0.99673200 0.66858000
H 2.73991800 1.23679600 1.62370500
H 4.26281100 1.36225900 0.77549700
C 2.53875000 1.73928000 -0.47137800
H 2.85537400 2.79201000 -0.51038700
H 2.79943100 1.30103900 -1.44706300
P 1.73610400 -1.34117700 -0.14979600
P 0.70146200 1.72608100 -0.26229800
C 1.92976200 -2.99658900 0.61361400
H 1.24531900 -3.72206800 0.16159900
H 2.95909300 -3.35829100 0.48896800
H 1.70446100 -2.93585200 1.68579900
C 2.14723400 -1.66282200 -1.91300400
H 3.09765400 -2.20506200 -2.00652500
H 1.36011500 -2.26028900 -2.38860600
H 2.22642000 -0.71656400 -2.46330000
C 0.14531700 2.51606000 -1.82473000

H -0.91903800 2.77524000 -1.76862600
H 0.71780300 3.43125700 -2.02611200
H 0.28653100 1.82062700 -2.66247400
C 0.55440600 3.10270000 0.95624700
H 0.85005000 4.04583500 0.47846300
H -0.45972500 3.21529200 1.35245100
H 1.22829600 2.92766500 1.80395100
Co -0.20872000 -0.33697600 0.14213000
C -4.06554600 -1.37505800 -0.02868800
H -4.77024200 -0.89123600 0.66114500
H -4.61691500 -1.62960200 -0.94456400
H -3.73878500 -2.31423000 0.43600700
C -3.32482000 0.98642500 -0.77063100
C -2.68547300 1.55543900 0.51783600
H -4.40422700 1.14560600 -0.86554200
H -2.84702700 1.32383000 -1.69999200
H -3.44483300 1.81214700 1.27185900
H -2.02343300 2.42218400 0.41717200
C -1.38880200 -0.52739000 1.77731900
H -1.65194700 -1.56646600 1.97295200
C -0.11447200 -0.08615500 2.19089300
H 0.49883600 -0.76073800 2.79162600
H 0.07797000 0.97266600 2.35768100
H -1.05939700 -0.22365500 -1.49641200
TSE4
C -2.87981400 -0.52191600 -0.32617100
C -1.77070800 -1.19325200 -1.10982100
C -2.06546800 0.19907300 0.74799900
C -0.98280200 -2.18247100 -0.48820600
H -1.79583700 -1.12300400 -2.20160000

H -0.33933300 -2.77830300 -1.13466700
H -1.33829800 -2.71669200 0.39042300
C 3.28207600 -0.45684800 0.48087400
H 3.53868100 -0.93163800 1.43844700
H 4.09667700 -0.70910800 -0.21567700
C 3.19371200 1.05454800 0.66770100
H 2.70355000 1.27371800 1.62886400
H 4.21190300 1.45344300 0.76590800
C 2.46718500 1.78195800 -0.46124000
H 2.75058400 2.84463600 -0.49384500
H 2.73315300 1.36036500 -1.44282900
P 1.76040300 -1.31630700 -0.15160700
P 0.63179000 1.73101400 -0.25549200
C 1.97175200 -2.95507400 0.64577800
H 1.30345400 -3.70048200 0.20177300
H 3.00706100 -3.30380800 0.53403300
H 1.73881800 -2.87918200 1.71529500
C 2.20253800 -1.66999200 -1.89999800
H 3.15987400 -2.20366400 -1.96837300
H 1.42777200 -2.28228500 -2.37680300
H 2.27806300 -0.73312400 -2.46626800
C 0.07805500 2.60197900 -1.77137300
H -1.00061300 2.79602500 -1.73723700
H 0.60319200 3.55939600 -1.88500400
H 0.28534100 1.97524400 -2.64801700
C 0.44627400 3.04167500 1.03035400
H 0.66688900 4.01855900 0.58076800
H -0.56018400 3.07455300 1.45961800
H 1.15807600 2.87988400 1.84872800
Co -0.21387800 -0.32392800 0.07930400

C -4.02977600 -1.42579100 0.06832300
H -4.73396500 -0.88271900 0.71365300
H -4.58177400 -1.76586900 -0.81833300
H -3.69355600 -2.31673500 0.61411500
C -3.30189800 0.87529400 -0.85295600
C -2.72169800 1.52490300 0.42446600
H -4.37759400 1.00822400 -1.00959600
H -2.77752500 1.16440100 -1.77320000
H -3.51371400 1.74275600 1.15699700
H -2.12301600 2.43561600 0.31047700
C -1.35419800 -0.48686900 1.77174600
H -1.63994900 -1.52080500 1.97374600
C -0.10285000 -0.08402800 2.23311800
H 0.47011700 -0.77297400 2.85520900
H 0.14999800 0.96514200 2.35730200
H -0.51031400 -0.02526500 -1.37216800
E5
C -2.94300100 -0.58190100 -0.28200200
C -1.84277800 -1.06071400 -1.18831200
C -2.04576100 0.10074700 0.73606000
C -0.97055100 -2.08511500 -0.82646500
H -1.77930400 -0.63102600 -2.18930600
H -0.32967500 -2.50080600 -1.60211200
H -1.21102900 -2.77155700 -0.01463700
C 3.26736800 -0.38919700 0.55353200
H 3.49715200 -0.80728000 1.54426700
H 4.11876700 -0.65130300 -0.09280900
C 3.13805500 1.13110100 0.66402400
H 2.64758100 1.38231300 1.61621700
H 4.14925900 1.55067100 0.74739200

C 2.40414200 1.82281700 -0.48871600
H 2.70329500 2.87951100 -0.55666300
H 2.65417500 1.36463100 -1.45825300
P 1.80310800 -1.32374500 -0.10652900
P 0.57165700 1.78644700 -0.27263900
C 1.91756400 -2.91906900 0.78785000
H 1.27028400 -3.66100500 0.30526600
H 2.94875700 -3.29658400 0.77739400
H 1.59368300 -2.80609600 1.82946800
C 2.39699000 -1.79666600 -1.77870600
H 3.36153000 -2.31692800 -1.71058200
H 1.68181100 -2.45964700 -2.27815900
H 2.52043800 -0.90358000 -2.40307300
C -0.03937400 2.70106500 -1.73704600
H -1.12832600 2.82211000 -1.68088200
H 0.42038200 3.69549400 -1.80493100
H 0.19082500 2.13411600 -2.64709300
C 0.38676300 3.05786200 1.05370400
H 0.64539600 4.04100100 0.63914800
H -0.63353400 3.10650900 1.44788100
H 1.06466800 2.85730800 1.89132600
Co -0.15697900 -0.29721300 -0.03288700
C -3.96474200 -1.60551400 0.16168500
H -4.61801600 -1.18030700 0.93623500
H -4.59774400 -1.91325400 -0.68108300
H -3.49987100 -2.50982500 0.57518500
C -3.50323800 0.81860400 -0.64260300
C -2.77392500 1.41951500 0.58158300
H -4.59528300 0.89795000 -0.62731900
H -3.14020200 1.19720100 -1.60686000

H -3.46007200 1.57494200 1.42787800
H -2.21544400 2.35058600 0.43438900
C -1.24338500 -0.62488900 1.66295400
H -1.44809000 -1.68942200 1.79862100
C -0.03638800 -0.13131900 2.13826500
H 0.61698300 -0.78527300 2.71676500
H 0.10982800 0.93154400 2.30842200
H 0.19228200 0.03826600 -1.44146300

TSE5

C -2.97628700 -0.35662000 -0.54347800
C -1.80842200 -0.57726900 -1.47895400
C -2.23627200 -0.03368900 0.74668200
C -0.94353400 -1.63784500 -1.33842000
H -1.71086000 0.08031700 -2.34575800
H -0.21179900 -1.82490900 -2.12329400
H -1.19754500 -2.48817700 -0.70647500
C 2.77772100 -0.92833400 -1.23449900
H 3.62019300 -1.63624600 -1.20899600
H 2.26400400 -1.07607400 -2.19781200
C 3.29302600 0.50548000 -1.12925100
H 3.78539200 0.66153600 -0.15570000
H 4.08598000 0.64351600 -1.87688200
C 2.23733600 1.58338100 -1.36070300
H 2.71753500 2.57219500 -1.42341600
H 1.72641200 1.41565400 -2.32280700
P 1.59744200 -1.39040800 0.10460800
P 0.90897500 1.71345400 -0.08750500
C 2.68685200 -1.39567800 1.58945900
H 2.21556100 -1.98570000 2.38500700
H 3.64692400 -1.86867100 1.34233900

H 2.88096300 -0.39373200 1.98337300
C 1.45628900 -3.21024000 -0.11978700
H 2.43794700 -3.68081000 0.02189500
H 0.76258600 -3.62367500 0.62400400
H 1.08842300 -3.46959100 -1.11787100
C 0.12526200 3.29494400 -0.60102700
H -0.69553900 3.55049000 0.08085700
H 0.85399400 4.11592900 -0.59288600
H -0.28997300 3.19658200 -1.61223600
C 1.77276500 2.29772200 1.42651300
H 2.47544000 3.10106400 1.16545200
H 1.02966900 2.70445400 2.12364900
H 2.31273500 1.49719700 1.93947900
Co -0.26235900 -0.13928200 0.11656200
C -4.03501100 -1.43989600 -0.55547500
H -4.79047300 -1.24219700 0.21670800
H -4.54632600 -1.47939100 -1.52623600
H -3.60704500 -2.43191300 -0.35989000
C -3.49578400 1.11037200 -0.53394300
C -2.89652500 1.31840600 0.87894500
H -4.58458300 1.20885400 -0.59680900
H -3.04602200 1.74208100 -1.31111900
H -3.67119900 1.29610500 1.65990400
H -2.27076400 2.20237700 1.05667100
C -1.45112500 -0.85530100 1.58077400
H -1.50891400 -1.94496000 1.55201800
C -0.39486400 -0.18605000 2.22089400
H 0.32866500 -0.73847400 2.81925400
H -0.52737900 0.85640900 2.51382600
H -0.75514700 1.01836800 -0.69633400

E6

C -2.95852600 -0.12878100 -0.62611800
C -1.79410200 0.52461100 -1.35263100
C -2.31343400 0.16193200 0.70941000
C -0.69076600 -0.12430300 -1.86248500
H -1.85846400 1.60750700 -1.47652200
H -0.00203500 0.43280900 -2.49770600
H -0.71028500 -1.19993300 -2.03010100
C 2.43667600 -1.64153200 -0.99516000
H 2.92778100 -2.62128300 -0.89706300
H 2.07031500 -1.57494800 -2.03217400
C 3.43179100 -0.51928200 -0.71374500
H 3.73011200 -0.52865000 0.34738900
H 4.35455300 -0.72300100 -1.27373000
C 2.92359600 0.86098300 -1.10925700
H 3.73556700 1.60219400 -1.04970700
H 2.58919100 0.85111700 -2.15923100
P 0.96987700 -1.65243900 0.12132300
P 1.52213900 1.53214100 -0.10759900
C 1.71397600 -2.19046200 1.71364500
H 0.92825800 -2.49521200 2.41618100
H 2.37604900 -3.05113300 1.55037300
H 2.29150500 -1.38346300 2.17914800
C 0.16576700 -3.22568300 -0.39710000
H 0.88538900 -4.05175900 -0.32242800
H -0.69004900 -3.46027200 0.24787500
H -0.18557300 -3.17657400 -1.43476500
C 1.21596900 3.09520000 -1.01300600
H 0.57945400 3.75081000 -0.40696000
H 2.15731900 3.61411900 -1.23666200

H 0.69482600 2.89271400 -1.95739500
C 2.32704400 2.10663800 1.42967300
H 3.18294500 2.75788900 1.20826600
H 1.59702700 2.66444500 2.02836400
H 2.66979400 1.25420300 2.02808500
Co -0.21988300 0.27068500 0.22902500
C -3.34899900 -1.51284400 -1.07107200
H -4.13114500 -1.91755800 -0.41672700
H -3.73629400 -1.50135800 -2.09784800
H -2.49981200 -2.20907100 -1.04199100
C -4.02556100 0.93863700 -0.29878300
C -3.17244200 1.40419800 0.91088100
H -4.96841800 0.47733500 0.01608000
H -4.23721500 1.67586600 -1.08162900
H -3.69376300 1.40196200 1.87603200
H -2.67646600 2.37353600 0.79424300
C -1.46304500 -0.57552100 1.54774100
H -1.43828900 -1.66561600 1.50605300
C -0.50153800 0.18041700 2.27203100
H 0.22375900 -0.33021200 2.90485400
H -0.76256300 1.18358700 2.60835400
H -0.52532200 1.72068200 0.44767000
TSE6
C 3.12874400 0.12658300 -0.73489800
C 1.78926400 -0.49310200 -1.00905700
C 2.36344500 0.16911000 0.54955700
C 0.66682100 0.24169900 -1.54252500
H 1.76222500 -1.58395700 -1.03527300
H 0.03769800 -0.32068300 -2.23533300
H 0.85031200 1.26150800 -1.89283300

C -2.63752200 1.06811800 -1.32450300
H -3.38980300 1.87033200 -1.36623700
H -2.07721800 1.10947000 -2.27129400
C -3.32752700 -0.28663900 -1.17012800
H -3.86444300 -0.32935600 -0.20852700
H -4.10835700 -0.36575900 -1.93871200
C -2.39877400 -1.49081100 -1.30613500
H -2.98663600 -2.42122700 -1.33148000
H -1.85203200 -1.44301600 -2.26010200
P -1.46385900 1.48149400 0.03365300
P -1.16087600 -1.68027900 0.05552400
C -2.59285700 1.77580300 1.45356200
H -2.05924600 2.30645200 2.25094600
H -3.45138000 2.38951000 1.14828900
H -2.95916800 0.83148400 1.87190600
C -0.97216300 3.19798800 -0.38251300
H -1.85822500 3.82391300 -0.55230100
H -0.39857000 3.63304700 0.44594300
H -0.34906500 3.21780000 -1.28466900
C -0.31348100 -3.22871100 -0.43404200
H 0.44540000 -3.49057500 0.31370600
H -1.03523200 -4.05229100 -0.51333000
H 0.17849800 -3.10833100 -1.40735700
C -2.20974200 -2.24745000 1.44630000
H -2.92070300 -3.01712400 1.11839200
H -1.56594900 -2.66486600 2.23008100
H -2.76597600 -1.41226400 1.88718300
Co 0.14313300 0.05008800 0.37480100
C 3.62115900 1.29966900 -1.52882200
H 4.49110700 1.75181300 -1.03609700

H 3.92556300 0.99165000 -2.53706000
H 2.86055700 2.08336800 -1.63544200
C 4.05902700 -0.93596300 -0.12726300
C 3.19500500 -0.94617400 1.16204000
H 5.06556300 -0.54186300 0.05045800
H 4.14268200 -1.87738300 -0.68351000
H 3.73960100 -0.62170800 2.05697600
H 2.66011500 -1.87485100 1.39611400
C 1.55087600 1.22977100 1.08925400
H 1.56919300 2.22985400 0.65355800
C 0.77012200 0.89855900 2.21188000
H 0.10419200 1.64392500 2.64744300
H 1.13205400 0.16313300 2.92864300
H 0.02930000 -0.82331300 1.61638300
E7
C -3.10162100 -0.13187400 -0.74052500
C -1.80454600 0.57893900 -1.00136800
C -2.31631900 -0.14078100 0.53451800
C -0.65895500 -0.07646100 -1.60023100
H -1.83450800 1.67053500 -1.00055700
H -0.05452500 0.54927700 -2.26307600
H -0.80078400 -1.08143300 -2.00945600
C 2.73003100 -1.07661900 -1.18393400
H 3.45702200 -1.90236200 -1.22266800
H 2.26336200 -1.02194000 -2.18057900
C 3.44190700 0.23661000 -0.86031500
H 3.80034000 0.22889100 0.18234800
H 4.35115600 0.29450000 -1.47406000
C 2.61273300 1.49177300 -1.12434200
H 3.24604800 2.38940200 -1.05273300

H 2.21983400 1.47149000 -2.15328700
P 1.41012500 -1.55989200 0.01009200
P 1.17682500 1.73310600 0.01142900
C 2.36986200 -2.06224500 1.49489200
H 1.72358200 -2.62793300 2.17711700
H 3.21603200 -2.70384500 1.21410200
H 2.75047300 -1.18828000 2.03718700
C 0.88516900 -3.18745300 -0.64923200
H 1.75136200 -3.83900400 -0.82568000
H 0.21807500 -3.68030200 0.06837500
H 0.34191000 -3.06349300 -1.59402900
C 0.45957900 3.29147000 -0.64084100
H -0.33733100 3.64371800 0.02640400
H 1.22622000 4.07406100 -0.71641600
H 0.03019900 3.13172000 -1.63819300
C 1.97821900 2.30570600 1.56209800
H 2.67686300 3.13029800 1.36664200
H 1.21138800 2.65542100 2.26443100
H 2.52452500 1.48468600 2.04249900
Co -0.14868200 -0.05048100 0.26271200
C -3.50909500 -1.33241000 -1.54034800
H -4.38041500 -1.81469600 -1.07976000
H -3.77793000 -1.05814600 -2.56828200
H -2.70981300 -2.08433900 -1.58959900
C -4.08383000 0.87082900 -0.11877800
C -3.18429700 0.95754300 1.14209300
H -5.05210200 0.40770400 0.10106200
H -4.25443900 1.79497800 -0.68400800
H -3.68794900 0.63882500 2.06259800
H -2.68709200 1.91836600 1.33248900

C -1.45779600 -1.14972200 1.10892900
H -1.63750800 -2.21037200 0.92131300
C -0.81872900 -0.71240700 2.39206500
H -0.28558600 -1.51191700 2.91498500
H -1.50766700 -0.21261100 3.08820500
H -0.04445000 0.10419800 2.18849300
TSE3 (triplet state)
C -3.10518200 -0.26933000 -0.28176400
C -2.15895200 -0.55873100 -1.45276500
C -2.24076400 0.22766300 0.86347300
C -1.16902400 -1.65060900 -1.17682000
H -2.67768600 -0.66057200 -2.42211300
H -0.70602100 -2.07723900 -2.07674300
H -1.50418500 -2.44031100 -0.49901900
C 2.57619000 1.65911400 0.79249700
H 3.15105400 2.58425200 0.63219300
H 2.20845200 1.68961000 1.83066900
C 3.47626700 0.44252700 0.59232500
H 3.78752000 0.36535600 -0.46241300
H 4.40642400 0.61089000 1.15204500
C 2.87273200 -0.87655200 1.06776400
H 3.65115100 -1.65317600 1.12845300
H 2.46239300 -0.75985500 2.08318800
P 1.09607300 1.73431700 -0.30944900
P 1.52058900 -1.55883300 0.01704100
C 0.41972100 3.38162200 0.14300000
H 1.20918700 4.14273700 0.08069200
H -0.38777900 3.66342900 -0.54361700
H 0.02187600 3.37470000 1.16484500
C 1.11283300 -3.11038700 0.89675300

H 0.41786000 -3.71277100 0.30069200	C -2.11787000 -0.54841100 -1.43471600
H 2.02464600 -3.69622200 1.07336700	C -2.29378500 0.19718500 0.90036700
H 0.64613200 -2.89199300 1.86490600	C -1.15240200 -1.66253700 -1.19287900
Co -0.11745200 -0.19151000 -0.44882200	H -2.59759000 -0.57905900 -2.42789600
C -4.08314600 -1.39793500 -0.01442300	H -0.71165000 -2.09150300 -2.10217200
H -4.71797900 -1.16282900 0.84932800	H -1.47669800 -2.44529000 -0.50260900
H -4.73908400 -1.55049200 -0.88266000	C 2.54213700 1.68495900 0.81323800
H -3.58025100 -2.35115000 0.19478800	H 3.10663500 2.61853800 0.66553200
C -3.72548400 1.15472500 -0.34824400	H 2.14865400 1.71111200 1.84210400
C -2.75379900 1.63876300 0.75663000	C 3.46327000 0.48056700 0.63631300
H -4.77829500 1.17802800 -0.04619500	H 3.79748700 0.40382800 -0.41142400
H -3.63500900 1.65960000 -1.31818400	H 4.37914400 0.66305200 1.21477900
H -3.23176900 2.01442400 1.67295700	C 2.86692200 -0.84482300 1.10367300
H -2.02556200 2.39700300 0.43754300	H 3.65356700 -1.61132300 1.18341100
C -1.35250100 -0.42255400 1.71371000	H 2.43403600 -0.72994700 2.10991200
H -1.35002100 -1.51558900 1.69461300	P 1.08883700 1.73436900 -0.32434900
C -0.51163600 0.22311700 2.61249000	P 1.54565900 -1.54661400 0.02728100
H 0.11506100 -0.33136900 3.30819300	C 0.35729400 3.35816800 0.12295900
H -0.52398900 1.30937200 2.70924000	H 1.11888700 4.14717000 0.06073500
H -1.58040300 0.42125200 -1.62642700	H -0.46080400 3.60853200 -0.56345500
C 2.39771400 -2.17025400 -1.47187100	H -0.03900200 3.33607600 1.14528400
H 3.25745000 -2.79127400 -1.18678000	C 1.14017800 -3.10192900 0.90131400
H 1.71226400 -2.77614000 -2.07623100	H 0.46268600 -3.71251700 0.29352300
H 2.75245200 -1.34023700 -2.09364400	H 2.05532600 -3.67714500 1.09468300
C 1.84085300 2.10867200 -1.94984200	H 0.65403300 -2.88848500 1.86103300
H 1.04780700 2.38513500 -2.65567100	Co -0.09151200 -0.20057000 -0.49200000
H 2.55384400 2.94163900 -1.88180400	C -4.08391700 -1.42500500 -0.08166900
H 2.35880600 1.23318800 -2.35937000	H -4.76286500 -1.20164700 0.75097700
E4 (triplet state)	H -4.69429700 -1.57700500 -0.98262000
C -3.10312900 -0.28593400 -0.29003200	H -3.58218000 -2.37442000 0.14659100

C -3.73292000 1.13467300 -0.35729500	H -1.70375300 1.54614500 -1.98218100
C -2.83273700 1.59816500 0.81444700	C -3.29982900 0.46746700 -0.98478300
H -4.80323000 1.14455900 -0.12408700	H -3.83269000 0.48228600 -0.02026300
H -3.58409700 1.66424000 -1.30691900	H -4.07436300 0.64355600 -1.74356000
H -3.36930000 1.92988600 1.71517800	C -2.69239300 -0.90830700 -1.23641700
H -2.10473000 2.38333200 0.56599300	H -3.48651300 -1.66655300 -1.31280500
C -1.36844200 -0.43483000 1.72169200	H -2.15735100 -0.90953300 -2.19982500
H -1.31401100 -1.52540200 1.67005000	P -1.09831500 1.66847700 0.35012400
C -0.55480800 0.22251100 2.63686000	P -1.48651300 -1.50551700 0.02790900
H 0.09785300 -0.32219600 3.31630300	C -2.16010400 2.01946400 1.79923800
H -0.61473700 1.30421600 2.76340100	H -1.52890600 2.40858700 2.60682800
H -1.51973200 0.44443700 -1.54137700	H -2.92552100 2.76569500 1.54678400
C 2.45881900 -2.14774000 -1.44408300	H -2.65008100 1.11421200 2.17285900
H 3.32025400 -2.75871300 -1.14280400	C -0.28384900 3.28343600 0.07483400
H 1.79177400 -2.76116700 -2.06141400	H -1.02196100 4.09041200 0.17540000
H 2.81543200 -1.31324600 -2.05887200	H 0.51781800 3.43735300 0.80670000
C 1.86263900 2.13437100 -1.94448900	H 0.14045100 3.32869200 -0.93521900
H 1.08022500 2.39493800 -2.66790800	C -1.12657400 -3.17345600 -0.65083100
H 2.55307800 2.98409300 -1.85521800	H -0.56771500 -3.77923500 0.07158100
H 2.41172700 1.27375900 -2.34489000	H -2.06686200 -3.69205300 -0.87919300
TSE4 (triplet state)	H -0.54156000 -3.09851100 -1.57614100
C 2.93922900 -0.26036000 0.34392400	C -2.54224700 -1.92336800 1.46838100
C 2.05031300 -0.76472400 1.45723400	H -3.37458300 -2.57370000 1.16744900
C 2.11293300 0.16624700 -0.86973100	H -1.94141100 -2.44609000 2.22237200
C 1.22251800 -1.84487900 1.27096900	H -2.94974400 -1.02119900 1.93772600
H 2.19307500 -0.35035600 2.45565700	Co 0.22230500 -0.05649300 0.60456300
H 0.69108500 -2.28551000 2.11481100	C 4.08530700 -1.21879600 0.03706300
H 1.32409500 -2.47234200 0.38581000	H 4.70067100 -0.82514200 -0.78346900
C -2.29205500 1.61079900 -1.05291500	H 4.73002500 -1.34657100 0.91684500
H -2.81320600 2.58065100 -1.06662600	H 3.71570300 -2.20888900 -0.26064300

C 3.38083500 1.22430200 0.47739300	P -1.22624000 1.65439700 0.08144000
C 2.70829800 1.54838500 -0.87578700	C -2.48728400 -1.75567300 -1.80653900
H 4.46337300 1.38396000 0.52704000	H -1.94985300 -2.11667800 -2.69121800
H 2.90911800 1.73326600 1.32791900	H -3.27549700 -2.47374300 -1.54322900
H 3.42485200 1.67388200 -1.70299900	H -2.94743500 -0.79689300 -2.06976700
H 2.03428400 2.41343500 -0.90262600	C -0.64390600 -3.26779200 -0.26598500
C 1.34592300 -0.53972900 -1.80300500	H -1.47456800 -3.98087100 -0.17824000
H 1.28037400 -1.62547400 -1.68832200	H -0.05275300 -3.52641300 -1.15298500
C 0.71108200 0.04339400 -2.88211700	H -0.00481400 -3.35785900 0.61997700
H 0.17050500 -0.54904500 -3.61701700	C -0.61955500 3.22715700 0.81983100
H 0.36702600 0.83335000 1.86497800	H -0.06346100 3.81318200 0.07834700
H 0.78761800 1.11638000 -3.06425900	H -1.46367900 3.83671200 1.16900200
E5 (triplet state)	H 0.04141900 3.03104300 1.67371200
C 2.93759500 0.28975500 -0.14714900	C -2.30857600 2.28644800 -1.25896800
C 2.16891000 0.56902000 -1.41894800	H -3.05274700 2.99625000 -0.87321100
C 1.93038800 -0.51626800 0.67603200	H -1.69075400 2.79488100 -2.00970400
C 1.37359600 1.66553500 -1.60275000	H -2.82655300 1.46332700 -1.76479900
H 2.26594400 -0.15119000 -2.23704300	Co 0.24398000 0.00197100 -0.68163100
H 0.88273800 1.83856800 -2.55876200	C 3.58987900 1.49691000 0.48884000
H 1.41014000 2.50670600 -0.91228200	H 4.07492900 1.21456900 1.43223700
C -2.40278200 -1.41052600 1.03791500	H 4.35137500 1.92544600 -0.17543700
H -3.06483900 -2.29024300 1.02489400	H 2.86435100 2.29048500 0.71711900
H -1.77594300 -1.49060400 1.93958500	C 3.76394900 -1.01723000 -0.25405100
C -3.23127100 -0.12826400 1.08158500	C 2.55999200 -1.83456300 0.27380000
H -3.79610200 -0.00399200 0.14347000	H 4.59371400 -1.01261100 0.46181500
H -3.99605100 -0.24389000 1.86188800	H 4.15134400 -1.27706200 -1.24638000
C -2.42917400 1.13368200 1.38638400	H 2.75616200 -2.54682900 1.08642900
H -3.11147900 1.97898000 1.56457400	H 2.02508900 -2.37092700 -0.52504700
H -1.84941100 0.99454900 2.31350500	C 1.21746600 -0.13158200 1.81809300
P -1.29610300 -1.56333900 -0.42914800	H 1.17124900 0.94110100 2.03088700

C 0.64423100 -1.00247700 2.72393500
H 0.14937000 -0.64399100 3.62372400
H 0.72699200 -2.08268000 2.60044500
H -0.20192200 -0.30320500 -2.09598800

E6 (triplet state)

C 2.72394600 0.38327700 0.64818300
C 1.48977500 0.69252000 1.46734300
C 2.25963700 -0.41694200 -0.57398100
C 0.72568900 -0.29416700 2.03815900
H 1.27714300 1.74029100 1.69613700
H -0.08603300 -0.04366700 2.71950600
H 1.06275800 -1.33220600 2.06380800
C -2.71253600 1.48128100 -0.99951900
H -3.28823100 2.41835500 -0.94673800
H -2.50293400 1.29291800 -2.06398000
C -3.53019600 0.33152700 -0.41254400
H -3.65345500 0.46614300 0.67507900
H -4.54664200 0.39933300 -0.82364000
C -2.99009400 -1.06447200 -0.71805200
H -3.76300100 -1.81965300 -0.50797200
H -2.74305400 -1.14902300 -1.78797000
P -1.08950100 1.79548400 -0.18861300
P -1.47574900 -1.56019000 0.21328300
C -1.57447900 2.56721300 1.40495100
H -0.69401900 2.96834600 1.92140800
H -2.28192000 3.39085200 1.23854200
H -2.04534600 1.82644100 2.06327600
C -0.44530000 3.21431400 -1.14930100
H -1.18085300 4.02924900 -1.18185800
H 0.47757700 3.59374800 -0.69349400

H -0.22062300 2.89626100 -2.17449100
C -1.15335100 -3.22456000 -0.47866800
H -0.35585200 -3.72144700 0.08742200
H -2.05736800 -3.84658400 -0.43478900
H -0.82633700 -3.12769500 -1.52119400
C -2.15735100 -1.96170000 1.87180600
H -2.99886500 -2.66205600 1.78494100
H -1.38469600 -2.42368700 2.49820100
H -2.50718400 -1.05409800 2.37971700
Co 0.18276300 -0.03396900 -0.04174300

C 3.86216300 -0.20403000 1.46697000
H 4.70233100 -0.47621800 0.81386000
H 4.22345700 0.52514700 2.20436700
H 3.54953300 -1.10431000 2.01208200
C 3.12305400 1.51831100 -0.33608600
C 2.65494100 0.67156500 -1.54456700
H 4.19646700 1.73698900 -0.33112500
H 2.58006000 2.46107000 -0.18866000
H 3.45844000 0.36917100 -2.23282900
H 1.84718300 1.10252700 -2.15307400
C 2.08374300 -1.80263100 -0.74158800
H 2.11239400 -2.42640700 0.15749200
C 1.93148400 -2.41368500 -1.96323300
H 1.84593700 -3.49378800 -2.05514000
H -0.30296900 -0.18783700 -1.45923700
H 1.90350200 -1.82734100 -2.88187800

TSE6 (triplet state)

C 3.00029300 -0.16945200 0.63785200
C 1.73839100 0.23583000 1.38023900
C 2.52810500 -0.56992700 -0.74764100

C 0.81230700 -0.64776100 1.84945800	H -2.46077300 -0.86308100 2.42672500
H 1.64310900 1.29363500 1.64339000	Co 0.16371000 -0.09927400 -0.23942600
H 0.01096500 -0.31288800 2.50530900	C 3.88047600 -1.12229600 1.42796200
H 0.97297800 -1.72620500 1.80218600	H 4.76235300 -1.40333600 0.83871900
C -2.58899600 1.84666100 -0.69466900	H 4.22529000 -0.65655300 2.36026700
H -3.01076600 2.84001900 -0.47641500	H 3.34621900 -2.04480200 1.69148600
H -2.48790500 1.77365200 -1.78871000	C 3.69776500 1.04597600 -0.03298400
C -3.52962200 0.75768600 -0.17807200	C 3.02621400 0.69813100 -1.38367400
H -3.58734200 0.79694400 0.92230600	H 4.78719300 0.93314200 -0.06010200
H -4.54298800 1.00354600 -0.52371100	H 3.46372100 2.02957700 0.39329200
C -3.20090700 -0.66139000 -0.64066300	H 3.70158700 0.56653600 -2.24089800
H -4.05864900 -1.32412300 -0.44852800	H 2.23208600 1.39582100 -1.70474500
H -3.02614400 -0.67410200 -1.72845300	C 1.61558200 -1.54371800 -1.15446200
P -0.88269600 1.81595600 -0.00510400	H 1.45027900 -2.41209300 -0.50988200
P -1.71231800 -1.42229800 0.14809500	C 0.91991200 -1.45017300 -2.36386300
C -1.12975700 2.41958900 1.71116300	H 0.23485600 -2.22829500 -2.68952700
H -0.16562200 2.60131100 2.20101800	H -0.48555800 0.10259600 -1.59748900
H -1.69563800 3.36105900 1.70453600	H 1.17129200 -0.67770700 -3.08881900
H -1.68272100 1.68502100 2.30901700	E7 (triplet state)
C -0.08653600 3.24591900 -0.82410900	C 2.99188800 0.07948100 0.62483300
H -0.67393300 4.16239500 -0.67901800	C 1.83955100 0.53328100 1.50452200
H 0.91767300 3.40222900 -0.40936300	C 2.33216700 -0.18184200 -0.73034100
H 0.01032100 3.04848100 -1.89869800	C 0.98689500 -0.30999400 2.13598700
C -1.74762300 -3.10317500 -0.59188400	H 1.70657100 1.61314600 1.63479900
H -0.94006900 -3.72127300 -0.17989300	H 0.20313300 0.06793100 2.79057400
H -2.70571700 -3.59875000 -0.38606400	H 1.15297300 -1.38870300 2.14995600
H -1.61721900 -3.03904200 -1.67853300	C -2.83463200 1.36529100 -0.94021700
C -2.33099900 -1.78345200 1.84399600	H -3.51162800 2.22896200 -0.84813900
H -3.29546200 -2.30705800 1.80083700	H -2.55432400 1.29787000 -2.00406000
H -1.61599700 -2.42182800 2.37750600	C -3.56060200 0.08993700 -0.51139500

H -3.80246100 0.13391200 0.56286000
H -4.53448900 0.07800500 -1.02009100
C -2.84895300 -1.22435800 -0.83947400
H -3.55548800 -2.06224300 -0.73347900
H -2.51988300 -1.22249700 -1.89192100
P -1.28859700 1.76472400 -0.00944100
P -1.36700700 -1.61127100 0.20261900
C -1.90495700 2.26288600 1.64729000
H -1.07490700 2.67399900 2.23618900
H -2.68656900 3.03018600 1.56236800
H -2.31156400 1.40376400 2.19393100
C -0.83018000 3.39033800 -0.73132400
H -1.66279800 4.10323100 -0.66246200
H 0.03191700 3.80630900 -0.19444300
H -0.55302700 3.27214300 -1.78594300
C -1.03599400 -3.35902900 -0.25986100
H -0.22828300 -3.76011500 0.36611100
H -1.92949900 -3.98099800 -0.11570700
H -0.72465700 -3.43346100 -1.30879900
C -2.11773400 -1.84749100 1.86539000
H -3.00930300 -2.48647800 1.80352200
H -1.39073600 -2.33125000 2.52936100
H -2.39965000 -0.89004300 2.31884800
Co 0.24533700 0.04173400 -0.06791800
C 3.85640900 -1.00375700 1.23389300
H 4.63255200 -1.31642100 0.52374400
H 4.34884900 -0.64440600 2.14647800
H 3.27274900 -1.89528100 1.50003400
C 3.70371000 1.28467200 -0.04381100
C 2.77200900 1.16690900 -1.27433600

H 4.74221900 1.04191300 -0.29615300
H 3.68970900 2.23213200 0.50772500
H 3.25205100 1.14927200 -2.26064600
H 1.97934000 1.93161100 -1.30366500
C 1.71472500 -1.26443200 -1.26622200
H 1.71686800 -2.20061100 -0.69951400
C 1.21517300 -1.30301500 -2.67901100
H 1.87719500 -1.90488500 -3.31737000
H 0.21534000 -1.75388200 -2.75128900
H 1.16092400 -0.29497400 -3.11224200

a

C 0.00000000 0.00000000 0.66358600
H 0.00000000 0.92487000 1.23894100
H 0.00000000 -0.92487000 1.23894100
C 0.00000000 0.00000000 -0.66358600
H 0.00000000 -0.92487000 -1.23894100
H 0.00000000 0.92487000 -1.23894100

b

C -2.56398100 0.16188500 0.00021700
H -3.12063600 -0.78417400 0.00053800
H -2.87831300 0.73093000 0.88519000
H -2.87886100 0.73064900 -0.88474200
C -1.13000900 -0.06574600 -0.00019500
C 0.06970500 -0.23730500 -0.00052700
C 1.46955900 -0.48281400 0.00010200
H 1.77911100 -1.53050900 0.00053700
C 2.40423800 0.47386500 0.00011200
H 2.13897500 1.52929600 -0.00034100
H 3.46265600 0.22448900 0.00057100

A2-1

C -2.09079100 -0.17222100 0.32533300
C -0.45253100 -0.77792700 -1.64252900
C -1.47450700 -1.85445600 -1.35547300
C -2.41912300 -1.33810900 -0.28702300
H 0.48479700 -1.12719600 -2.09501300
H -0.87084200 0.04497500 -2.23467300
H -0.99765000 -2.79828800 -1.04289600
H -2.05475400 -2.11528500 -2.26083000
C -3.63384800 -2.16378900 -0.00338700
H -3.35742000 -3.20904400 0.19506800
H -4.20413700 -1.78292400 0.84974200
H -4.29628800 -2.17866100 -0.88251400
C -2.90104400 0.70587400 1.14567000
H -2.47080900 1.05867800 2.08864700
C -4.11581000 1.14932800 0.78913400
H -4.57551000 0.83990400 -0.14974300
H -4.68687200 1.82852500 1.41855000
C 3.10129500 -0.23743000 -0.65298700
H 4.10485900 -0.61281300 -0.40166600
H 2.90911100 -0.53555300 -1.69583000
C 3.05412200 1.28398400 -0.52859200
H 3.16938700 1.58812200 0.52468200
H 3.93118600 1.69926500 -1.04315200
C 1.80832100 1.93164200 -1.13118900
H 1.94756500 3.02103800 -1.21490700
H 1.63730900 1.55948000 -2.15403100
P 1.87968700 -1.12472000 0.41006200
P 0.24075800 1.67992700 -0.20196200
C 2.67529300 -1.08673600 2.06556400
H 2.09468600 -1.69155000 2.77184300

H 3.69515800 -1.49065600 2.01280900
H 2.72306500 -0.06406600 2.45814900
C 2.13095700 -2.86911000 -0.09867700
H 3.19506100 -3.13704300 -0.05647000
H 1.57342000 -3.53774600 0.56789500
H 1.77067600 -3.02481700 -1.12309900
C -0.95303900 2.70804900 -1.11995700
H -1.93279100 2.66057800 -0.62934400
H -0.60992200 3.75058700 -1.14856100
H -1.06090700 2.34621000 -2.14894200
C 0.46279500 2.58563000 1.37434700
H 0.86957500 3.58853000 1.18477100
H -0.50963900 2.69271900 1.86976500
H 1.13795800 2.05110900 2.05250000
Co -0.24353700 -0.33113200 0.21793900
A2-2
C -1.91662900 0.81699600 0.49349200
C -0.76430600 -0.27653700 -1.57829600
C -2.11074900 -0.88788900 -1.26071700
C -2.72374100 -0.09646600 -0.11836500
H -0.05324600 -0.94400000 -2.08341500
H -0.85549500 0.66400700 -2.13432800
H -2.01909900 -1.95541200 -1.00407500
H -2.77950000 -0.85297800 -2.14007000
C -2.27656200 1.89725200 1.44912900
H -2.30875400 2.87321100 0.94084100
C 2.75818100 -1.30028500 -0.76893700
H 3.52814200 -2.06070800 -0.56899300
H 2.40771500 -1.47453900 -1.79862000
C 3.34868200 0.10284800 -0.64931300

H 3.63558400 0.31206600 0.39423600
H 4.28963200 0.13128500 -1.21522700
C 2.44934000 1.21690800 -1.18285900
H 3.01946600 2.15482800 -1.27466500
H 2.08944900 0.97018400 -2.19464700
P 1.33248700 -1.61854000 0.36019600
P 0.96505700 1.61302700 -0.16986500
C 2.14934600 -1.95741100 1.97009100
H 1.40239500 -2.27702300 2.70609100
H 2.89886600 -2.75271500 1.86215800
H 2.64369300 -1.05987800 2.36007200
C 0.79944000 -3.29376600 -0.16283200
H 1.64974000 -3.98865100 -0.16697300
H 0.03553900 -3.67592500 0.52469400
H 0.36916200 -3.26004100 -1.17136500
C 0.27910400 3.07249000 -1.02491400
H -0.57595700 3.46832200 -0.46604600
H 1.04458300 3.85546300 -1.10697200
H -0.05956500 2.80673200 -2.03266800
C 1.62037300 2.30681000 1.39331800
H 2.39089200 3.06135500 1.18318900
H 0.80534700 2.78705200 1.94805400
H 2.05300400 1.52516700 2.02825200
Co -0.29568800 -0.02173400 0.26959400
H -3.27021000 1.75089700 1.89646900
H -1.55762000 1.98517000 2.27630200
C -4.10661600 -0.35721700 0.26134600
H -4.51742300 0.25495800 1.06519100
C -4.88708700 -1.28716300 -0.30133200
H -4.54294300 -1.94071500 -1.10174800

H -5.91562300 -1.42803700 0.02138700

A2-3

C -2.03188300 0.34897300 0.37459200
C -0.58148300 -0.48859400 -1.63977100
C -1.81939300 -1.32566600 -1.40865300
C -2.63524100 -0.65711000 -0.31509900
H 0.25958000 -1.01457000 -2.11117100
H -0.80422500 0.43046700 -2.19517000
H -1.56261900 -2.36258000 -1.13514400
H -2.42417000 -1.41062600 -2.32974200
C -2.61456500 1.27707200 1.38107000
H -3.09019300 2.15061500 0.90973500
C 2.99645800 -0.81035400 -0.72804100
H 3.89769500 -1.40614600 -0.51840100
H 2.70828500 -1.03623400 -1.76675700
C 3.29631100 0.67972200 -0.58203500
H 3.51947500 0.92559500 0.46899900
H 4.22248300 0.90064500 -1.12966700
C 2.20517100 1.60461300 -1.11966000
H 2.58219900 2.63740800 -1.18548800
H 1.91918400 1.31080200 -2.14213000
P 1.64076900 -1.42136300 0.36726500
P 0.65723400 1.68529500 -0.12756200
C 2.48258900 -1.62168400 1.98763200
H 1.79913800 -2.08541000 2.70841100
H 3.36959200 -2.26062000 1.88325600
H 2.79490800 -0.65277600 2.39468100
C 1.45900200 -3.16043600 -0.18802300
H 2.43187600 -3.66969400 -0.19614000
H 0.78512700 -3.70084000 0.48733700

H 1.03520100 -3.19713400 -1.19919000
C -0.29027500 3.00853500 -0.95329500
H -1.19235900 3.23613000 -0.37449000
H 0.32061400 3.91732700 -1.03514100
H -0.59464000 2.69708700 -1.95886400
C 1.15587500 2.45114700 1.46002800
H 1.77104800 3.34232300 1.27354100
H 0.26357200 2.75721100 2.01885700
H 1.72533000 1.75090600 2.08151900
Co -0.26850900 -0.17637200 0.23357900
H -3.39701600 0.77098300 1.96808100
H -1.86559300 1.65412300 2.09234900
C -3.98045300 -1.19238800 -0.08631000
H -4.08647200 -2.26800400 -0.25799500
C -5.06433900 -0.48700300 0.25046400
H -5.04393000 0.59432400 0.37406200
H -6.03106300 -0.96920500 0.37507800

B1

C -1.93361200 -1.01395900 1.32051000
C -0.03112800 -1.12720000 -2.20497800
C -1.37580600 -1.02995700 -2.00369100
C -2.79956900 -0.66600800 0.51080800
H 0.45059400 -2.10337500 -2.20679900
H 0.53018300 -0.29928600 -2.64052200
H -1.97080200 -1.92367100 -1.81702200
H -1.92501200 -0.12314200 -2.25323400
C -4.04818700 -0.41154100 -0.19055000
H -4.30534000 -1.24777200 -0.85335800
H -4.86161300 -0.30518400 0.53871000
H -4.02211100 0.50261200 -0.79581300

C -0.66991200 -1.53327300 1.66229300
H -0.13871900 -1.24269800 2.56699500
C -0.27051500 -2.54892800 0.74366300
H -1.03219000 -3.15914300 0.25579100
H 0.67391400 -3.06683200 0.91871400
Co -0.37445700 -0.67505500 -0.07091700
C 2.69430400 0.85820100 -0.70564400
C 2.28031200 2.23145500 -0.19341800
C 0.87995600 2.63563900 -0.63473100
H 2.36449900 2.27444400 0.90446000
H 2.99777600 2.97379200 -0.56843200
P -0.47314800 1.59801900 0.07069400
P 1.81653000 -0.58414700 0.03971600
C -0.54283300 2.16939400 1.81492400
H -0.64065900 3.26190800 1.87189800
H -1.40828100 1.71121100 2.30961900
H 0.35640100 1.86669500 2.36462700
C -1.93260400 2.46811800 -0.63033800
H -1.80643300 3.55459300 -0.53301600
H -2.06733100 2.22846400 -1.69227600
H -2.83700900 2.18151200 -0.08164700
C 2.49443100 -0.62389900 1.74569400
H 2.27440300 -1.59022400 2.21560900
H 3.58475600 -0.49540500 1.72300800
H 2.05885400 0.16553800 2.36864000
C 2.75638800 -1.94550500 -0.75824100
H 2.73810200 -1.83248400 -1.84826300
H 3.80265000 -1.90682200 -0.42797800
H 2.34465400 -2.92777500 -0.50503900
H 0.79796400 2.57624300 -1.73244800

H 0.67544200 3.68130900 -0.35984700

H 3.76638800 0.68595100 -0.52520800

H 2.55117700 0.80271100 -1.79638700

TSBI

C -2.00155600 -0.63100000 1.15636800

C -0.42544100 -0.70794700 -1.92729500

C -1.86227300 -0.60579400 -1.62799200

C -2.62404500 -0.55475200 0.01008300

H -0.09715500 -1.68298700 -2.29812800

H 0.00752900 0.12967100 -2.48307500

H -2.40048500 -1.51911500 -1.90452300

H -2.34184500 0.28543500 -2.04250300

C -4.09091600 -0.53207300 -0.26520400

H -4.39710600 -1.39846700 -0.86590800

H -4.64990000 -0.54461000 0.67520400

H -4.37558300 0.36849000 -0.82830100

C -0.96420300 -1.31127900 1.78187500

H -0.46911600 -0.97123600 2.69001700

C -0.51358600 -2.40356300 0.97087000

H -1.24758100 -2.97038400 0.39620600

H 0.33545100 -2.99637200 1.31608600

Co -0.37171700 -0.57455000 0.00074400

C 2.74082100 0.47585000 -0.87095100

C 2.57659800 1.86938200 -0.26967300

C 1.23774100 2.52330300 -0.59444100

H 2.73399000 1.83766600 0.82076000

H 3.38101200 2.50865000 -0.65785900

P -0.22188800 1.69358100 0.16771400

P 1.74176400 -0.86153900 -0.08970200

C -0.20514400 2.29589900 1.90005100

H -0.18077600 3.39292600 1.94256100

H -1.11156800 1.94502600 2.41039600

H 0.66212400 1.90135900 2.44349400

C -1.59509600 2.67757300 -0.55064100

H -1.44192100 3.74832100 -0.36156300

H -1.65060800 2.52404400 -1.63594400

H -2.54883300 2.37687300 -0.09986100

C 2.51862300 -1.02139800 1.56438700

H 2.19805500 -1.94950200 2.05089900

H 3.61274500 -1.04149800 1.46964300

H 2.23524700 -0.18356400 2.21187700

C 2.36132100 -2.33386200 -0.98119600

H 2.19855300 -2.21707400 -2.05902000

H 3.43749000 -2.45899500 -0.80379900

H 1.83668800 -3.23616400 -0.64841600

H 1.07615100 2.52213700 -1.68456000

H 1.23431900 3.57781400 -0.27983600

H 3.79053800 0.15196700 -0.79756300

H 2.49373600 0.48978700 -1.94401300

TSC1

C -1.82443200 0.78917000 0.50266300

C -1.10433200 1.70239600 -1.74302900

C -1.86816200 0.47438700 -1.86316900

C -2.48903900 0.17843300 -0.56525200

H -0.43542400 1.97112500 -2.56139100

H -1.55693800 2.55140100 -1.23257700

H -0.71260300 -0.39945800 -2.01037900

H -2.31227400 0.08446700 -2.78433400

C -3.57119400 -0.84472000 -0.40028800

H -3.62879500 -1.22133800 0.62845500

H -4.54913200 -0.41390200 -0.65692500
H -3.40956200 -1.69668600 -1.07523500
C -2.32633400 1.35778000 1.71710600
H -3.36212700 1.70610800 1.74153900
C -1.57326000 1.44448200 2.82764100
H -0.54417000 1.08806500 2.82802900
H -1.96318800 1.85203100 3.75787500
C 2.04672900 -2.20103800 -0.27450300
H 2.25257000 -3.18591000 0.17196400
H 2.11068800 -2.32320700 -1.36732400
C 3.07058200 -1.17281000 0.19902000
H 2.99433700 -1.03300900 1.28978000
H 4.07507400 -1.58460800 0.03180700
C 2.97519300 0.17183200 -0.51560200
H 3.85430900 0.79065700 -0.27853200
H 2.97639200 0.02099300 -1.60696400
P 0.30245100 -1.76501000 0.10719300
P 1.47889000 1.17922100 -0.12153500
C 0.15953100 -2.05818700 1.91046900
H -0.88722600 -1.91900000 2.21095400
H 0.47396600 -3.07732800 2.17341200
H 0.76943200 -1.34285300 2.47500600
C -0.61786700 -3.19121900 -0.58033400
H -0.19709600 -4.13863700 -0.21767900
H -1.66933600 -3.13655300 -0.27269400
H -0.57459600 -3.17379400 -1.67576600
C 1.84789900 2.71580200 -1.04822500
H 1.07716700 3.47076300 -0.85473700
H 2.82306800 3.11696100 -0.74183100
H 1.87382000 2.51297500 -2.12510900
C 1.81177500 1.72903500 1.59787600
H 2.81791200 2.16328700 1.67532500
H 1.07905100 2.49557300 1.87932000
H 1.73496200 0.89713400 2.30861300
Co -0.40936800 0.22739000 -0.52154500
C1
C 1.61225600 -0.80978300 0.73297500
C 0.64471700 -2.35247000 -1.31374800
C 1.72499600 -1.49953500 -1.55766700
C 2.36335100 -0.83602100 -0.47127100
H 0.05458000 -2.69236600 -2.16214600
H 0.62279600 -2.98879200 -0.43227200
H -0.39737800 0.03541100 -1.79270900
H 2.00362600 -1.23072200 -2.57852500
C 3.64331900 -0.07519500 -0.66258800
H 3.72396800 0.77933000 0.02127900
H 4.50605900 -0.72936700 -0.47324300
H 3.73636500 0.29132900 -1.69322500
C 2.18443100 -0.67450600 2.04108900
H 3.27124700 -0.74998100 2.15211600
C 1.42625100 -0.52915900 3.14219400
H 0.34070300 -0.48145800 3.06459400
H 1.85800200 -0.47015900 4.13905300
C -1.56676300 2.42525100 -0.54050800
H -1.50642100 3.49555400 -0.29216700
H -1.76077000 2.35222000 -1.62150300
C -2.68825500 1.75294100 0.24506900
H -2.44675300 1.73454100 1.32101700
H -3.59262600 2.37049000 0.16271000
C -3.01519100 0.35003500 -0.25233500

H -3.94640400 -0.01418200 0.20803900
H -3.18217000 0.36548900 -1.34076700
P 0.09432800 1.70511800 -0.24305100
P -1.73716100 -0.93789600 0.05909200
C 0.57908600 2.44837500 1.35945700
H 1.60829400 2.16387800 1.60904300
H 0.51289600 3.54337300 1.30888500
H -0.07106800 2.09099300 2.16740600
C 1.15197500 2.59926600 -1.43509000
H 1.01141100 3.68471600 -1.34270200
H 2.20750500 2.36640400 -1.25029000
H 0.90007800 2.28220800 -2.45343100
C -2.48352500 -2.36324700 -0.80988400
H -1.95079900 -3.28952900 -0.56713200
H -3.53418800 -2.47511000 -0.51015800
H -2.43555600 -2.20248500 -1.89328300
C -1.99590300 -1.37561200 1.81948700
H -3.02046900 -1.73543600 1.98557500
H -1.28870400 -2.16274300 2.10883000
H -1.82376200 -0.50127300 2.45993800
Co 0.28731700 -0.43343400 -0.49365300

4a

C 0.28625700 -0.02910400 -0.00003000
C 0.08812800 -1.52700800 -0.00004900
C -1.43665600 -1.21554600 0.00004000
C -1.03840800 0.23987000 0.00009200
H 0.45355400 -2.05697300 0.89100800
H 0.45331600 -2.05665900 -0.89140600
H -1.98238100 -1.56316500 0.88966300
H -1.98224300 -1.56285000 -0.88982300

C -1.85491200 1.47578500 0.00003200
H -2.51031000 1.52222700 0.88233600
H -1.23020400 2.37797800 -0.00238200
H -2.51370200 1.51977100 -0.87986800
C 1.48314200 0.77543200 -0.00010800
H 1.34919900 1.86044900 -0.00041800
C 2.71857800 0.26154500 0.00010200
H 2.88011600 -0.81683000 0.00035000
H 3.60587800 0.89019900 0.00007100

4b

C 0.12987400 -0.53195700 -0.05622100
C -1.03036400 -1.49822800 0.03734300
C -1.93570700 -0.23629100 0.10895600
C -0.66246600 0.56296300 -0.01330900
H -1.05341400 -2.14037800 0.92902800
H -1.19797200 -2.13028700 -0.84640800
H -2.49082700 -0.11654600 1.05090300
H -2.64896400 -0.12660400 -0.72156600
C -0.42956500 2.02338700 -0.10705200
H -0.48018900 2.51017200 0.87892700
H 0.55885300 2.24229200 -0.53283700
H -1.19050400 2.50684700 -0.73580500
C 1.55649600 -0.75622000 -0.18223800
H 1.85570800 -1.71600700 -0.61263400
C 2.50814300 0.10735200 0.19099500
H 2.26440400 1.05420300 0.67244200
H 3.56443800 -0.10972500 0.04709900
dppp (open-shell singlet)
C 1.54559600 -0.72929000 1.29241000
H 2.22720800 -0.55190100 2.13908400

H 1.40313100 -1.81938100 1.22922800
C 2.16873600 -0.20172400 0.00000000
H 2.18247100 0.90037700 0.00000000
H 3.22697900 -0.49641200 0.00000000
C 1.54559600 -0.72929000 -1.29241000
H 2.22720800 -0.55190100 -2.13908400
H 1.40313100 -1.81938100 -1.22922800
P -0.08168400 0.00596800 1.76395000
P -0.08168400 0.00596800 -1.76395000
C 0.35144100 1.70609100 2.29474500
H -0.52233100 2.18917400 2.74704200
H 1.16209700 1.68230600 3.03541700
H 0.66874600 2.31578300 1.44077800
C -0.45836900 -0.83648300 3.34536700
H 0.38025200 -0.72231400 4.04495800
H -1.35649300 -0.40595400 3.80232500
H -0.63625100 -1.90462000 3.17701200
C -0.45836900 -0.83648300 -3.34536700
H -1.35649300 -0.40595400 -3.80232500
H 0.38025200 -0.72231400 -4.04495800
H -0.63625100 -1.90462000 -3.17701200
C 0.35144100 1.70609100 -2.29474500
H 1.16209700 1.68230600 -3.03541700
H -0.52233100 2.18917400 -2.74704200
H 0.66874600 2.31578300 -1.44077800
Co -1.47733600 -0.09713600 0.00000000
dppp (triplet state)
C 1.52851100 -0.69607900 1.29904700
H 2.23196700 -0.52334900 2.12891300
H 1.40520900 -1.78745000 1.21916700

C 2.11028900 -0.13209200 0.00000000
H 2.05891100 0.96900100 0.00000000
H 3.18464300 -0.36116500 0.00000000
C 1.52851100 -0.69607900 -1.29904700
H 2.23196700 -0.52334900 -2.12891300
H 1.40520900 -1.78745000 -1.21916700
P -0.09966300 -0.00416500 1.84175100
P -0.09966300 -0.00416500 -1.84175100
C 0.32402600 1.68544700 2.41217300
H -0.54619000 2.14786400 2.89187600
H 1.14826600 1.65097700 3.13719800
H 0.61987200 2.31917900 1.56754600
C -0.42153200 -0.90520900 3.40131500
H 0.43453900 -0.80266800 4.08121000
H -1.31288300 -0.50290500 3.89539100
H -0.59044300 -1.96912000 3.20066200
C -0.42153200 -0.90520900 -3.40131500
H -1.31288300 -0.50290500 -3.89539100
H 0.43453900 -0.80266800 -4.08121000
H -0.59044300 -1.96912000 -3.20066200
C 0.32402600 1.68544700 -2.41217300
H 1.14826600 1.65097700 -3.13719800
H -0.54619000 2.14786400 -2.89187600
H 0.61987200 2.31917900 -1.56754600
Co -1.43956000 -0.06538200 0.00000000
D1 (open-shell singlet)
C -2.84283200 0.37311600 0.31171200
C -2.03259600 0.16216400 1.59729900
C -1.95485500 -0.08007600 -0.86107200
C -1.31873700 -1.14429500 1.68202100

H -2.55706500 0.47753100 2.51446600
H -1.82593400 -2.01894100 1.27304100
H -0.86640900 -1.36216300 2.65821900
C 2.66661400 1.23827700 -1.07140900
C 3.29996700 -0.15115800 -1.05158400
H 4.10621200 -0.16842900 -1.79766600
H 3.80065800 -0.32830100 -0.08582700
C 2.34140900 -1.29691400 -1.36988300
H 2.90944300 -2.21786900 -1.57473500
P 1.45797000 1.55046200 0.28587000
P 1.10203700 -1.71227700 -0.06668500
C 1.12361800 3.34399200 0.07714000
H 0.38569700 3.68187700 0.81540600
H 2.04778000 3.92200700 0.21034300
H 0.72766100 3.54297400 -0.92504200
C 2.52665900 1.57706000 1.78621400
H 3.43061500 2.17864600 1.61824200
H 1.96708300 2.01856400 2.62024800
H 2.82659600 0.56611100 2.08681700
C 2.09653600 -2.46925300 1.27364000
H 2.75854200 -3.25002400 0.87561100
H 2.70621800 -1.72018500 1.79204000
H 1.41870900 -2.91964400 2.00909500
C 0.29016000 -3.17096900 -0.81584600
H 1.04642000 -3.91177500 -1.10789200
H -0.39731800 -3.63580600 -0.09966400
H -0.27520400 -2.87695100 -1.70871400
Co -0.12198500 -0.06866700 0.62235400
C -3.47528700 1.75086900 0.28605300
H -3.91609800 1.97392700 -0.69369600

H -4.27837800 1.80254900 1.03442200
H -2.75361300 2.54567300 0.52703000
C -3.78541500 -0.80662200 -0.04043400
C -2.75382000 -1.35496000 -1.05282700
H -4.70373000 -0.45556700 -0.52518800
H -4.05913200 -1.46922000 0.78932800
H -3.12033300 -1.50091900 -2.07816400
H -2.27122500 -2.28789600 -0.73844200
C -1.29452000 0.61578100 -1.89895600
H -0.94701200 -0.01843500 -2.72360400
C -1.10180400 1.96406100 -2.01132900
H -0.61740200 2.39003300 -2.88798500
H -1.48002700 2.66160600 -1.26654000
H 1.77257300 -1.06968800 -2.28630100
H 3.44765600 2.01195200 -1.01130200
H 2.13108900 1.39840400 -2.02107000
H -1.23114900 1.01476000 1.57174800
TSD1
C 2.75836500 -0.80837500 -0.17893700
C 1.83690500 -1.14572300 -1.33704600
C 1.83129100 0.13122200 0.62599800
C 0.81102500 -2.05985700 -1.26830700
H 2.07944900 -0.67515100 -2.29157500
H 0.76429100 -2.78808200 -0.46124000
H 0.24100600 -2.30731700 -2.16490400
C -2.13034300 1.89628900 1.06892400
C -3.24452900 0.85602400 1.07878300
H -3.98235900 1.15067700 1.83754200
H -3.79110600 0.87785300 0.12211800
C -2.78185000 -0.56355700 1.39138000

H -3.65139300 -1.21792600 1.55603600
P -0.88372600 1.72608100 -0.28167000
P -1.72973900 -1.35168900 0.09702100
C -0.05229300 3.35320000 -0.16907200
H 0.77483200 3.40878300 -0.88579900
H -0.78612100 4.13680200 -0.39993500
H 0.34730200 3.53119800 0.83394600
C -1.84404600 1.96656500 -1.82930900
H -2.58260500 2.77075600 -1.70766700
H -1.14416300 2.24938600 -2.62514300
H -2.35677100 1.05472500 -2.15091200
C -2.91375700 -1.65984200 -1.27408400
H -3.76258600 -2.25258500 -0.90735400
H -3.30208700 -0.72903600 -1.70017100
H -2.41597400 -2.21875000 -2.07554400
C -1.58518500 -3.05452500 0.77716100
H -2.57257800 -3.40235200 1.10795800
H -1.22080700 -3.74397200 0.00680100
H -0.89953400 -3.09174600 1.63238900
Co 0.18861300 -0.16095300 -0.51582000
C 4.13858800 -0.40680200 -0.64494500
H 4.73630400 0.00799100 0.17579200
H 4.66550600 -1.28910000 -1.03359300
H 4.10252400 0.33339000 -1.45643900
C 2.68951400 -1.78993700 1.01262800
C 1.55908500 -0.96324300 1.65837300
H 3.61086700 -1.72310600 1.60275700
H 2.49774300 -2.84754900 0.79383200
H 1.70351700 -0.64943200 2.70107100
H 0.56152600 -1.42691700 1.59253200

C 2.15605900 1.46414800 1.12198800
H 1.63411200 1.73523600 2.04828100
C 3.01928600 2.34207900 0.59757300
H 3.20666400 3.30070100 1.07680500
H 3.56391700 2.14687500 -0.32411300
H -2.19470100 -0.57403000 2.32479700
H -2.55892100 2.90708200 0.98687900
H -1.57176300 1.86625600 2.01935800
H 0.92463500 0.84318600 -1.32428000
D2
C -2.76126000 -1.07838200 -0.04567000
C -1.69465400 -1.64036300 0.83473600
C -2.00249200 0.25518300 -0.28675100
C -0.62720300 -2.39792300 0.42067700
H -1.79459100 -1.38268000 1.89143500
H -0.62337500 -2.87596600 -0.55902400
H 0.02448400 -2.84028500 1.17087500
C 2.38856700 2.01060000 -0.67483000
C 3.46343500 1.13754400 -0.04828400
H 4.44704000 1.55793300 -0.29791500
H 3.40299500 1.17265000 1.05197400
C 3.40186400 -0.29817800 -0.54606500
H 4.30228100 -0.85637600 -0.24829500
P 0.64949200 1.75526000 -0.09991400
P 1.95482100 -1.25974300 0.07406800
C -0.16028700 2.91762700 -1.27042700
H -1.14367200 3.22200000 -0.90500600
H 0.46809600 3.81297800 -1.36645000
H -0.26716200 2.46265000 -2.26239700
C 0.62255100 2.67622500 1.47874500

H 0.97211400 3.70645300 1.33150000
H -0.40206400 2.69498500 1.86773500
H 1.26297800 2.17730200 2.21616200
C 2.50412400 -1.63895400 1.78394500
H 3.48757700 -2.12735200 1.77518300
H 2.57091000 -0.71093200 2.36496700
H 1.78919900 -2.29302400 2.29504400
C 2.24766200 -2.84016000 -0.81627200
H 3.31205400 -3.10490800 -0.76786300
H 1.66990400 -3.66163800 -0.38011400
H 1.96027400 -2.73595700 -1.87003800
Co -0.11753100 -0.32961500 0.06437500
C -4.14627600 -1.10651200 0.54500400
H -4.84334200 -0.51337300 -0.06027600
H -4.52496800 -2.13612900 0.59190100
H -4.16002100 -0.69428200 1.56295900
C -2.59848900 -1.38925500 -1.54422500
C -1.61475300 -0.21759400 -1.67684800
H -3.53404800 -1.16034300 -2.06755100
H -2.27121500 -2.39092100 -1.85038000
H -1.71406700 0.48455900 -2.51344700
H -0.52711700 -0.58107800 -1.76037900
C -2.65056000 1.52802800 0.05224800
H -3.04014400 2.10999400 -0.79115300
C -2.89251500 1.95623100 1.29432400
H -3.46962500 2.85717300 1.48809200
H -2.52334100 1.41000700 2.16491500
H 3.36862100 -0.31552900 -1.64686700
H 2.60229800 3.07516500 -0.49501000
H 2.38746300 1.87422300 -1.76839100

H 0.04082900 -0.01514400 1.48552600

A1-dppm

C -1.56614600 0.98198100 -0.58845500
C 0.93497400 -1.87172600 -1.51163300
C -0.40328800 -2.24602600 -1.47420100
C -2.10676200 -0.18233100 -0.70525600
H 1.66240900 -2.30737200 -0.82237300
H 1.36251500 -1.48283300 -2.43686300
H -0.78473300 -2.95041400 -0.73387600
H -1.01841400 -2.13974900 -2.36838600
C -3.29749800 -1.04224400 -0.77408400
H -3.31635300 -1.73771000 0.07866400
H -4.22285400 -0.45279700 -0.75389100
H -3.30103900 -1.66037200 -1.68096700
C -1.69961300 2.39818700 -0.36183700
H -0.99312800 3.06117700 -0.86417700
C -2.63625500 2.91118400 0.44647500
H -3.35337400 2.27053300 0.95999700
H -2.71882600 3.98239600 0.61593300
P 0.26587800 -0.81135800 1.30346300
P 1.69234000 0.82409100 -0.32965500
C -0.69717000 0.11455900 2.53880100
H -1.72658500 -0.26519100 2.55482700
H -0.25620100 0.00232500 3.53774400
H -0.73379600 1.17659400 2.26799600
C 0.28891600 -2.52320300 1.92550900
H 0.68550000 -2.54524800 2.94866300
H -0.73544200 -2.91690000 1.93770300
H 0.90376400 -3.16915100 1.28916300
C 3.27085500 0.66416200 -1.24534300

H 3.20709100 1.22097900 -2.18786400
H 4.10398500 1.06662100 -0.65522100
H 3.47214100 -0.38654000 -1.48233300
C 1.71741300 2.58379600 0.18285700
H 2.65749300 2.82498600 0.69574500
H 1.62644700 3.22926800 -0.69923300
H 0.87409800 2.80032300 0.84990200
Co -0.23318400 -0.35408800 -0.71196100
C 1.95872300 -0.10006600 1.27948500
H 2.70749300 -0.89210700 1.14125200
H 2.23562300 0.51092000 2.14953000

TSA1-dppm

C 1.97478800 -0.37761900 0.07930000
C -0.16686200 1.61063200 -1.69477600
C 1.16327700 2.00416300 -1.25620000
C 2.19698700 0.91537100 -0.08418400
H -0.95261600 2.35972400 -1.58455900
H -0.24923900 1.03799700 -2.62338700
H 1.22512300 2.95553000 -0.72492300
H 1.94472700 1.89918900 -2.01459300
C 3.36430300 1.79282100 0.20014800
H 3.06573600 2.73503900 0.67697900
H 4.05966500 1.26761400 0.86549300
H 3.90858600 2.04935600 -0.71902400
C 2.72840700 -1.54694900 0.45730600
H 3.64246400 -1.74010900 -0.11097500
C 2.40575200 -2.35174500 1.47632700
H 1.51756300 -2.16896500 2.08155300
H 3.04149800 -3.18357200 1.76893300
P -1.50728300 0.88674500 0.73064400

P -0.95088000 -1.37462000 -0.56385500
C -1.32557000 0.53105900 2.51355700
H -0.75154100 1.33470000 2.98956000
H -2.30556200 0.45461800 3.00317700
H -0.77068900 -0.40399600 2.65481200
C -2.51261900 2.41153500 0.68533300
H -3.37448300 2.31099400 1.35692900
H -1.91069300 3.26814500 1.01223200
H -2.87775300 2.60789700 -0.32868200
C -1.28467800 -1.93209600 -2.27271900
H -0.40117400 -2.44815700 -2.66642800
H -2.13974500 -2.61934400 -2.29959800
H -1.49459500 -1.06964200 -2.91534000
C -0.82834200 -2.93299900 0.37898600
H -1.63010800 -3.62435800 0.09045200
H 0.14371900 -3.40345000 0.18597500
H -0.90076300 -2.73486100 1.45496900
Co 0.33119700 0.37055200 -0.28426100
C -2.48880800 -0.51415300 0.03607300
H -3.07868800 -0.17083900 -0.82572300
H -3.14111400 -1.06041300 0.73048100

A2-dppm

C -1.85691600 0.15837700 0.26068200
C 0.02540900 -2.20063800 -0.88015200
C -1.42806900 -2.32986400 -0.48324500
C -2.30151000 -1.07387000 -0.01982100
H 0.65947600 -2.99865500 -0.48629700
H 0.19762300 -2.04500400 -1.95268200
H -1.55144700 -3.07753200 0.30977200
H -1.99498800 -2.67463500 -1.36075800

C -3.74484300 -1.48376600 0.04447100
H -3.85622400 -2.42258800 0.60512100
H -4.36024300 -0.71943400 0.52935800
H -4.14057600 -1.66345400 -0.96590300
C -2.61608600 1.34527800 0.60851800
H -3.49434900 1.57048200 -0.00483100
C -2.33187400 2.13414000 1.64980200
H -1.47822500 1.92622600 2.29703700
H -2.95633800 2.98492700 1.91226000
P 1.88159400 -0.63933400 0.47638900
P 0.64689900 1.40367600 -0.66587000
C 2.11208200 -0.18516200 2.23186400
H 1.81516600 -1.02375500 2.87214100
H 3.16216600 0.06401700 2.43500400
H 1.47484500 0.67070300 2.48477400
C 3.10275100 -1.96465700 0.19439600
H 4.10374100 -1.61645400 0.47853600
H 2.85416000 -2.84648500 0.79719600
H 3.10976800 -2.25632400 -0.86218700
C 0.33296300 1.79808800 -2.41887800
H -0.71701700 2.09776300 -2.52760400
H 0.97844500 2.61435500 -2.76731400
H 0.49987800 0.90683300 -3.03485700
C 0.52333300 3.00978600 0.18730300
H 1.16360100 3.74359400 -0.31894800
H -0.51473700 3.36055100 0.17603000
H 0.84141400 2.91706000 1.23238500
Co -0.18479400 -0.49790700 -0.10744400
C 2.40706000 0.85313400 -0.48479000
H 2.81825900 0.55838400 -1.45991900

H 3.10183600 1.54270700 0.01397400

A1-dppf

C -3.20813400 0.48044000 0.38673500
C -0.64963300 -0.59548800 -2.33127600
C -1.90133100 -1.18108900 -2.37041000
C -3.54887900 -0.40732200 -0.50088200
H 0.24730300 -1.17527800 -2.11737600
H -0.47810100 0.32951400 -2.88347300
H -2.04953800 -2.23742700 -2.14937400
H -2.69775100 -0.71673000 -2.94963900
C -4.65974400 -1.17420000 -1.09201000
H -4.39402400 -2.22818600 -1.24755200
H -5.55518700 -1.13059100 -0.45920700
H -4.92913700 -0.76890500 -2.07721500
C -3.80718000 1.33952200 1.38198300
H -4.71815600 1.84747900 1.05203300
C -3.41269600 1.49127600 2.65041700
H -2.53306900 0.98718400 3.04825300
H -3.98623400 2.09647100 3.34784300
Fe 2.56204400 -0.04200400 0.02437800
P -0.34597100 1.62470500 -0.19919600
P -0.50687600 -1.46456600 0.59789500
C 1.30205900 -1.49131800 0.64427400
C 2.17488100 -1.99171400 -0.38037400
C 3.51447400 -1.85416300 0.07427200
H 4.40321400 -2.10753000 -0.49340000
C 3.48820700 -1.26849900 1.37005000
C 2.13149800 -1.04116500 1.72981000
H 1.78921700 -0.58923800 2.65615700
C 2.45645800 1.93713000 0.45725300

C 1.44695900 1.55275600 -0.49095700	C -2.36022600 -1.28571500 -1.95786400
C 2.12966400 1.02846900 -1.64042600	C -3.46272400 -0.63553600 -0.57327300
C 3.52799500 1.08192600 -1.39068800	H -0.21317400 -1.61534400 -2.19918800
C 3.72863400 1.63638900 -0.09736100	H -0.78366800 0.02550500 -2.73692600
H 4.68313300 1.76352000 0.40200800	H -2.50224000 -2.36060600 -1.82765700
H 4.35418600 -0.99735200 1.96419600	H -3.05380100 -0.86531700 -2.69306600
H 1.87667900 -2.39725700 -1.34305500	C -4.64677200 -1.53490500 -0.63545300
Co -1.70739000 -0.11532000 -0.57878500	H -4.37984800 -2.57912400 -0.42412800
H 2.28568900 2.33784100 1.45077300	H -5.39165400 -1.20637800 0.09928400
H 4.30342100 0.71512400 -2.05454800	H -5.12034800 -1.51396900 -1.62647500
C -0.93249700 -3.19538200 0.18028700	C -4.05691600 1.55797300 0.63180400
H -0.45589600 -3.87666400 0.89705100	H -4.76091800 2.10462200 -0.00228500
H -2.02164800 -3.32197400 0.22362500	C -4.01963800 1.81242900 1.94571600
H -0.58434000 -3.45272200 -0.82664500	H -3.35166400 1.26214900 2.60988200
C -0.97762000 -1.35506600 2.35942900	H -4.68808900 2.53675500 2.40403400
H -2.06251300 -1.49118700 2.44123700	Fe 2.60169300 0.05705800 -0.04599100
H -0.46318200 -2.13181400 2.94023700	P -0.41368300 1.63246800 -0.01733200
H -0.72152000 -0.37121600 2.76900800	P -0.29748500 -1.58891500 0.59620600
H 1.67231300 0.63243300 -2.54003400	C 1.50427400 -1.51770000 0.58256600
C -0.40719200 2.46249000 1.42568200	C 2.34900900 -1.89813800 -0.51207300
H 0.15073200 3.40666700 1.39200600	C 3.69828900 -1.66738100 -0.12771400
H -1.45233800 2.67509400 1.67550200	H 4.56944900 -1.81815300 -0.75607500
H 0.01664200 1.82710800 2.21414000	C 3.70181400 -1.13841600 1.19273100
C -0.93262400 2.95929400 -1.31496600	C 2.35470900 -1.04184100 1.63846300
H -1.97797200 3.18978300 -1.07259600	H 2.02979100 -0.65673500 2.60057300
H -0.32136100 3.86224700 -1.18939300	C 2.43407400 2.02353300 0.44563800
H -0.88129300 2.64151400 -2.36274000	C 1.35624200 1.60120900 -0.40211000
TSA1-dppf	C 1.93606900 1.12869500 -1.62596400
C -3.25358800 0.55355200 -0.02096800	C 3.34910700 1.25457900 -1.52367300
C -0.97778200 -0.84145900 -2.09767600	C 3.65515400 1.80042300 -0.24597600

H 4.64961200 1.96847300 0.15350400	H -2.89119200 1.24996000 -2.97591700
H 4.57700600 -0.81895600 1.74816000	H -2.53516200 2.40722500 -1.71926500
H 2.02158300 -2.27029400 -1.47870100	C -5.22690100 1.02497500 -1.53249800
Co -1.58970800 -0.17060700 -0.39003800	H -5.40452400 0.55627600 -2.51023700
H 2.34286000 2.40056700 1.45930900	H -5.95084000 0.61972500 -0.81876300
H 4.07034300 0.93655000 -2.26890800	H -5.42517300 2.09900100 -1.65818600
C -0.65720700 -3.34690600 0.22055900	C -3.43780700 -0.68737600 1.11007400
H -0.07799600 -3.99956000 0.88581500	H -3.55158300 -0.24645700 2.10499800
H -1.72731200 -3.53854000 0.37423300	C -2.84970200 -1.96009100 0.96163700
H -0.39985900 -3.59502300 -0.81581800	H -3.05463300 -2.51811200 0.04216100
C -0.75095200 -1.47601900 2.36639200	H -2.61178300 -2.56335500 1.83760100
H -1.82703300 -1.66973200 2.45798100	Fe 2.47253900 0.40530600 -0.29475800
H -0.19655700 -2.21202000 2.96358600	P -0.64316500 1.13749000 0.98199400
H -0.55566800 -0.47044700 2.75627900	P 0.11903100 -1.93916600 0.15441300
H 1.39643200 0.71183500 -2.47117000	C 1.69669600 -1.42770300 -0.57235500
C -0.44671200 2.34237200 1.66797000	C 1.85174800 -0.75738700 -1.83140000
H 0.04519000 3.32330800 1.68747900	C 3.22870600 -0.44453500 -1.99809300
H -1.49244000 2.46728200 1.97443400	H 3.65854500 0.10568800 -2.82817600
H 0.05787800 1.67797900 2.38075600	C 3.93336300 -0.91662100 -0.85630600
C -1.01653000 3.02882100 -1.04319300	C 2.99911100 -1.53142700 0.02006600
H -2.04347400 3.27856100 -0.75064500	H 3.23067800 -1.95166400 0.99356800
H -0.37318600 3.90859400 -0.91445000	C 2.20851500 1.26760200 1.51571500
H -1.01377900 2.74018400 -2.10151700	C 1.09148000 1.53142600 0.64875100
A2-dppf	C 1.59994900 2.22541100 -0.50060700
C -3.43539800 0.10901400 -0.02421200	C 3.00269900 2.38386900 -0.33771700
C -1.42040400 0.52529100 -1.55374500	C 3.37777700 1.79337400 0.90024600
C -2.66570400 1.32705700 -1.89713800	H 4.38750200 1.71392600 1.28835200
C -3.81704600 0.80428900 -1.08896900	H 4.99240900 -0.78525000 -0.66167000
H -1.42838900 -0.44959900 -2.08515300	H 1.05321400 -0.50189200 -2.52172700
H -0.48041000 1.03656900 -1.79585600	Co -1.62297100 -0.52588100 0.10753400

H 2.17460100 0.74196700 2.46559000
H 3.67600700 2.83139300 -1.06073400
C -0.28119800 -3.45745800 -0.80244700
H 0.60396200 -4.10091600 -0.88388600
H -1.08689400 -4.01498600 -0.30970400
H -0.61162700 -3.18610700 -1.81329900
C 0.64516100 -2.63365400 1.76846500
H -0.23047700 -3.01370600 2.30682700
H 1.35541900 -3.45802700 1.62526500
H 1.12421800 -1.86181300 2.38360600
H 1.02439100 2.55776700 -1.35965500
C -0.68241300 0.83189700 2.79189200
H -0.10580500 1.60135600 3.32197700
H -1.72297500 0.87887900 3.13355300
H -0.28648000 -0.15934800 3.03989300
C -1.43835700 2.78124800 0.87751500
H -2.50804600 2.69633300 1.10266900
H -0.96149100 3.45567800 1.60003000
H -1.31893300 3.21023200 -0.12292200

TSE3-1

C -2.35937400 -0.88096600 -0.60667400
C -1.65333800 -0.63306600 -1.98220400
C -1.87058000 0.12511600 0.52760800
C -0.16413600 -0.89475100 -1.91833100
H -2.15426000 -1.28021000 -2.72430800
H 0.45225000 -0.28473200 -2.59256500
H 0.09291000 -1.95527000 -2.04075000
C 3.26505000 -0.41323800 -0.40299800
H 4.14387100 -0.94990100 -0.01362400
H 3.29523600 -0.51048000 -1.50016600

C 3.31100200 1.05856500 -0.00289600
H 3.18427800 1.16455200 1.08734400
H 4.31882000 1.44097000 -0.21406800
C 2.30326200 1.92900500 -0.74576000
H 2.56276300 2.99392200 -0.64051800
H 2.33735300 1.70635300 -1.82468400
P 1.76843600 -1.31260100 0.18036200
P 0.53840700 1.76115000 -0.22494100
C 2.04605900 -1.47881600 1.98939900
H 1.35547900 -2.22543700 2.40035600
H 3.07460700 -1.80318000 2.19946000
H 1.85619900 -0.52695300 2.50044700
C 2.08979600 -3.00978500 -0.43180500
H 3.03995000 -3.38868500 -0.03296600
H 1.28297200 -3.68546400 -0.12244200
H 2.14420800 -3.01636100 -1.52698800
C -0.25345800 2.85657500 -1.46354200
H -1.29815600 3.06064700 -1.20719800
H 0.28311300 3.81389600 -1.50964600
H -0.22029800 2.38885900 -2.45525300
C 0.43775800 2.73900200 1.31840700
H 0.86290800 3.74195700 1.18021600
H -0.61424500 2.83477400 1.61494900
H 0.96885200 2.23171400 2.13324700
Co -0.13314900 -0.27928800 -0.10129700
C -2.48661800 -2.35929000 -0.29440400
H -2.95197800 -2.52252200 0.68682100
H -3.12455800 -2.84491100 -1.04725100
H -1.51845400 -2.88244500 -0.29856400
C -3.67956100 -0.06784200 -0.54526000

C -3.01374300 1.08034200 0.23331000
H -4.41880600 -0.59113500 0.07353700
H -4.12544600 0.17014900 -1.52053200
H -3.56540900 1.45798800 1.10204300
H -2.75004100 1.93208800 -0.40419100
C -1.60048600 -0.36375400 1.87999100
H -1.17554200 -1.37082200 1.97031400
C -1.81457000 0.32654600 3.01482600
H -1.54678700 -0.07867200 3.98754800
H -2.29826000 1.30359500 3.01182300
H -1.84351900 0.40638600 -2.28667200

E3-1

C -3.09486400 -0.19057200 -0.51725600
C -2.29304900 0.58792100 -1.57000000
C -2.08976600 -0.59191800 0.55102600
C -0.86670900 0.05951700 -1.59444400
H -2.75123500 0.51869600 -2.57214100
H -0.21534100 0.63921100 -2.26737200
H -0.83075700 -0.99817300 -1.91651800
C 3.10705100 -0.13448000 -1.16996500
H 4.07456400 -0.65386900 -1.24112800
H 2.66331400 -0.14646500 -2.17890200
C 3.29298400 1.30215300 -0.69572500
H 3.64122500 1.32156400 0.34971800
H 4.09859000 1.76935100 -1.27784200
C 2.03698300 2.15180500 -0.84921100
H 2.24772300 3.19914200 -0.58464200
H 1.70929300 2.15747500 -1.90099400
P 2.00334400 -1.13298800 -0.08501500
P 0.58466400 1.63991500 0.16470000

C 3.10282000 -1.56479800 1.31812500
H 2.58989400 -2.23822600 2.01404000
H 4.01074200 -2.06131100 0.95056400
H 3.39992900 -0.66746800 1.87378900
C 1.89473000 -2.70122500 -1.02899600
H 2.89742600 -3.05346300 -1.30692000
H 1.39915500 -3.47868100 -0.43664200
H 1.31222100 -2.54143200 -1.94488600
C -0.52432100 3.06640500 -0.15177800
H -1.47567400 2.97007200 0.38347800
H -0.02591400 3.98413000 0.18760100
H -0.73158500 3.16391600 -1.22378400
C 1.10646300 1.95224500 1.89974600
H 1.58039800 2.93962600 1.99096300
H 0.22648900 1.92701900 2.55501000
H 1.80615700 1.18496500 2.25001300
Co -0.05571300 -0.39643000 0.17017700
C -3.92856300 -1.29922400 -1.13016400
H -4.36979200 -1.94652800 -0.35992200
H -4.74971800 -0.87780500 -1.72508100
H -3.33163000 -1.93159100 -1.80427900
C -3.79587900 0.68017100 0.56307400
C -2.63173600 0.41471800 1.55558500
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C -1.46787300 -1.83787000 0.69831300
H -1.64205300 -2.60565400 -0.06288400
C -0.33561100 -1.93702200 1.51274800

H 0.23115400 -2.86491100 1.57574500
H -0.23653500 -1.26455200 2.37660000
H -2.29640600 1.65710900 -1.32105300
F1
C -3.62313300 -0.04920600 -0.03788300
C -0.29772900 0.63519200 -1.99965700
C -2.54278200 0.34740000 0.69491000
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H -0.15338300 -1.47764400 -2.32569700
H -1.79904800 -0.91429800 -1.73815200
C 2.40679600 -1.70629700 -0.87321100
H 2.89752700 -2.68662200 -0.76445400
H 2.11814000 -1.61605800 -1.93160200
C 3.38784200 -0.59365100 -0.49300600
H 3.59800700 -0.62596200 0.58803100
H 4.34835300 -0.82551900 -0.97363000
C 2.99051800 0.82204400 -0.91066000
H 3.84663600 1.50085600 -0.77320200
H 2.74711400 0.84327300 -1.98375000
P 0.86542600 -1.77522900 0.14063300
P 1.55610000 1.55450600 0.00781400
C 1.50399800 -2.18070700 1.81440400
H 0.67260300 -2.41013700 2.49236900
H 2.15081600 -3.06650100 1.75486000
H 2.08048000 -1.35473300 2.24472200
C 0.10130100 -3.38367800 -0.29772400
H 0.80677900 -4.20336400 -0.10719700
H -0.78892900 -3.54257600 0.32411900
H -0.20486900 -3.41870100 -1.34769400

C 1.41894500 3.21914900 -0.75437800
H 0.68252400 3.81397400 -0.19940900
H 2.38338800 3.74349200 -0.72585700
H 1.08579400 3.14849200 -1.79588700
C 2.33656200 1.98338000 1.61515300
H 3.23560100 2.59333200 1.45537600
H 1.63618500 2.55465900 2.23590700
H 2.61831200 1.08116600 2.17120600
Co -0.13913900 0.11127400 -0.05579500
C -4.17702400 -1.35872800 -0.43320500
H -5.15919400 -1.52779800 0.03170100
H -4.34282800 -1.40879700 -1.51952000
H -3.51763300 -2.18739100 -0.14323200
C -4.08647700 1.35707700 -0.29386500
C -2.88221000 1.82575900 0.56936400
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H -4.05911500 1.66909500 -1.34889500
H -3.16453500 2.31609400 1.51049700
H -2.15574900 2.46808500 0.05025700
C -1.47583600 -0.34958700 1.37013500
H -1.60556700 -1.41040800 1.59810300
C -0.43567100 0.42160900 1.92998600
H 0.27323500 -0.02350500 2.62572500
H -0.61264300 1.48686800 2.09279800
H 0.60624000 0.85579300 -2.56823300
TSF1
C 2.69400100 0.61442000 -0.24803100
C 1.47787300 -0.02916900 -1.79272600
C 2.10920600 0.12756500 0.96166800
C 0.07210900 0.23501000 -1.91107800

H 2.13340800 0.63314000 -2.35980000
H -0.55183100 -0.56868800 -2.30358900
H -0.19782600 1.19963500 -2.34522000
C -2.85830700 0.91942400 -0.65637900
H -3.66814800 1.64014000 -0.46322200
H -2.75714100 0.85292500 -1.75051800
C -3.22633500 -0.45006700 -0.07337500
H -3.10583700 -0.44625900 1.02378100
H -4.30125300 -0.60475400 -0.23995600
C -2.48485700 -1.64370000 -0.67793200
H -3.03771100 -2.57243300 -0.46915200
H -2.46071100 -1.54984900 -1.77458400
P -1.30350600 1.65631600 0.02058400
P -0.74041700 -1.91026900 -0.08951100
C -1.92939200 2.33126600 1.61944200
H -1.12162900 2.77059500 2.21734400
H -2.66900700 3.11626600 1.41473800
H -2.42114200 1.55594900 2.21779400
C -1.15877500 3.23794700 -0.91056400
H -2.13325700 3.74196800 -0.96357300
H -0.45903700 3.89768400 -0.38140300
H -0.78869300 3.09548600 -1.93144300
C -0.16839000 -3.17376200 -1.30605200
H 0.76163600 -3.63474200 -0.94911100
H -0.92018400 -3.96521200 -1.42903600
H 0.02574700 -2.72999100 -2.29030000
C -1.03378300 -3.00444000 1.36364900
H -1.58904500 -3.90247600 1.06283700
H -0.08165600 -3.32311800 1.80794900
H -1.61198200 -2.47954800 2.13446600

Co 0.34536500 0.13193400 0.06333500
C 2.98747500 2.03679300 -0.60882300
H 3.70350600 2.45312100 0.11373700
H 3.44297400 2.12333200 -1.60311700
H 2.08234400 2.65730700 -0.58747500
C 3.69801800 -0.53846900 -0.23785000
C 2.92888600 -1.15147700 0.96510900
H 4.68868200 -0.16747200 0.05747200
H 3.81581600 -1.13951800 -1.14643800
H 3.53873700 -1.30458700 1.86410400
H 2.37721000 -2.07709900 0.75303300
C 1.12825500 0.77679200 1.76300900
H 1.08771800 1.85997300 1.87819100
C 0.12214400 -0.10816700 2.17226600
H -0.77506500 0.24858200 2.67472600
H 0.39753300 -1.13653300 2.39713100
H 1.78106900 -1.07653100 -1.83949600
TSS1
C 0.68607700 0.47510700 0.02441800
C -0.52270900 0.92308400 -0.21136100
C -1.75539700 0.30978500 -0.52449300
C -2.72745000 -0.00980900 0.35514500
H -2.63576800 0.23162800 1.41297100
C 2.01375600 1.16591700 0.08948100
H 1.85484300 2.20432000 0.40213300
H 2.69982300 0.69078300 0.80428200
H 2.51646100 1.19001000 -0.88643200
H -1.90508600 0.07207300 -1.58407400
H -3.62979700 -0.52456400 0.03591000
C 0.69204000 -1.07624600 0.70281600

C 1.17010800 -1.49764700 -0.53732400
H -0.33534600 -1.32047200 0.98386700
H 1.38357200 -1.03492400 1.54720400
H 0.48079300 -1.75653200 -1.33712400
H 2.23196300 -1.49346100 -0.77082900

S1

C 0.69571600 -0.22851200 -0.02722600
C -0.43621000 -0.89430000 0.53201400
C -1.72462400 -0.30569800 0.53460500
C -2.40876300 -0.01986700 -0.60181200
H -1.93084900 -0.07792900 -1.57930600
C 1.93275600 -1.04271900 -0.33330000
H 1.79323900 -1.62669200 -1.25203900
H 2.81661300 -0.40559000 -0.47707800
H 2.13245700 -1.74776700 0.48231700
H -2.28114700 -0.33141400 1.47724400
H -3.48997600 0.10397000 -0.59415000
C 0.62251700 1.17813600 -0.63871500
C 0.94013100 1.07340800 0.79110700
H -0.35745600 1.56016600 -0.91334700
H 1.42753500 1.41483000 -1.33253000
H 0.18966600 1.37035200 1.52076200
H 1.97078300 1.17739400 1.12808400

TSS2

C -0.76053700 0.26665500 -0.35967200
C 0.31651400 -0.49762300 -0.82768300
C 1.65659000 -0.03760600 -0.59114100
C 2.40446000 -0.14657200 0.52088000
H 2.00934500 -0.58751500 1.43671300
C -0.70799800 1.64959200 0.23761200

H -0.98699600 2.38119400 -0.53176100
H -1.41803200 1.76681100 1.06704500
H 0.30264600 1.88613400 0.59084800
H 2.12649900 0.36746100 -1.49505800
H 3.45244200 0.14253500 0.53048400

C -1.98407200 -0.55593100 -0.16444800
C -0.80479000 -1.01010600 0.65408200
H -2.26015900 -1.23422500 -0.96863700
H -2.81416000 -0.08958900 0.36452700
H -0.43423200 -2.02076200 0.51754500
H -0.69835100 -0.62249800 1.67051600

TSS3

C -0.64956300 0.50943600 -0.00359700
C 0.57015000 0.14204600 -0.19998300
C 1.88605700 -0.17410100 -0.45142800
C 2.91063700 -0.07918500 0.44552600
H 2.74428500 0.28033000 1.45843500
H 2.11626900 -0.53854200 -1.45802900
H 3.92270500 -0.36244800 0.17018800
C -1.63369000 -0.58396000 0.52174000
C -1.44586500 -1.79781200 -0.24357300
H -2.70068700 -0.28074000 0.56742800
H -1.32516900 -0.63924900 1.58319700
H -2.16901900 -2.61006300 -0.19945400
H -0.60243800 -1.90187000 -0.91726200
C -1.25582700 1.87796100 -0.16690700
H -1.69801000 2.22028200 0.78020600
H -0.51196000 2.61363100 -0.48706400
H -2.06736800 1.85234700 -0.90831200

MECP1

C -0.39760315 0.32197017 0.04693399
H 0.21536697 0.53117017 0.93643893
H -0.59582249 -0.76090290 0.03851120
C 0.33694345 0.73181985 -1.22727746
H 0.53241733 1.81608151 -1.22727752
H 1.32770903 0.25869225 -1.22727769
C -0.39760333 0.32197059 -2.50148922
H 0.21536640 0.53116991 -3.39099372
H -0.59582317 -0.76090304 -2.49306588
P -2.01927624 1.15925764 0.27258211
P -2.01927642 1.15925788 -2.72713706
C -1.59155640 2.86725402 0.77107345
H -2.49936761 3.39921506 1.07765765
H -0.88657199 2.85479274 1.61324677
H -1.14091820 3.42400548 -0.05788101
C -2.68145726 0.41826452 1.81384540
H -1.94930032 0.52550922 2.62538936
H -3.60666671 0.92126795 2.11966073
H -2.89100489 -0.64770069 1.66877009
C -2.68145665 0.41826592 -4.26840136
H -3.60666645 0.92126717 -4.57421597
H -1.94930052 0.52550894 -5.07994373
H -2.89100464 -0.64770197 -4.12332468
C -1.59155789 2.86725484 -3.22562805
H -0.88657126 2.85479270 -4.06780263
H -2.49936669 3.39921493 -3.53221280
H -1.14091818 3.42400551 -2.39667438
Co -3.43228481 0.91900831 -1.22727745

MECP2

C -2.43548307 -0.23143344 0.13414620

C -0.72585211 -0.76974517 -1.65012330
C -2.02939443 -1.56485583 -1.78278095
C -2.98212396 -1.08075271 -0.73314603
H 0.15260839 -1.34157178 -1.98394983
H -0.78189382 0.13787615 -2.26920905
H -1.84543697 -2.63502601 -1.58130478
H -2.46496828 -1.53402609 -2.79539419
C -4.37228827 -1.61734847 -0.64233387
H -4.35608773 -2.71383539 -0.57008879
H -4.91655933 -1.21587703 0.21821646
H -4.93338508 -1.37025349 -1.55461193
C -2.20586591 0.45403427 1.32186287
H -2.42124842 1.52438348 1.40082829
C -1.29819292 -0.14635565 2.21864844
H -1.32718042 -1.23082480 2.35798559
H -0.87610082 0.43222918 3.04082861
C 2.80826796 -0.58980441 -0.53522756
H 3.72275113 -1.12816027 -0.24377129
H 2.50915787 -0.98272862 -1.51872278
C 3.08486074 0.91139432 -0.63190722
H 3.31165015 1.32366775 0.36471448
H 4.00477761 1.05222819 -1.21543430
C 1.97500858 1.72334001 -1.30152342
H 2.32476441 2.74672181 -1.50780928
H 1.71088474 1.27751516 -2.27386178
P 1.48661762 -1.04319937 0.66324587
P 0.41524968 1.85476474 -0.33652138
C 2.29212468 -0.85935648 2.29753582
H 1.61808711 -1.24462149 3.07246615
H 3.23467151 -1.42135753 2.33538792

H 2.49714728 0.19343908 2.52514532
C 1.32912623 -2.85911454 0.49409759
H 2.29998859 -3.35437585 0.62623371
H 0.63596332 -3.23510196 1.25734665
H 0.92611869 -3.11712524 -0.49229314
C -0.64508989 2.94795547 -1.34556010
H -1.58564786 3.13556490 -0.81325050
H -0.14882255 3.90771162 -1.54115346
H -0.88552569 2.47087179 -2.30201036
C 0.83714281 2.89504339 1.11159330
H 1.34416171 3.81884935 0.80125687
H -0.08516866 3.16337772 1.64170159
H 1.47993502 2.35239358 1.81420129
Co -0.49951754 -0.12886411 0.25712650

MECP3

C 2.85910168 -0.60048797 0.36707062
C 1.92622076 -1.10212408 1.47232684
C 2.12183791 0.35915537 -0.59170417
C 0.86274800 -0.05866717 1.75050711
H 2.50744647 -1.36707155 2.37493972
H 1.45008152 -2.04684588 1.14601646
H 1.29211588 0.91578171 2.02240015
H 0.12546273 -0.35265670 2.50753002
C -2.49440305 2.05145289 -0.86524337
H -2.92310403 3.06445823 -0.81072279
H -2.22215701 1.88195045 -1.92041935
C -3.53443431 1.02395089 -0.41930718
H -3.76097825 1.15163070 0.65131878
H -4.47423227 1.25696143 -0.93816854
C -3.18922043 -0.43544878 -0.71480471

H -4.07083452 -1.07224233 -0.54187005
H -2.91496478 -0.55549843 -1.77561809
P -0.91326549 2.06782064 0.09438638
P -1.79829497 -1.13252087 0.27908439
C -1.39983860 2.65042821 1.75904239
H -0.49776073 2.82904558 2.35641786
H -1.96914307 3.58720053 1.69036070
H -2.00566497 1.90300372 2.28307980
C -0.06741212 3.54049482 -0.59360757
H -0.73866610 4.40946945 -0.57427096
H 0.82172969 3.77859964 0.00142274
H 0.24772486 3.35815140 -1.62804257
C -1.81167704 -2.89972894 -0.20172896
H -1.01837490 -3.43684173 0.33348256
H -2.77679530 -3.36259143 0.04373269
H -1.63187774 -3.00085403 -1.27827501
C -2.47285024 -1.21477023 1.98198020
H -3.47970544 -1.65412817 1.97348021
H -1.82199712 -1.84913282 2.59665748
H -2.51899266 -0.22650977 2.45294383
Co 0.07802769 0.01387025 -0.08322909
C 3.63602316 -1.72004483 -0.30151575
H 4.27614414 -1.33744817 -1.10736095
H 4.28360903 -2.21693914 0.43416643
H 2.97632055 -2.48643061 -0.73090105
C 3.74772677 0.60866940 0.77746270
C 2.98040625 1.53271079 -0.19398303
H 4.80610248 0.47250828 0.52704468
H 3.67788914 0.89064043 1.83512732
H 3.57557752 1.96238718 -1.01074128

H 2.43896240 2.35487029 0.29372457
C 1.33706690 0.13033779 -1.72585047
C 0.53297322 -1.02713660 -1.80947782
H 1.13706201 0.97017898 -2.39872972
H 0.89665473 -1.96874769 -1.38941879
H -0.18212839 -1.13501415 -2.62520325

MECP4

C 3.25453201 0.39961131 -0.20631637
C 2.45800247 1.21125712 -1.23149241
C 2.32202727 -0.54040493 0.58843136
C 1.23864682 0.42120202 -1.66306486
H 3.10056957 1.49605172 -2.08473237
H 2.14493321 2.16893747 -0.77120793
H 1.49970629 -0.56762050 -2.06451841
H 0.59291891 0.94117551 -2.38042009
C -2.58623730 -1.33774659 0.49156239
H -3.18668983 -2.22681326 0.24156203
H -2.39094980 -1.38479726 1.57572786
C -3.36668563 -0.06885542 0.15445903
H -3.50983667 0.01408620 -0.93513875
H -4.37870173 -0.18186400 0.56658960
C -2.77563358 1.22538058 0.71173784
H -3.50590568 2.04427274 0.61983382
H -2.55867695 1.11393465 1.78661237
P -0.94854006 -1.53057074 -0.34552083
P -1.21051844 1.78391725 -0.08961721
C -1.36936022 -1.81120800 -2.10351449
H -0.47537581 -2.14960586 -2.64114767
H -2.14924109 -2.57808195 -2.20068202
H -1.71432782 -0.88678203 -2.58002102

C -0.45291342 -3.20121162 0.22197572
H -1.23983575 -3.93281440 -0.00593776
H 0.47231610 -3.52066000 -0.27079286
H -0.28288136 -3.19417404 1.30540759
C -0.94302121 3.42381447 0.68088004
H -0.03576620 3.88618552 0.27263649
H -1.79509266 4.08812318 0.48379943
H -0.81791139 3.31735558 1.76470110
C -1.72991625 2.25783260 -1.78264400
H -2.63234635 2.88280916 -1.74477490
H -0.92702456 2.83568753 -2.25754250
H -1.92844705 1.38183430 -2.41065019
Co 0.39777791 0.25484496 0.13831124
C 4.19320892 1.25740628 0.62307722
H 4.72255813 0.66065663 1.37781483
H 4.94769209 1.72198845 -0.02750480
H 3.66547459 2.06761876 1.14526941
C 3.92316234 -0.87837920 -0.78978351
C 2.94983162 -1.77956110 0.00251557
H 4.97312143 -0.98965137 -0.49675950
H 3.85974579 -0.97167349 -1.88095609
H 3.41023442 -2.45685156 0.73389823
H 2.27645991 -2.37602568 -0.62942526
C 1.56339003 -0.34401185 1.74632950
C 0.98575425 0.91650665 2.01021056
H 1.19404443 -1.22420288 2.28138350
H 1.52557470 1.82801442 1.73972212
H 0.28091199 1.02915334 2.83402423

MECP5

C -2.87489337 -0.89036389 -0.32578059

C -1.60485104 -1.39069728 -0.97982847
C -2.42071807 0.36345152 0.42617716
C -0.86698887 -0.64876522 -1.88023149
H -1.31872617 -2.42826064 -0.77971946
H -0.87678540 -1.43296317 1.92342387
H -1.24780569 0.28265945 -2.30327479
H -0.06131366 -1.10891145 -2.45202942
C 3.00455318 -0.65639158 -1.15572261
H 3.86400762 -1.34164801 -1.09715670
H 2.63386459 -0.70043834 -2.19288277
C 3.44012896 0.76802294 -0.81965737
H 3.75620441 0.83295935 0.23428054
H 4.34214430 0.99511723 -1.40394812
C 2.39180101 1.83441882 -1.12533161
H 2.84044009 2.83834606 -1.07005675
H 2.01710593 1.71054374 -2.15466193
P 1.67421072 -1.34885914 -0.08201818
P 0.91800153 1.81494171 -0.01502615
C 2.51508998 -1.60536399 1.53117191
H 1.87777880 -2.21822574 2.18112494
H 3.47496093 -2.12245305 1.39740603
H 2.69216628 -0.65023778 2.03992984
C 1.55506651 -3.06937554 -0.71052324
H 2.54472489 -3.54518524 -0.72306130
H 0.89280691 -3.66024145 -0.06581813
H 1.14907380 -3.08720994 -1.72938570
C -0.02729346 3.24745678 -0.66725268
H -0.91138711 3.44169011 -0.04782137
H 0.59735884 4.15107388 -0.68145721
H -0.36118610 3.03634763 -1.69123710

C 1.58713160 2.49777166 1.55627723
H 2.25059704 1.77632282 2.04838903
H 2.14491471 3.42716625 1.37767232
H 0.76224618 2.71596142 2.24633828
Co -0.20829655 -0.14371960 0.07770792
C -3.61233196 -1.96951394 0.43911048
H -4.42975822 -1.53977636 1.03136464
H -4.04838745 -2.69879859 -0.25676893
H -2.95035842 -2.51686366 1.12409903
C -3.75179242 0.03867533 -1.21336098
C -3.14926783 1.28590139 -0.52259749
H -4.82086485 -0.09263480 -1.01046720
H -3.58965052 -0.04646862 -2.29328194
H -3.86625699 1.96252344 -0.04037302
H -2.50015173 1.89750708 -1.16438362
C -1.64139783 0.56844165 1.52346718
C -1.17206135 -0.51036967 2.46022885
H -1.50809739 1.60091178 1.85938457
H -1.96829002 -0.81347656 3.15649219
H -0.31559374 -0.17543957 3.05878778
Z
C 0.64824000 0.06874400 0.45272400
C 1.08760700 1.35973900 -0.17718900
C -0.38919100 -0.70523100 -0.35512800
C 0.52191600 1.96166000 -1.21971900
H 1.96880100 1.81112100 0.29352200
H -2.03651800 1.13081300 0.69348200
H -0.35565900 1.53866400 -1.71013200
H 0.91139500 2.89597800 -1.61958200
C 0.39004100 0.25935700 1.94173300

H 0.02391400 -0.67271200 2.39362100
H 1.32138800 0.54367900 2.45402700
H -0.34854700 1.04739800 2.13755500
C 1.64665900 -1.08722600 0.12133300
C 0.66138300 -1.61653700 -0.94132800
H 1.75722700 -1.77373600 0.97122900
H 2.64286000 -0.78507700 -0.22510000
H 0.45419200 -2.69419800 -0.94827300
H 0.95158800 -1.31555300 -1.95871000
C -1.71742400 -0.68464500 -0.42426900
C -2.60822000 0.30216900 0.25864400
H -2.20848300 -1.44651000 -1.03710800
H -3.19789600 -0.16323900 1.06251100
H -3.33031300 0.73518800 -0.44785100
E
C 0.73306900 -0.23190600 0.25453600
C 1.55432700 0.32552500 -0.87075000
C -0.75835800 -0.07692800 -0.04687700
C 2.57070600 1.17896200 -0.77330000
H 1.25195000 -0.02097900 -1.86517600
H 3.10013800 1.53052900 -1.65676800
H 2.92071100 1.56441000 0.18363900
C 1.17821100 0.22796400 1.62748600
H 0.52871200 -0.20218200 2.40079500
H 2.21266100 -0.07955300 1.83572500
H 1.12591900 1.32185700 1.71945500
C 0.51533300 -1.77033700 0.08514600
C -0.88951700 -1.50982900 -0.50471100
H 0.47438700 -2.27540600 1.05853800
H 1.23654100 -2.29467300 -0.55344700

H -1.72168600 -2.09555700 -0.09172700
H -0.92050500 -1.61431900 -1.59975600
C -1.60449600 0.92869900 0.14859000
H -1.20613700 1.86589700 0.54940700
C -3.06798200 0.87697100 -0.14071700
H -3.35685400 1.62640800 -0.89172900
H -3.66749600 1.08697100 0.75672300
H -3.36609500 -0.10813200 -0.52209100
Z4 (open-shell singlet)
C -2.87041500 -0.37704200 -0.62205600
C -1.67200400 -0.91116700 -1.36677800
C -2.38646300 0.06654700 0.76881900
C -0.74467900 -0.19215900 -2.05170100
H -1.55008400 -2.00087100 -1.33898100
H -1.45854000 -2.53960100 0.93823600
H -0.86573200 0.86890600 -2.26549500
H 0.05282800 -0.69756400 -2.59488300
C 3.13735100 -0.55093100 -1.02655600
H 4.03142600 -1.19303500 -1.00944700
H 2.81612700 -0.48438300 -2.07851300
C 3.46500500 0.84104600 -0.48999200
H 3.66738000 0.79673200 0.59304600
H 4.41079300 1.16786200 -0.94353600
C 2.40664700 1.89893900 -0.79030300
H 2.82220100 2.90433600 -0.61981200
H 2.12757300 1.85511700 -1.85656800
P 1.80582300 -1.41771500 -0.09358100
P 0.82530200 1.79873900 0.16890300
C 2.65759500 -1.91020000 1.45930100
H 2.03207500 -2.62169300 2.01247800

H 3.62179100 -2.39104900 1.24492800
H 2.82948900 -1.04177400 2.10609300
C 1.68407700 -3.02488300 -0.97278000
H 2.66447200 -3.51499600 -1.04314100
H 0.99872400 -3.69076200 -0.43262900
H 1.29175000 -2.87981700 -1.98707000
C -0.01148700 3.28533300 -0.52565100
H -0.91277400 3.53822400 0.04354900
H 0.66636100 4.14925700 -0.49499900
H -0.30033300 3.11199700 -1.56993000
C 1.30686100 2.40807900 1.83469700
H 1.92078100 1.66461600 2.35762500
H 1.86223400 3.35417700 1.77802800
H 0.39995100 2.56862900 2.43261100
Co -0.15136700 -0.27453500 0.18256800
C -4.04965700 -1.33476500 -0.63520200
H -4.86239200 -0.95949800 0.00064300
H -4.44207700 -1.44701400 -1.65467800
H -3.76959800 -2.33120600 -0.26746100
C -3.26688700 1.10805800 -0.87172200
C -2.97992600 1.43849300 0.60964400
H -4.30284400 1.24508700 -1.19992100
H -2.61538200 1.63815000 -1.57433100
H -3.89804000 1.54012100 1.20613100
H -2.34353500 2.30219100 0.83853100
C -1.65466400 -0.52218900 1.75123200
C -1.39984200 -1.99930200 1.89335400
H -1.42645700 0.09304200 2.62798900
H -2.15503500 -2.44711300 2.55669300
H -0.42218600 -2.20411900 2.34982100

TSZ4-E (open-shell singlet)

C -2.61106300 -0.39455200 -0.88209000
C -1.40381500 -0.91609100 -1.63095300
C -2.02626100 0.09660500 0.45622000
C -0.44529000 -0.13940000 -2.20463700
H -1.28852800 -2.00449500 -1.67159500
H -3.42905500 -1.56695200 2.30299800
H -0.58628100 0.92959000 -2.35718500
H 0.39537100 -0.58849600 -2.73270400
C 3.23577900 -0.54692500 -0.74467300
H 4.11529600 -1.19788300 -0.62476400
H 3.06396700 -0.44637000 -1.82849200
C 3.49503200 0.82564700 -0.12678000
H 3.54032800 0.74922500 0.97233200
H 4.49662800 1.15788500 -0.43182400
C 2.49211000 1.89769900 -0.54358700
H 2.86795100 2.89664900 -0.27298800
H 2.37720800 1.89495800 -1.64047400
P 1.78398100 -1.42967900 -0.03075500
P 0.79010700 1.74839100 0.16191100
C 2.43119800 -2.02633600 1.58184800
H 1.70668600 -2.71667400 2.03189000
H 3.38737400 -2.55270600 1.45936300
H 2.57339700 -1.18905000 2.27626000
C 1.74473300 -2.97604100 -1.01658900
H 2.72317400 -3.47471600 -1.00606700
H 0.99541000 -3.66129600 -0.60161400
H 1.47274300 -2.76151600 -2.05754600
C 0.01747000 3.22531300 -0.61024700
H -0.99639900 3.38865400 -0.22920300

H 0.61839400 4.11909400 -0.39508100
H -0.03848700 3.10447100 -1.69926500
C 0.99263900 2.29098900 1.90376900
H 1.55309300 1.54152300 2.47672900
H 1.51233900 3.25617200 1.97259200
H 0.00048000 2.38919100 2.36366800
Co -0.16496600 -0.28534600 0.06187900
C -3.71664200 -1.42722700 -0.78003200
H -4.53861300 -1.06901200 -0.14554200
H -4.13476000 -1.64941800 -1.77153600
H -3.33991600 -2.36810100 -0.35212000
C -3.12315400 1.05470900 -1.09541100
C -2.89859200 1.33779200 0.40850100
H -4.15067000 1.13523500 -1.46709100
H -2.47447900 1.65965800 -1.74001900
H -3.82081500 1.20054600 0.99676200
H -2.46152600 2.30078900 0.70566800
C -1.60288700 -0.76555900 1.53133500
C -2.44618000 -1.23702500 2.66508000
H -0.49153200 -0.88213100 1.75568000
H -2.63494600 -0.41425800 3.37555400
H -1.98154300 -2.05448400 3.22703100
Z4-E (open-shell singlet)
C -2.82579300 -0.66206800 -0.68221500
C -1.58759200 -1.19419600 -1.35651500
C -2.41059700 -0.19567300 0.71578000
C -0.68448800 -0.50014700 -2.09477700
H -1.40539400 -2.26457700 -1.19552900
H -1.77915400 -0.64846500 3.79964600
H -0.86389700 0.52328200 -2.42202200

H 0.15501100 -1.01087300 -2.56480800
C 3.19010600 -0.52523100 -0.94265000
H 4.13549200 -1.07569400 -0.81738700
H 2.90890000 -0.62087300 -2.00383900
C 3.37874900 0.94761100 -0.58354100
H 3.54708400 1.05900500 0.50058100
H 4.30990300 1.29403900 -1.05252900
C 2.24934600 1.86914000 -1.04201600
H 2.58783500 2.91678300 -1.01773800
H 1.98839600 1.65039100 -2.09092700
P 1.89793200 -1.39379000 0.04611200
P 0.67546400 1.78515400 -0.07078500
C 2.72541700 -1.65238500 1.66638900
H 2.09524500 -2.28722200 2.30183300
H 3.70216200 -2.13935200 1.54182600
H 2.87060300 -0.69763300 2.18661900
C 1.93112300 -3.08273200 -0.67265300
H 2.95201400 -3.48777700 -0.68843800
H 1.29701400 -3.75268400 -0.07899900
H 1.54441800 -3.06752600 -1.69934200
C -0.26615600 3.13141800 -0.90080100
H -1.22020400 3.31541500 -0.39293700
H 0.31492300 4.06355100 -0.89728500
H -0.47776500 2.86315800 -1.94364700
C 1.13562200 2.59738300 1.51381300
H 1.76121300 1.93621000 2.12597900
H 1.67499000 3.53858000 1.34021700
H 0.22541200 2.81656500 2.08645700
Co -0.13136100 -0.35520600 0.15481900
C -3.97356600 -1.65704500 -0.70437700

H -4.82551200 -1.28367300 -0.12089300
H -4.31674200 -1.83506600 -1.73195300
H -3.66868700 -2.62070700 -0.27281600
C -3.25454800 0.80837800 -0.95739700
C -3.07368900 1.14250800 0.54386300
H -4.26798600 0.91926700 -1.35751200
H -2.56669100 1.36207000 -1.60564000
H -4.03008500 1.18647100 1.08504700
H -2.50171300 2.04060400 0.81299700
C -1.63934300 -0.79874500 1.65488100
C -1.24885800 -0.17808400 2.96033100
H -1.42072600 -1.86950300 1.51915300
H -1.48193000 0.89426000 2.97543300
H -0.17272500 -0.29870700 3.15973700

TSZ4-E (triplet)

C -2.52414800 -0.56281900 -0.85186600
C -1.33738400 -1.06125600 -1.62909500
C -1.95668200 0.20526200 0.43672800
C -0.47379000 -0.27089800 -2.32007000
H -1.13853800 -2.13878800 -1.59115800
H -3.58117500 -0.47774300 2.60323100
H -0.68176500 0.77932400 -2.51859500
H 0.37790000 -0.69890600 -2.84801100
C 3.28116800 -0.53769900 -0.61129000
H 4.16412400 -1.16754000 -0.42280400
H 3.17233800 -0.46630100 -1.70580500
C 3.47729800 0.85404100 -0.01304900
H 3.45344300 0.80526300 1.08837100
H 4.49143400 1.19519500 -0.26159400
C 2.48908700 1.89986000 -0.52145200

H 2.84273000 2.91240100 -0.27205300
H 2.42971900 1.85368000 -1.62175700
P 1.80410500 -1.43405900 0.03254000
P 0.75362000 1.76766200 0.09976600
C 2.34885600 -1.95277200 1.70884700
H 1.60660500 -2.63567600 2.14040200
H 3.31941000 -2.46574600 1.67307100
H 2.43071200 -1.08392800 2.37408300
C 1.88037800 -3.01278600 -0.89947800
H 2.87116000 -3.47718300 -0.80604500
H 1.12816600 -3.71241000 -0.51507000
H 1.67499800 -2.83901100 -1.96313900
C -0.00160400 3.16966500 -0.80997600
H -1.03310600 3.34353200 -0.48616400
H 0.57634700 4.08710500 -0.63558100
H -0.00661200 2.96542300 -1.88778800
C 0.83996800 2.40707600 1.81508900
H 1.38891600 1.70741600 2.45806600
H 1.32779600 3.38993500 1.85717400
H -0.17945200 2.49678800 2.21273700
Co -0.14057300 -0.26484500 -0.00688000
C -3.50788800 -1.66998400 -0.52859200
H -4.31819200 -1.30793900 0.11767700
H -3.96580600 -2.06254600 -1.44722200
H -3.00980800 -2.50398100 -0.01291500
C -3.18686200 0.77643700 -1.24680200
C -2.95247800 1.32071700 0.17238000
H -4.22828200 0.69003200 -1.57753100
H -2.63003600 1.33065900 -2.01146200
H -3.84182500 1.20869500 0.81337700

H -2.60801200 2.35738300 0.28678900
C -1.63358200 -0.40501200 1.70700700
C -2.58946300 -0.93160300 2.72545400
H -0.55283600 -0.55349800 1.96505700
H -2.24734500 -0.73058000 3.74862800
H -2.72063900 -2.02365700 2.64420400

Z4-E (triplet)

C -2.95302500 -0.07213700 -0.66111600
C -1.74443900 -0.27801200 -1.55077000
C -2.34268400 0.18374400 0.72081800
C -0.90411500 0.68630900 -2.02115500
H -1.54399000 -1.32040600 -1.81444200
H -1.16014000 0.94468300 2.97508400
H -1.13578000 1.74957300 -1.93519400
H -0.08904200 0.42734100 -2.69699000
C 2.56987100 -1.59275000 -1.04020400
H 3.11553300 -2.54844800 -1.00085200
H 2.25394200 -1.45550100 -2.08752700
C 3.49135000 -0.44717100 -0.62027100
H 3.70609200 -0.50425100 0.45971900
H 4.46315100 -0.59882000 -1.10985600
C 3.00136400 0.95341300 -0.98803600
H 3.82556500 1.67753600 -0.89078600
H 2.68526300 0.97796300 -2.04359500
P 1.03059400 -1.77827900 -0.03264700
P 1.58756800 1.60186600 0.00943900
C 1.67266300 -2.45043900 1.55499900
H 0.83399000 -2.79992400 2.17101700
H 2.35261100 -3.29603800 1.38365700
H 2.20666300 -1.67867800 2.12316200

C 0.29048800 -3.28345700 -0.78418500
H 0.98409700 -4.13373700 -0.73905100
H -0.63217500 -3.55534600 -0.25470600
H 0.03947300 -3.09684000 -1.83605800
C 1.40761000 3.29522200 -0.67404700
H 0.64508400 3.85123900 -0.11508400
H 2.35615200 3.84595700 -0.61761900
H 1.09458700 3.24267700 -1.72421900
C 2.34933000 1.92047400 1.65089900
H 2.55365200 0.97855900 2.17463500
H 3.28691600 2.48468000 1.55361200
H 1.65316300 2.50064300 2.26921900
Co -0.22814500 0.16966100 0.06466200
C -3.95552700 -1.19807400 -0.79444200
H -4.76837100 -1.08782000 -0.06600100
H -4.39619500 -1.21565900 -1.79990500
H -3.47826900 -2.17417400 -0.62160900
C -3.50164200 1.37801600 -0.61275300
C -2.70214600 1.65825100 0.68344500
H -4.58428200 1.38715000 -0.44341400
H -3.28578400 2.01383400 -1.47830200
H -3.28308100 2.01195500 1.54511000
H -1.85110200 2.34868400 0.55831200
C -1.72234700 -0.62887000 1.61181100
C -1.17249100 -0.15253100 2.92187500
H -1.74744100 -1.70880400 1.43292700
H -0.14550300 -0.51236800 3.08515600
H -1.77284900 -0.52223000 3.76464600

E7 (open-shell singlet)

C -2.83119100 -0.53293400 -0.72673200

C -1.62188500 -0.34695700 -1.61944000	H 1.37344200 3.54055500 1.47114100
C -2.32016500 -0.34119500 0.70230400	H -0.03617500 2.68859300 2.15340300
C -0.67624100 -1.29615900 -1.87093100	H 1.55003600 1.90374100 2.16667200
H -1.52773300 0.61892100 -2.12211400	Co -0.09504200 -0.40229600 0.06099200
H 0.11405300 -1.10609500 -2.59763200	C -3.62953300 -1.79063800 -1.01332600
H -0.79532400 -2.33481300 -1.55145900	H -4.46015500 -1.88640300 -0.30205800
C 3.21991200 -0.23977100 -0.96221700	H -4.04654600 -1.76575800 -2.02835900
H 4.21472100 -0.70095100 -0.86080400	H -3.01267300 -2.69517800 -0.92605600
H 2.93196000 -0.33967000 -2.02149700	C -3.64920100 0.77691500 -0.53711900
C 3.27791500 1.23648300 -0.57236500	C -3.05632300 0.96404200 0.88168400
H 3.44677100 1.34061100 0.51215700	H -4.73173800 0.60917400 -0.54199400
H 4.17087600 1.67243700 -1.04111600	H -3.42366000 1.57407000 -1.25622000
C 2.07098400 2.06703600 -1.00471200	H -3.79340700 0.93871100 1.69568200
H 2.31476400 3.13923600 -0.94327600	H -2.43594400 1.85765100 1.03449100
H 1.83407700 1.86093200 -2.06188300	C -1.55956600 -1.13004200 1.50217000
P 2.03366400 -1.25647500 0.01829900	H -1.35311200 -2.15935900 1.17377400
P 0.50489500 1.80960600 -0.05112600	C -1.16360100 -0.76136200 2.89912200
C 2.85814300 -1.39139700 1.65503500	H -1.39334100 0.29091800 3.11061700
H 2.33834700 -2.14035300 2.26532500	H -0.08709400 -0.91415000 3.06933400
H 3.90689800 -1.69877300 1.54341800	H -1.69083900 -1.37694900 3.64077500
H 2.82394100 -0.43698800 2.19412500	TSE7-Z (open-shell singlet)
C 2.30048000 -2.93179400 -0.67949800	C -2.64965400 -0.10303800 -0.90881800
H 3.35921300 -3.21736700 -0.61923800	C -1.40319300 -0.08430500 -1.75916000
H 1.70518900 -3.66894900 -0.12708100	C -2.00514600 -0.00960500 0.49413600
H 1.98867600 -2.95757200 -1.73064400	C -0.59057900 -1.16932700 -1.93819000
C -0.53587200 3.11748500 -0.81976700	H -1.13217900 0.86358300 -2.23122300
H -1.51248800 3.18783600 -0.32654900	H 0.27375600 -1.09979400 -2.59832600
H -0.03880900 4.09424400 -0.74738800	H -0.91006200 -2.17679000 -1.66562000
H -0.70238800 2.89318100 -1.88091100	C 3.21711200 -0.41362500 -0.90228200
C 0.89217600 2.55921400 1.58262700	H 4.14393300 -1.00141600 -0.81668000

H 2.94323800 -0.40425600 -1.96980200
C 3.44198400 1.01255000 -0.40636100
H 3.65178600 1.01313900 0.67561200
H 4.35738900 1.39830000 -0.87538900
C 2.30444100 1.97729800 -0.72717500
H 2.62522400 3.01422100 -0.54226800
H 2.05091400 1.91364400 -1.79887400
P 1.89083100 -1.32276000 -0.00577500
P 0.72022900 1.72930400 0.19239900
C 2.63891900 -1.61777000 1.64744800
H 2.02698000 -2.34449700 2.19686000
H 3.65673700 -2.02059100 1.55422100
H 2.67501600 -0.69726600 2.24140500
C 1.99976400 -2.99767400 -0.74513700
H 3.00950400 -3.41037600 -0.61949200
H 1.28110200 -3.66794200 -0.25748400
H 1.76479100 -2.96431800 -1.81519300
C -0.21569600 3.17846300 -0.43604000
H -1.18938100 3.26630600 0.05775300
H 0.35416400 4.09861800 -0.25010300
H -0.38022600 3.08673000 -1.51665300
C 1.11757000 2.25736900 1.90422600
H 1.59832500 3.24499300 1.91587400
H 0.19066000 2.30855600 2.48927000
H 1.77882300 1.53374200 2.39498100
Co -0.12499300 -0.31486300 0.05234400
C -3.61671200 -1.23469300 -1.17289400
H -4.45918000 -1.19343500 -0.46791200
H -4.02786300 -1.17076300 -2.18939300
H -3.13706700 -2.21729200 -1.06222900

C -3.29332500 1.28143000 -0.64435300
C -2.86015400 1.20125400 0.83553400
H -4.37352800 1.32632400 -0.82075500
H -2.82200500 2.09852300 -1.20478600
H -3.69453100 0.91549000 1.49670400
H -2.37338700 2.07559900 1.29073500
C -1.64014900 -1.12542600 1.32956700
H -0.56024300 -1.43081900 1.47041400
C -2.55801400 -1.81853700 2.27858400
H -2.73803800 -1.19386900 3.16958300
H -2.15959700 -2.77732000 2.62696000
H -3.53915000 -1.99006500 1.81467000
E7-Z (open-shell singlet)
C -2.90179700 -0.24272200 -0.59111100
C -1.70725200 0.01823000 -1.48711800
C -2.29783800 -0.10978400 0.81344700
C -0.79693300 -0.91181600 -1.90174200
H -1.58859600 1.04520100 -1.84072800
H -0.02184600 -0.63513000 -2.61742500
H -0.94993800 -1.98339800 -1.75482500
C 3.20335500 -0.37778400 -0.93112200
H 4.14239200 -0.95048500 -0.87844400
H 2.90928800 -0.35021700 -1.99301900
C 3.41856900 1.04235300 -0.40809900
H 3.56763200 1.03123300 0.68415700
H 4.36786700 1.41226800 -0.81933700
C 2.32708100 2.04185400 -0.78555300
H 2.68072600 3.06832600 -0.60072700
H 2.11873200 1.97431900 -1.86614100
P 1.91400700 -1.34435200 -0.03461400

P 0.69876300 1.86200200 0.07770800
C 2.71659600 -1.69398500 1.58131900
H 2.12266100 -2.42880600 2.13833700
H 3.72760600 -2.09940500 1.43804900
H 2.78157300 -0.78583600 2.19226900
C 2.00082000 -2.97471200 -0.86956600
H 3.02176700 -3.37833900 -0.83928400
H 1.32643000 -3.68628900 -0.37712000
H 1.69135900 -2.87662000 -1.91726700
C -0.17673800 3.31373600 -0.63784600
H -1.17055400 3.44375600 -0.19375700
H 0.40181600 4.23189500 -0.46875700
H -0.30040200 3.17926400 -1.71993900
C 1.06965100 2.43135800 1.78531300
H 1.59322100 3.39711200 1.79009300
H 0.13148600 2.53515900 2.34567100
H 1.68555600 1.68977200 2.30990100
Co -0.12227400 -0.28966300 0.08685300
C -3.73228000 -1.45515700 -0.96092800
H -4.47909900 -1.66014900 -0.18270800
H -4.26481400 -1.27371700 -1.90379100
H -3.12918200 -2.36213200 -1.09226300
C -3.68459000 1.06679900 -0.30052700
C -2.90228300 1.26067600 1.02014700
H -4.75121100 0.87743900 -0.13497100
H -3.58758200 1.85838000 -1.05384100
H -3.51917400 1.34237200 1.92401000
H -2.19502100 2.09938700 1.02944200
C -1.57828000 -0.93286900 1.62275900
H -1.29617900 -0.52233300 2.59940900

C -1.41685200 -2.42094800 1.46576800
H -2.19337300 -2.94535000 2.04293800
H -0.45000500 -2.76799500 1.85281600
H -1.51065000 -2.75492300 0.42496500
TSE7-Z (triplet)
C -2.73790000 0.65999100 0.62472500
C -1.61673000 1.27453600 1.40261600
C -1.86824700 -0.24755200 -0.29359700
C -0.78373700 2.25532900 0.91156800
H -1.43663500 0.89729600 2.41693200
H -0.07881800 2.74153600 1.58219500
H -1.01991800 2.78830300 -0.01246500
C 3.51323900 0.21126300 -0.01499000
H 4.29277600 0.77451600 -0.55046000
H 3.87307500 0.08667300 1.01836600
C 3.29466300 -1.15613000 -0.65461400
H 2.82810300 -1.04609200 -1.64916100
H 4.27520800 -1.61243200 -0.84502600
C 2.47499600 -2.09896800 0.22317400
H 2.63425500 -3.14695500 -0.07223100
H 2.80803000 -2.01826300 1.26986600
P 2.01265400 1.28640500 0.04564800
P 0.65108400 -1.80193900 0.19435800
C 2.04060000 2.07794800 -1.61371200
H 1.20216800 2.77892000 -1.70883200
H 2.98040500 2.62586800 -1.76499000
H 1.94432600 1.32128300 -2.40242200
C 2.60901000 2.65410300 1.11430200
H 3.63669400 2.92463500 0.83757200
H 1.97586200 3.54018000 0.98890000

H 2.59423300 2.36144800 2.17078300
C 0.13288200 -2.81191400 1.63472800
H 0.50700700 -3.84017500 1.53945900
H 0.55122300 -2.37134100 2.54820600
H -0.95644800 -2.83893000 1.73953100
C 0.15148800 -2.77064300 -1.27983700
H 0.44243500 -3.82257100 -1.16014200
H -0.92858500 -2.71116600 -1.44955700
H 0.65337600 -2.36538300 -2.16787000
Co -0.03541300 0.31539800 0.32799800
C -3.73337500 1.61427600 0.00842400
H -4.46007500 1.07561800 -0.61506000
H -4.29470200 2.14316900 0.79096000
H -3.24477600 2.36929200 -0.62213300
C -3.33551800 -0.62236000 1.24628900
C -2.75811700 -1.43646600 0.07711300
H -4.42493900 -0.63265400 1.36014300
H -2.88273200 -0.87806400 2.21415400
H -3.51142200 -1.58700400 -0.71423100
H -2.31666300 -2.41921100 0.28709200
C -1.44489700 0.14224900 -1.63385400
H -0.37278300 0.35293700 -1.82697700
C -2.35187100 0.34183100 -2.80145200
H -3.32899100 -0.12901500 -2.63637100
H -1.92396800 -0.07980500 -3.72134700
H -2.53654800 1.40971000 -3.00621500
E7-Z (triplet)
C -2.91791600 -0.24730900 -0.57209200
C -1.74006200 -0.01405200 -1.49794900
C -2.28602500 -0.10072400 0.81930000
C -0.84511700 -0.96126700 -1.90539400
H -1.61687500 1.00505900 -1.87285800
H -0.07597900 -0.70722100 -2.63579900
H -1.00402000 -2.02810000 -1.73279200
C 3.21789700 -0.38395200 -0.90624000
H 4.15835500 -0.95398500 -0.84840200
H 2.93688900 -0.34690800 -1.97138500
C 3.42362000 1.03224600 -0.36649700
H 3.53953100 1.01245600 0.72977300
H 4.38790100 1.39784000 -0.74550500
C 2.35235700 2.04426800 -0.77034200
H 2.71724400 3.06717600 -0.58778700
H 2.16182700 1.97130400 -1.85374300
P 1.92250800 -1.36836900 -0.03565600
P 0.70773100 1.89220200 0.06881300
C 2.70696500 -1.73420700 1.58529300
H 2.11103700 -2.48075100 2.12436700
H 3.72159200 -2.13253700 1.44789700
H 2.76014300 -0.83524800 2.21048500
C 2.02468600 -2.98965300 -0.88564700
H 3.04492400 -3.39398600 -0.84407200
H 1.34266200 -3.70530300 -0.40958900
H 1.73014600 -2.88206600 -1.93669200
C -0.15699600 3.32371900 -0.69817800
H 0.42046700 4.24660500 -0.55276000
H -0.27391900 3.15588300 -1.77627900
H -1.15402300 3.46673000 -0.26469000
C 1.05564700 2.51383700 1.76342200
H 1.55977100 3.48957200 1.74278600
H 0.11343000 2.61525800 2.31711000

H 1.68431200 1.80124800 2.31191400
Co -0.13150300 -0.28994200 0.07094100
C -3.76815700 -1.45719900 -0.90454400
H -4.50259100 -1.63967500 -0.10907600
H -4.31612900 -1.28716000 -1.84065300
H -3.17717000 -2.37296100 -1.02980900
C -3.68334300 1.07311900 -0.28528700
C -2.87829900 1.27604000 1.02020200
H -4.74922400 0.89695200 -0.10158200
H -3.58968000 1.85447800 -1.04958300
H -3.47956400 1.37242200 1.93318500
H -2.16606600 2.11063200 1.00666700
C -1.55530900 -0.92248900 1.62329000
H -1.25329900 -0.50553800 2.59134000
C -1.41312100 -2.41426300 1.47675300
H -1.49948000 -2.75277100 0.43658500
H -2.20216400 -2.92694300 2.04701600
H -0.45401400 -2.77020500 1.87461600

TSZE

C -0.65505800 0.20274700 0.29392700
C -1.63489000 -0.33042600 -0.70916600
C 0.71675600 0.39577500 -0.36126400
C -2.34987900 -1.45005200 -0.61768800
H -1.72034200 0.27876600 -1.61637800
H -3.01633400 -1.76342800 -1.41910800
H -2.30781700 -2.09956800 0.25600200
C -0.62377300 -0.56938900 1.59894800
H 0.11647300 -0.12993900 2.28199500
H -1.60292200 -0.56073500 2.09910300
H -0.33658600 -1.61678700 1.42774300

C -0.72067100 1.75645900 0.41481900
C 0.56902800 1.89307200 -0.42522100
H -0.59818900 2.09260100 1.45198000
H -1.62261200 2.22473600 0.00170700
H 1.38448200 2.48821800 0.01565300
H 0.40210800 2.28990800 -1.44224800
C 1.71531900 -0.55457800 -0.77836000
H 1.65605200 -1.00967000 -1.77446200
C 2.74636500 -1.08910800 0.16037400
H 3.69919600 -1.29516400 -0.34766700
H 2.42963100 -2.04053000 0.62497600
H 2.93767800 -0.38540900 0.98248100

A3-dppm

C -1.98992600 -0.61813700 0.60489500
C -0.86048500 0.02626800 -1.63399400
C -2.34558300 0.34272100 -1.53396100
C -2.90957500 -0.31946900 -0.30596700
H -0.70271900 -1.00989200 -1.99761100
H -0.31205300 0.70757900 -2.30171500
H -2.88146600 -0.00544600 -2.43479800
H -2.53531400 1.42858600 -1.49931300
C -4.36511500 -0.64791000 -0.22261400
H -4.63324800 -1.08560200 0.74380200
H -4.97106600 0.25634500 -0.37633500
H -4.64908200 -1.35464600 -1.01452600
C -1.32254900 -1.08889800 1.73015200
H -1.28514600 -0.48918700 2.64450000
C -0.33979500 -2.07039400 1.50082400
H -0.53786800 -2.85475900 0.76291400
H 0.39195100 -2.31685700 2.26901200

P 2.03436700 -0.58129300 -0.40030600
P 0.39393400 1.45893700 0.31253100
C 3.35775600 -1.05656100 0.76972400
H 3.40465300 -2.15005000 0.83941100
H 4.33626300 -0.68001600 0.44559900
H 3.13320500 -0.66652800 1.76986100
C 2.68311200 -1.11497900 -2.02631000
H 3.68137000 -0.69665500 -2.20701400
H 2.74828200 -2.20894500 -2.05568100
H 2.00445800 -0.79206700 -2.82453700
C -0.45085800 2.94860800 -0.30813600
H -1.44881900 3.01639500 0.14285800
H 0.12254100 3.84052300 -0.02544200
H -0.55530700 2.92280600 -1.39775700
C 0.67908100 1.83800300 2.07658400
H 1.26192900 2.76238000 2.18585100
H -0.28448500 1.96837700 2.58438200
H 1.21399700 1.01120800 2.55977100
Co -0.14969800 -0.56935600 0.09969000
C 2.06125900 1.29067600 -0.44869300
H 2.04844700 1.63993800 -1.49050800
H 2.88286700 1.78489000 0.08723600
TSA3-dppm
C -1.81922800 -0.92003200 0.19752800
C -1.68534300 0.13798700 -1.52928200
C -2.88317300 0.75787900 -0.81450600
C -3.00407500 -0.29256300 0.24377400
H -2.00925300 -0.68336400 -2.17843700
H -1.02641500 0.81277000 -2.10046700
H -3.77691500 0.85272800 -1.44991800

H -2.67484400 1.76121400 -0.40935800
C -4.22790800 -0.67171100 0.99182100
H -4.05315500 -1.52672500 1.65390900
H -4.59393200 0.16838600 1.59819300
H -5.04103000 -0.93386500 0.29986900
C -0.97239700 -1.99091300 0.58318500
H -0.69998000 -2.17275300 1.62729600
C -0.23965000 -2.57021700 -0.44693500
H -0.62547400 -2.60405900 -1.46755500
H 0.57468400 -3.25806800 -0.22175000
P 2.11232200 -0.51814600 0.01678600
P 0.48378700 1.61398200 0.12860400
C 2.57486100 -1.23185500 1.63545500
H 2.45614300 -2.32229700 1.60314600
H 3.61737200 -0.99850800 1.88689000
H 1.91944500 -0.84252400 2.42373100
C 3.39924600 -1.13942000 -1.12153500
H 4.40276600 -0.91538400 -0.73858200
H 3.29183400 -2.22616500 -1.22632500
H 3.27877600 -0.68894400 -2.11270100
C 0.21224300 3.17075700 -0.79380400
H -0.85846500 3.40894700 -0.81935900
H 0.74647200 4.00310600 -0.31864400
H 0.56222600 3.06308300 -1.82724900
C 0.01295400 2.02635900 1.84764500
H 0.54690300 2.91628900 2.20561100
H -1.06706700 2.21107600 1.89621700
H 0.23463600 1.17866700 2.50712000
Co -0.07041900 -0.46766100 -0.41464900
C 2.31690800 1.31873500 0.18100300

H 2.78949100 1.72555000 -0.72451100

H 2.85883900 1.69011200 1.06146300

A-dppm

C -1.95994700 -1.36628700 -0.16199100

C -2.52264400 -0.88179100 -1.48542700

C -3.02602300 0.36310300 -0.69875100

C -2.33071600 -0.20730900 0.52413100

H -3.32358200 -1.51318600 -1.88895700

H -1.79742500 -0.68183600 -2.28657300

H -4.11893800 0.39865100 -0.59449300

H -2.69057700 1.34389400 -1.06054600

C -2.48089100 0.13389800 1.96230100

H -1.82450300 -0.47035100 2.60049400

H -2.27050900 1.19309800 2.15635300

H -3.51844300 -0.04581600 2.28239000

C -1.01181500 -2.33746800 0.29456300

H -1.03454600 -2.66096000 1.33773500

C 0.11845400 -2.55394700 -0.48121200

H 0.09615500 -2.42126100 -1.56567800

H 0.92661600 -3.17824900 -0.09919600

P 2.01204800 -0.33127200 0.13444200

P 0.23215900 1.61160900 -0.05719700

C 3.00690500 -1.07817600 1.47263300

H 3.01928500 -2.16870900 1.35412500

H 4.03916800 -0.70671100 1.44489400

H 2.56286600 -0.84526200 2.44671300

C 2.97779100 -0.68355100 -1.37671500

H 4.00983200 -0.32481000 -1.27391200

H 2.99635400 -1.76580100 -1.55573100

H 2.51559300 -0.20425700 -2.24757800

C 0.20359000 2.24459800 -1.77646000

H -0.83059400 2.33639800 -2.12980800

H 0.68607100 3.22900600 -1.83749600

H 0.72431600 1.54639000 -2.44271000

C -0.48960900 2.98481500 0.91272600

H 0.03577400 3.92163300 0.68781200

H -1.55038900 3.10845500 0.66115400

H -0.40765300 2.77880300 1.98612400

Co -0.14699000 -0.54397700 0.08891000

C 2.03660500 1.50959900 0.36303100

H 2.73475100 2.09539400 -0.25031100

H 2.19581100 1.75289800 1.42297900

TSA3-dppf

C 3.42832900 0.09005000 0.06442200

C 2.59551300 -0.48224900 -1.65272900

C 3.63000300 -1.57664400 -1.39731300

C 4.30049300 -0.87738900 -0.26176900

H 3.00394900 0.28717500 -2.31744900

H 1.59959000 -0.80148200 -2.00625800

H 4.29848800 -1.73114800 -2.25813300

H 3.20605200 -2.55729900 -1.14795600

C 5.69626000 -1.05845800 0.20789300

H 5.95798800 -0.34051400 0.99300800

H 5.84986700 -2.07324700 0.60063700

H 6.40636200 -0.93500000 -0.62207200

C 3.21014800 1.34716500 0.68850900

H 3.17454400 1.48104200 1.77418900

C 2.76310600 2.34607500 -0.17020000

H 3.04229900 2.35166200 -1.22493100

H 2.44250500 3.30268200 0.23806400

Fe -2.63599500 -0.47446200 -0.17205600
P 0.55281800 -1.22214700 0.64656200
P -0.19193200 1.93481200 0.07996000
C -1.93232700 1.41131400 -0.01044700
C -2.66842700 1.24816200 -1.23077800
C -3.99660900 0.86197900 -0.90094300
H -4.78120200 0.62201500 -1.61042200
C -4.09522600 0.77812100 0.51540100
C -2.82880700 1.11546400 1.07080800
H -2.58835000 1.12992900 2.13017500
C -2.20269600 -2.11798800 0.94162000
C -1.09798000 -1.72173000 0.11691700
C -1.53638800 -1.77741100 -1.24788500
C -2.89839700 -2.18786300 -1.25530100
C -3.30814000 -2.39307000 0.09206900
H -4.30737700 -2.65996400 0.41933100
H -4.97019900 0.46724900 1.07604900
H -2.27134300 1.36086400 -2.23561800
Co 1.57510100 0.56003900 -0.19874500
H -2.21569500 -2.14712900 2.02688200
H -3.53138000 -2.27419800 -2.13191400
C -0.19789400 3.26785900 -1.18896900
H -1.09699100 3.88598700 -1.07368400
H 0.68915400 3.90151000 -1.09141700
H -0.19429500 2.83198200 -2.19470400
C -0.16404000 2.88055800 1.65482800
H 0.77514800 3.43872200 1.74110000
H -1.00366200 3.58613700 1.69017400
H -0.23182500 2.20599200 2.51642600
H -0.94696800 -1.50187500 -2.11866500

C 0.35636500 -0.85876000 2.43629900
H 0.03956000 -1.75056700 2.99243500
H 1.32034800 -0.52183800 2.83893300
H -0.38500900 -0.06649400 2.59060700
C 1.39093600 -2.85744600 0.71858000
H 2.41549400 -2.75723700 1.09567600
H 0.82284800 -3.52159300 1.38283400
H 1.40960300 -3.31480900 -0.27761800
A-dppf
C 3.64150200 -0.41173200 0.51910400
C 3.63012700 0.39163600 -0.61534400
C 3.61904600 -0.12942600 1.97775300
H 4.63363600 -0.22276900 2.39465900
H 2.98404600 -0.83609700 2.52838400
H 3.26599500 0.88907700 2.18715400
C 4.18051800 -1.60014900 -0.25423900
C 4.08832200 -0.72217800 -1.53531200
H 5.21370400 -1.85043100 0.02271900
H 3.59987400 -2.53117300 -0.24073900
H 5.05839100 -0.52678400 -2.00829700
H 3.38633600 -1.05252600 -2.31169300
C 3.07565800 1.70894900 -0.74531800
H 3.30549000 2.48957500 -0.01644200
C 2.04506000 1.85104100 -1.66868600
H 1.52118500 2.79832600 -1.78045900
H 1.96138900 1.16849700 -2.51877400
Fe -2.62021000 -0.23561100 -0.15434500
P -0.01869100 1.71404600 0.52623300
P 0.55004000 -1.46072500 0.12516100
C -1.25928900 -1.66027700 0.23504900

C -2.12508300 -2.07634900 -0.83311700	C 0.21983200 3.53689200 0.46215400
C -3.45980600 -2.09562200 -0.34599600	H 1.22039600 3.81587000 0.81592600
H -4.34389100 -2.32062500 -0.93267000	H -0.52919200 4.02153600 1.10199100
C -3.43944000 -1.70328800 1.01929400	H 0.08326900 3.91216000 -0.55800700
C -2.09098200 -1.43671900 1.38517800	TS1 (open-shell singlet)
H -1.76393700 -1.10271200 2.36571700	C 0.87418153 -2.68744040 -1.01904129
C -2.93383700 1.64928900 0.53488700	C -0.12535672 -1.81750011 -2.41623581
C -1.67621200 1.52197900 -0.14331800	C 0.85786032 -2.20108109 0.38277055
C -1.95137100 1.11512000 -1.49263300	C 0.19061050 -0.44250014 -2.66190002
C -3.35981900 0.98007800 -1.63041700	H -1.16990073 -2.02425126 -2.16876072
C -3.96208800 1.30576900 -0.38333400	H 0.28294659 -2.55668188 -3.11001068
H -5.02092100 1.24881500 -0.15460200	H -0.62069130 0.28292942 -2.76106393
H -4.30532100 -1.58065000 1.66085200	H 1.07132253 -0.21545578 -3.27135405
H -1.82619800 -2.28909000 -1.85443800	C 2.18693179 -2.97840155 -1.70458624
Co 1.61899100 0.47675600 -0.15489600	H 2.85331047 -3.53262604 -1.02726557
H -3.07926000 1.90168600 1.58081100	H 2.04226618 -3.58347092 -2.61041195
H -3.88180700 0.63504100 -2.51637600	H 2.70878897 -2.05499475 -1.99867281
C 0.88848400 -2.37602700 -1.43405100	C -0.09007363 -3.81148298 -0.59919556
H 0.37482900 -3.34579100 -1.43448900	C -0.22567735 -3.17596292 0.80076266
H 1.96344800 -2.54861200 -1.54710300	H 0.45499934 -4.76420210 -0.55933044
H 0.54556100 -1.78383600 -2.29267000	H -0.99810163 -3.95213253 -1.20029316
C 1.07169800 -2.65324100 1.42558800	H 0.07830775 -3.83394048 1.62622007
H 2.15555500 -2.81269500 1.40620500	H -1.20432589 -2.75424603 1.05706904
H 0.56241900 -3.61354000 1.27601400	C 1.98279430 -1.78523810 1.16777543
H 0.79782900 -2.26871000 2.41616700	H 2.86174192 -1.42953016 0.62319987
H -1.20278500 0.89771100 -2.25127200	C 2.02749804 -1.82909064 2.52143323
C -0.15849400 1.47835700 2.34229100	H 2.91108968 -1.50565813 3.06928417
H -1.00996800 2.03106000 2.76003400	H 1.18892958 -2.20285359 3.11019212
H 0.75887500 1.86614300 2.80374000	C -1.63796010 1.91763287 0.07548459
H -0.24946600 0.41957600 2.60471400	C -2.87927435 2.41399325 0.48575409

H -3.64715689 1.71886874 0.82419472
C -3.16492948 3.77221938 0.46559633
H -4.14354977 4.12544390 0.78473751
C -2.19397694 4.67109879 0.03728227
H -2.40029127 5.73906279 0.01563809
C -0.95167947 4.20376139 -0.35741171
H -0.19324077 4.91043315 -0.68017769
C -0.65117589 2.83057970 -0.34478317
C 0.70978815 2.45857197 -0.75464080
C 2.79252728 2.99631010 -1.40619082
H 3.47809362 3.40702111 -0.65539171
H 3.08236689 3.35586560 -2.39718592
C 2.65250316 1.47159753 -1.31960054
N 1.26903097 1.29307083 -0.80878694
P -1.39518186 0.09181473 0.17000637
Co 0.60595059 -0.53925638 -0.73791486
O 1.47588386 3.49143494 -1.11803793
C -2.82576743 -0.53947590 -0.78901683
C -3.36331734 -1.81198569 -0.55097512
C -3.25757627 0.16903996 -1.91860069
C -4.31282061 -2.35329488 -1.41240669
H -3.04488883 -2.39580518 0.31157342
C -4.19964522 -0.37894875 -2.78311338
H -2.85585683 1.15977359 -2.13211867
C -4.72977491 -1.64141021 -2.53352155
H -4.72583561 -3.33884550 -1.20399077
H -4.52176568 0.18778381 -3.65512593
H -5.46791506 -2.06858913 -3.21003356
C -1.73919312 -0.17821597 1.94748408
C -2.96495875 -0.58378914 2.48244286

C -0.67398281 0.10909491 2.80949127
C -3.11507573 -0.71232243 3.86058471
H -3.81015076 -0.79448040 1.82826047
C -0.83100767 -0.01051420 4.18604992
H 0.28689506 0.42575902 2.39672715
C -2.05105627 -0.42771789 4.71251695
H -4.07214637 -1.03170442 4.26982912
H 0.00472946 0.21501428 4.84701332
H -2.17403379 -0.52922512 5.78952502
C 3.69107069 0.82154245 -0.44573966
C 4.58524345 -0.10024393 -0.98747124
C 3.78287627 1.14991779 0.90993642
C 5.55875024 -0.69509109 -0.18641545
H 4.52126345 -0.34930703 -2.04797609
C 4.75557262 0.56193135 1.70929486
H 3.08038904 1.86679950 1.34095229
C 5.64364467 -0.36506831 1.16264679
H 6.25274398 -1.41374193 -0.61924687
H 4.82067311 0.82288859 2.76461046
H 6.40455864 -0.82589532 1.79041729
H 2.69577159 1.01662938 -2.32037845
TS2(open-shell singlet)
C -1.73619915 1.79937594 -0.64031244
C -3.07266702 2.18256989 -0.74324351
H -3.85355274 1.51863661 -0.37562706
C -3.42900977 3.40764613 -1.30316509
H -4.48020555 3.68012835 -1.37599371
C -2.44576900 4.27732811 -1.75717885
H -2.71577995 5.23740054 -2.19156038
C -1.10827058 3.91714840 -1.65646837

H -0.33576192 4.59300982 -2.01452199
C -0.74204179 2.68106959 -1.11304055
C 0.68543353 2.35149635 -1.08155758
C 2.85795324 2.86484934 -1.12709554
H 3.23661668 3.21145337 -0.15708235
H 3.47570133 3.27377802 -1.92992954
C 2.68856109 1.34483104 -1.18133503
N 1.23201125 1.18622139 -0.93782174
P -1.25960430 0.21854378 0.17146961
O 1.51898114 3.37262005 -1.28123253
C -2.81726182 -0.72639944 0.24482670
C -3.44876463 -1.06468768 1.44351463
C -3.31214982 -1.23527803 -0.96306123
C -4.55932278 -1.90534340 1.43248752
H -3.06354028 -0.69186416 2.39202167
C -4.42378776 -2.06917647 -0.97083638
H -2.81968637 -0.97767850 -1.90368706
C -5.04495342 -2.41002466 0.23009284
H -5.04355740 -2.16950066 2.37112210
H -4.80315928 -2.45890860 -1.91391989
H -5.90947818 -3.07172697 0.22657943
C -0.89587452 0.76601749 1.87945748
C 0.25410119 0.28543659 2.50948410
C -1.72791392 1.66519233 2.55737660
C 0.56831208 0.69170834 3.80351982
H 0.90589432 -0.40868101 1.97770137
C -1.41454179 2.06698985 3.85113915
H -2.62537658 2.05310606 2.07381515
C -0.26667755 1.58049749 4.47426632
H 1.46692283 0.31138046 4.28752952
H -2.06623740 2.76543329 4.37327275
H -0.02184334 1.89907559 5.48623301
C 3.57100044 0.60582682 -0.21455335
C 4.56304981 -0.24966495 -0.69304922
C 3.43501588 0.79298472 1.16370347
C 5.40655606 -0.91764375 0.19165941
H 4.67575508 -0.39054126 -1.76912301
C 4.26913463 0.11923664 2.04868101
H 2.66593778 1.46793286 1.54407479
C 5.25712203 -0.73736953 1.56347108
H 6.17981044 -1.58071559 -0.19267308
H 4.15472864 0.26887897 3.12146829
H 5.91362344 -1.25981582 2.25734924
H 2.88342115 0.96634746 -2.19791733
C 0.43295220 -2.77855779 -1.42050243
C -0.03562221 -1.71875714 -2.90263742
C 0.47075828 -2.34487666 0.00582475
C 0.24846553 -0.31210867 -2.92276661
H -1.09357624 -1.97504510 -2.99246195
H 0.60110571 -2.33332074 -3.54654856
H -0.57995538 0.39115103 -3.03606382
H 1.18751155 0.02025603 -3.37520585
C -0.43619545 -3.96666031 -1.75907809
H -0.16030731 -4.80498748 -1.10215605
H -1.50306340 -3.75651360 -1.60367716
H -0.29601037 -4.28547574 -2.80131330
C 1.96009716 -2.97052599 -1.39656005
C 1.97430759 -2.60761723 0.10433143
H 2.51999624 -2.28414522 -2.05114092
H 2.26876105 -3.99867825 -1.62796769

H 2.62330161 -1.77328202 0.40413021
H 2.19868359 -3.46430213 0.75672775
C -0.49525654 -2.79688358 0.99481553
H -1.51579696 -2.95501066 0.63504914
C -0.22407229 -3.06476412 2.28013516
H -0.99750016 -3.42213846 2.95862728
H 0.77457878 -2.93382723 2.70092336
Co 0.45301339 -0.60620999 -0.99109473

TS3

C -0.76198015 -2.79123298 -1.69043811
C -0.82545794 -1.17276371 -2.78292296
C -1.32571892 -2.60201006 -0.35442150
C -0.26204776 0.10851298 -2.41257713
H -0.29468477 -1.71724643 -3.56752971
H -1.90359245 -1.14393287 -2.95947553
H 0.70698010 0.38164216 -2.83379277
H -0.95578859 0.95321494 -2.32440166
C 0.55974717 -3.45816921 -1.93551394
H 0.48089935 -4.51408219 -1.63510452
H 1.36549908 -3.01112722 -1.33720749
H 0.85748423 -3.43549183 -2.99272787
C -2.09170989 -3.40096511 -2.14521334
C -2.74972212 -2.85749250 -0.86160106
H -2.49610554 -3.12479530 -3.12881598
H -2.00041883 -4.49453879 -2.09029177
H -3.35756221 -1.95814413 -1.02315920
H -3.33766794 -3.58153270 -0.28352665
C -0.77902841 -3.16675132 0.86794329
H 0.30805888 -3.29509131 0.89662688
C -1.49842726 -3.51671299 1.94462418

H -1.02395807 -3.93410896 2.83152714
H -2.58434368 -3.41196071 1.97444197
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C 3.34281168 -1.46788891 2.93755581
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C 2.37798689 -1.62994072 3.92323997
H 2.63880179 -2.07497219 4.88102896
C 1.06850344 -1.22769165 3.67965530
H 0.29806981 -1.36193205 4.43674632
C 0.72823130 -0.67854116 2.44553637
C -0.66350439 -0.32498227 2.17456126
C -2.68206908 0.48993510 2.62543001
H -2.66347776 1.58450440 2.71446751
H -3.51887166 0.08561261 3.19933098
C -2.63423011 0.01988753 1.16794604
N -1.19734889 -0.28823913 1.00385273
P 1.22669170 0.30791417 -0.15140227
Co -0.53949182 -0.79345877 -0.72068829
O -1.45196710 -0.01190728 3.20142655
C 2.78332980 0.30569256 -1.11301572
C 3.79218941 1.22827218 -0.80816564
C 3.00838636 -0.64908922 -2.10784085
C 5.00396588 1.19129363 -1.48889611
H 3.63477368 1.97382322 -0.02849147
C 4.22230263 -0.68388493 -2.78789780
H 2.22834089 -1.36460711 -2.36475574
C 5.21979287 0.23599293 -2.47941409
H 5.78195472 1.91246184 -1.24497359

H 4.38482663 -1.42903773 -3.56458223
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C 1.00190699 2.08241216 0.25446728
C 0.84316440 2.97893445 -0.81042390
C 0.94554513 2.56416608 1.56497729
C 0.62727171 4.32993204 -0.56582152
H 0.89936108 2.62354836 -1.83969127
C 0.71693925 3.91754983 1.80631410
H 1.08955639 1.89330183 2.41127411
C 0.55481011 4.80085681 0.74400420
H 0.51314585 5.01772005 -1.40216065
H 0.67508033 4.28038640 2.83189976
H 0.38099774 5.85845131 0.93486852
C -3.14017567 1.00655854 0.14962331
C -2.53423839 2.25758997 0.00231625
C -4.21703019 0.67271164 -0.67258619
C -2.99038619 3.14965849 -0.96232727
H -1.69102785 2.53102001 0.63937040
C -4.67532733 1.56515938 -1.63871750
H -4.70698732 -0.29362189 -0.54703086
C -4.05885134 2.80376133 -1.78822093
H -2.50751504 4.12015952 -1.07010492
H -5.51759057 1.29188060 -2.27223852
H -4.41402347 3.50346208 -2.54304722
H -3.18065362 -0.92939196 1.04953934
TS4(open-shell singlet)
C -1.00579725 3.20437457 -0.89225241
C 0.05202378 2.25765490 -2.18030058
C -1.79622323 2.41646981 0.08103190
C 1.22142739 1.62371136 -1.64841640

H 0.19177105 3.21782923 -2.68511347
H -0.65597004 1.61716576 -2.71797955
H 2.07984756 2.26622345 -1.42865974
H 1.48774581 0.60948037 -1.94813012
C -0.13321540 4.35356240 -0.46085773
H 0.71806361 4.02445818 0.15375295
H 0.26851316 4.90357626 -1.32303547
H -0.72306597 5.05573218 0.14634721
C -2.28746840 3.40619555 -1.70965372
C -2.97908473 2.31470322 -0.86984697
H -2.22707861 3.28126735 -2.79927165
H -2.69588907 4.40041084 -1.48336437
H -3.08052820 1.35640237 -1.39351562
H -3.95312040 2.58030137 -0.43893058
C -1.80725383 2.55975777 1.50934587
H -0.90761858 2.99281761 1.96072398
C -2.83628431 2.21251177 2.31967569
H -2.77721220 2.34604085 3.39793981
H -3.76933843 1.81422224 1.91891215
C -0.85902599 -1.37978741 1.54463220
C -1.74162270 -2.39193966 1.92804924
H -2.45111810 -2.78663036 1.20325841
C -1.73528075 -2.91572331 3.21697479
H -2.43763191 -3.70396742 3.48081685
C -0.83323841 -2.43279453 4.15676561
H -0.82664490 -2.82572487 5.17108439
C 0.07954653 -1.45591871 3.78893979
H 0.80673162 -1.09669218 4.51201689
C 0.08682712 -0.92717160 2.49079814
C 1.16365598 0.01471812 2.17059691

C 3.04564074 1.11385431 2.64835069
H 4.07797158 0.79058783 2.80417248
H 2.82107318 1.97811800 3.28550239
C 2.66873281 1.34439131 1.18520416
H 2.63647090 2.41712118 0.95795468
N 1.29819780 0.78388582 1.13575584
P -0.92610178 -0.70801908 -0.16936054
Co -0.03657111 1.42399957 -0.14115063
O 2.17321244 0.03621613 3.04460417
C -2.65461030 -1.04447614 -0.68491780
C -2.95907280 -1.49286903 -1.97296171
C -3.70370141 -0.68464127 0.17230123
C -4.28426442 -1.57579283 -2.39526752
H -2.16479024 -1.78734760 -2.65730885
C -5.02457020 -0.77675877 -0.24801749
H -3.48516790 -0.32856564 1.17897385
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H -4.50528617 -1.93003082 -3.40081557
H -5.82758578 -0.49885826 0.43299193
H -6.35287337 -1.28213228 -1.87040833
C 0.09168210 -1.89322381 -1.13155379
C 0.63041817 -3.05657869 -0.57329941
C 0.36193728 -1.59454964 -2.47420406
C 1.42065075 -3.90492256 -1.34543494
H 0.43732814 -3.30976375 0.46870440
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H -0.04555902 -0.68668243 -2.92296067
C 1.67515371 -3.60517038 -2.68063417
H 1.83443824 -4.80779292 -0.89910863
H 1.33640281 -2.20875195 -4.28963197

H 2.29138624 -4.27152073 -3.28191882
C 3.59641441 0.65106499 0.21404108
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C 5.52669433 0.77026477 -1.24279707
H 4.71243624 2.45162310 -0.16685886
C 4.38309073 -1.32646798 -0.93431586
H 2.67898241 -1.30245321 0.37154130
C 5.40539976 -0.58811322 -1.52476293
H 6.32096339 1.35601331 -1.70293512
H 4.27712369 -2.38868009 -1.15299149
H 6.10464558 -1.06965811 -2.20640944

E3

C -2.74710600 -0.00980200 -0.51742300
C -1.91413100 -0.14612600 -1.78978700
C -1.71528500 0.01684600 0.63946800
C -1.06422500 -1.36042400 -1.75489600
H -2.44422200 0.08610900 -2.72757600
H -0.52239600 -1.60740700 -2.67583400
H -1.48877800 -2.24691900 -1.27818800
C 2.88866400 -1.02534400 -0.82451200
H 3.61930200 -1.83491000 -0.67147600
H 2.67752000 -0.99453700 -1.90602600
C 3.47542300 0.30683200 -0.35770000
H 3.62288000 0.29345100 0.73406800
H 4.48545700 0.39484700 -0.78112700
C 2.68630900 1.54740100 -0.76939700
H 3.26172000 2.45685100 -0.53699800
H 2.53030500 1.54766500 -1.86069500
P 1.32808600 -1.53439400 0.03271100
P 1.01206900 1.72462200 0.00532700
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H 1.89243200 -0.74715400 2.29776200
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H 2.03202200 3.05963900 1.78429500
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H 1.93865500 1.34189000 2.24685600
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H -1.12491800 -1.67137200 3.60271800
H -1.17915600 0.15773900 3.31960700
H -1.20119700 0.78929700 -1.77518300

TSE3

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C -1.94647300 -0.03290500 0.68365000
C -0.93128400 -1.89089400 -1.20142100
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H -0.32288000 -2.30017800 -2.01053000
H -1.30698000 -2.66429200 -0.52754300
C 3.21729700 -0.50391900 -0.78583300
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H 3.09007800 -0.58032900 -1.87705700
C 3.39787300 0.95561200 -0.38102600
H 3.46820700 1.04354600 0.71567100
H 4.37262000 1.29475900 -0.75787700
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H 2.17570700 1.70663600 -2.00098300
P 1.77542100 -1.35205400 -0.00444300

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H 2.27833300 -0.56229800 2.26710700
C 2.00578900 -3.06787100 -0.60613500
H 3.00050700 -3.43985900 -0.32753600
H 1.24634800 -3.72753200 -0.16978500
H 1.90967300 -3.10868100 -1.69736400
C -0.20076900 3.09726900 -1.07489700
H -1.20940400 3.27991500 -0.68731100
H 0.36563900 4.03689900 -1.02562900
H -0.28805100 2.79727100 -2.12701300
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H 1.46958700 3.56921000 1.32635500
H 0.00017400 2.81767000 1.98601100
H 1.56142600 1.98793800 2.14701300
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