

Supplementary Information

Stereoselectivity in Butadiene Polymerization Promoted by Zieger-Natta Catalysts Based on (Anilidomethyl)pyridine Group (IV) Complexes

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Cartesian coordinates and energies of calculated structures

Zirconium - Path 1**1_{Zr} anti-P/cis-P**

E: -1010.28016020 A.U.

Zr	-0.10735600	0.80314500	-0.07033800
N	-2.07496100	-0.47405800	-0.23453400
N	0.30656300	-1.04822100	0.60416000
C	-1.96631000	-1.76093900	0.21644600
C	-3.06622100	-2.63789800	0.20845800
H	-2.94635300	-3.66486100	0.58683200
C	-4.29897400	-2.19420300	-0.28740800
H	-5.16892700	-2.86904500	-0.30645700
C	-4.40663800	-0.87091600	-0.75686300
H	-5.35549000	-0.47728800	-1.15080700
C	-3.28194200	-0.04618100	-0.70520000
H	-3.34167300	1.00123000	-1.03951800
C	-0.60167500	-2.18011100	0.71189900
H	-0.23514600	-3.06009000	0.13541000
C	1.69834900	-1.12483900	0.31861000
C	2.15423700	-1.56834700	-0.98628100
C	3.53403800	-1.57129700	-1.24494700
H	3.89826500	-1.90496400	-2.22996600
C	4.45925000	-1.17005200	-0.26262800
H	5.53668100	-1.18398700	-0.49143500
C	4.02379100	-0.78996000	1.01574600
H	4.76506900	-0.53439600	1.78970600
C	2.65507000	-0.78919500	1.35080000
C	1.20636400	-2.07888200	-2.04933700
H	0.15467600	-1.75259300	-1.91347500
C	2.25172600	-0.59933800	2.79011900
H	1.15553900	-0.59315000	2.93151400
H	1.53701400	-1.78491700	-3.06668800
H	1.19002700	-3.19144100	-2.04962600
H	2.68469300	0.32538200	3.22457300
H	2.65853800	-1.43869600	3.39510100
C	-2.00964100	0.88595100	2.68203100
H	-2.75690500	0.11606200	2.40767200
H	-0.67225200	-2.52409200	1.77204400
H	-1.07218200	0.38364400	2.99275000
C	-1.83228600	1.92306000	1.60060400
C	-0.68281200	2.69763500	1.39490900
C	1.02751500	2.64350500	-1.63322700
H	1.18535100	3.59928500	-1.10468100
C	2.04632400	1.72432200	-1.64733700
H	2.02997200	0.82852300	-2.29006400
C	-0.28327200	2.45600800	-2.27566500
H	-0.93087900	3.34760400	-2.34616900
C	-0.77610900	1.24808300	-2.68894400
H	-0.15428800	0.32846700	-2.72354200
H	-1.77195400	1.15798600	-3.14925400
H	2.98567800	1.91709300	-1.10523100
H	-2.76965800	2.32368200	1.17461800
H	-0.80834100	3.60120300	0.76560800
C	0.64582600	2.24994000	1.65926100
H	1.48311600	2.93713700	1.45632400
H	0.82158500	1.56523200	2.50743700
H	-2.40878500	1.39908300	3.58717800

TS_{1-2Zr} anti-P/cis-P

E: -1010.25310770 A.U.

Zr	-0.04551600	0.63948700	-0.34229500
N	-2.10587500	-0.43837500	-0.24010800
N	0.19606700	-1.14754900	0.54339000
C	-2.11114200	-1.69070800	0.31405400
C	-3.29542300	-2.44309300	0.40126200
H	-3.27277600	-3.44494200	0.85720800
C	-4.48864900	-1.91245000	-0.10841000
H	-5.42342200	-2.49212500	-0.05477900
C	-4.47373300	-0.63217200	-0.69581700
H	-5.38581600	-0.18274400	-1.11577800
C	-3.26877900	0.07118600	-0.73628100
H	-3.21997700	1.07836900	-1.18291000
C	-0.76728000	-2.20201300	0.78406000
H	-0.50858000	-3.14159900	0.24169000
C	1.61624600	-1.23414100	0.40887300
C	2.20007800	-1.77713100	-0.80228100
C	3.59176400	-1.66450600	-0.97674600
H	4.05073600	-2.05947700	-1.89717300
C	4.40709400	-1.08400900	0.01171200
H	5.49349400	-1.00821100	-0.15296500
C	3.85242800	-0.64562900	1.22360700
H	4.51148500	-0.25603900	2.01593900
C	2.46676800	-0.73827900	1.46535100
C	1.38694400	-2.54800700	-1.81699700
H	0.32313800	-2.24386900	-1.86769600
C	1.93563500	-0.44710000	2.84638100
H	0.83090100	-0.42663800	2.88191600
H	1.82331200	-2.47035500	-2.83240600
H	1.40166300	-3.62984500	-1.55620600
H	2.34189300	0.49600600	3.26728200
H	2.26622500	-1.25277900	3.53820100
C	-1.63654900	1.31148600	2.95392500
H	-2.25045400	0.38644000	2.93231900
H	-0.81036600	-2.48257700	1.86460600
H	-0.60143100	1.07586500	3.26148200
C	-1.74786000	2.07843400	1.68309900
C	-0.74523800	2.68023400	0.94621500
C	0.78009500	2.79725600	-1.87859400
H	0.61464900	3.88333700	-1.97791300
C	1.70258800	2.37345200	-0.86484700
H	2.15375000	1.34688000	-0.91340100
C	-0.01513300	1.95218900	-2.68103400
H	-0.77650700	2.45008100	-3.30809900
C	-0.01715800	0.52659600	-2.64485500
H	0.96239600	0.01495600	-2.46236600
H	-0.65496000	-0.03204700	-3.34768600
H	2.46784200	3.08687800	-0.52922900
H	-2.78030600	2.29798000	1.35386900
H	-1.08112400	3.38034900	0.15616800
C	0.70647500	2.53424600	1.10423300
H	1.25058300	3.49059400	1.09523700
H	1.07904800	1.88643900	1.92084600
H	-2.09112200	1.93600900	3.75920600

1_{Zr} anti-P/cis-S

E: -1010.27519411 A.U.

Zr	-0.09234300	0.71828900	-0.13581300
N	-1.88768300	-0.80327500	-0.19449000
N	0.60269300	-1.15650800	-0.07627100

C	-1.55250200	-2.13186000	-0.19825600
C	-2.53011300	-3.13936400	-0.26321200
H	-2.22054200	-4.19579200	-0.26515400
C	-3.88429600	-2.78581700	-0.32475600
H	-4.66329900	-3.56231900	-0.37733400
C	-4.22952000	-1.42123300	-0.31722100
H	-5.27915200	-1.09474600	-0.36353500
C	-3.21016400	-0.47015500	-0.24962100
H	-3.44488000	0.60392100	-0.24022400
C	-0.07606500	-2.43132500	-0.12763200
H	0.23859100	-3.03627500	-1.01225500
C	1.99889300	-0.92059600	0.11678500
C	2.84999800	-0.73022800	-1.03637000
C	4.18934600	-0.35174200	-0.82025600
H	4.85037700	-0.18978600	-1.68679100
C	4.70594100	-0.23339000	0.47939700
H	5.75873600	0.05584700	0.62457000
C	3.90537500	-0.53005400	1.59669100
H	4.34554800	-0.49322000	2.60596000
C	2.55705900	-0.89895400	1.44849400
C	2.39770300	-1.06978900	-2.43625400
H	1.29926600	-1.16232900	-2.53507300
C	1.77454800	-1.35352400	2.65607700
H	0.67968200	-1.36285300	2.49281400
H	2.77422100	-0.34473900	-3.18655200
H	2.82860400	-2.05360500	-2.72615500
H	1.99891900	-0.73554000	3.54897800
H	2.07261300	-2.39230500	2.92042300
C	-2.52701600	1.16505600	2.69967000
H	-3.44267300	0.70480200	2.27521200
H	0.15031800	-3.06159600	0.76548600
H	-1.80192700	0.36816700	2.95374800
C	-1.98226800	2.25682100	1.83867700
C	-0.63586900	2.56399200	1.63528500
C	0.08704500	1.55619100	-2.60725600
H	0.33843100	0.87451000	-3.43708000
C	1.11857300	2.14387200	-1.90764100
H	0.94378600	2.93195600	-1.14168300
C	-1.32674000	1.64333300	-2.24661800
H	-1.99899800	0.90881000	-2.72130900
C	-1.86606500	2.59315600	-1.40238100
H	-1.29525100	3.47460000	-1.06734000
H	-2.94947200	2.62221800	-1.21036200
H	2.16797000	2.00601300	-2.20757700
H	-2.71282900	3.01370200	1.50088200
H	-0.42588000	3.53820600	1.15420000
C	0.47980400	1.69858100	1.88749900
H	1.49705200	2.13312000	1.84445400
H	0.37534400	0.88925900	2.63333000
H	-2.85789500	1.62906000	3.65962700

TS_{1-2Zr} anti-P/cis-S

E: -1010.27455352 A.U.

Zr	-0.10895000	0.69968900	-0.42247900
N	-2.14624100	-0.45840900	-0.24780000
N	0.17641000	-0.87860800	0.77708500
C	-2.13540000	-1.51766400	0.61877100
C	-3.30018500	-2.26039400	0.88264200
H	-3.25924900	-3.10583000	1.58678200
C	-4.49575800	-1.92176600	0.23482300
H	-5.41514000	-2.49764400	0.42386700

C	-4.50042800	-0.83902400	-0.66575100
H	-5.41442900	-0.54208600	-1.20125000
C	-3.31258900	-0.13647600	-0.87561000
H	-3.28419900	0.71671000	-1.57286900
C	-0.79811600	-1.84920500	1.24233300
H	-0.50028300	-2.88770700	0.96939200
C	1.58786000	-1.08630500	0.64453500
C	2.08708400	-1.96259500	-0.39029000
C	3.47513000	-2.03572400	-0.58490100
H	3.87399100	-2.69322600	-1.37389700
C	4.36563400	-1.28616100	0.20990500
H	5.44971600	-1.35497300	0.02800700
C	3.88196400	-0.48428600	1.25114400
H	4.59050200	0.05354100	1.90121000
C	2.49817200	-0.39325000	1.51775900
C	1.17065300	-2.82106400	-1.23163600
H	0.18559200	-2.35289400	-1.43854600
C	2.04210400	0.30778700	2.77346100
H	0.94117200	0.35195400	2.85760700
H	1.64056900	-3.07870000	-2.20095300
H	0.96599700	-3.78972800	-0.72375500
H	2.46352100	1.33116600	2.86432400
H	2.41403600	-0.24990400	3.66002500
C	-1.59902800	1.77486800	2.57427700
H	-2.12255000	0.80587800	2.70856400
H	-0.87425200	-1.84553900	2.35691500
H	-0.55272100	1.69401300	2.92054500
C	-1.75876500	2.32086000	1.19309700
C	-0.81171400	2.95480800	0.40047000
C	1.74966500	1.09841900	-1.93822800
H	2.69302200	0.56430100	-1.73344700
C	1.62210400	2.42893400	-1.42953500
H	0.96182600	3.14390200	-1.95247700
C	0.79270800	0.42163200	-2.76765100
H	1.12095400	-0.53869000	-3.20102200
C	-0.56544100	0.72695500	-2.84178600
H	-0.93797200	1.75463300	-2.61266400
H	-1.24806900	0.11251800	-3.44745700
H	2.54437400	2.87707200	-1.03214100
H	-2.80317500	2.40092900	0.83994600
H	-1.20651900	3.52175700	-0.46697700
C	0.63956700	2.92213300	0.52639800
H	1.14686400	3.86457500	0.27624500
H	1.08131400	2.45738200	1.43101200
H	-2.11942200	2.48324200	3.26182500

1_{Zr} anti-S/cis-P

E: -1010.28475131 A.U.

Zr	0.27065800	0.80328200	-0.11790300
N	2.14572000	-0.60963100	0.08539600
N	-0.38581700	-1.09500200	0.06129600
C	1.86268000	-1.94547300	0.14038300
C	2.88011500	-2.90820500	0.26273300
H	2.61680200	-3.97653700	0.29970200
C	4.21635300	-2.49423600	0.33940600
H	5.02622700	-3.23425900	0.43398400
C	4.50392000	-1.11684900	0.29898700
H	5.53685600	-0.74365800	0.36326000
C	3.44695100	-0.21376200	0.17126400
H	3.64252800	0.86878600	0.13471200
C	0.40272000	-2.31675100	0.06725500

H	0.12258600	-2.96372100	0.93257200
C	-1.81722200	-1.07157300	0.04248700
C	-2.54194400	-0.95335000	1.28591400
C	-3.94192900	-0.81732400	1.23565600
H	-4.50793900	-0.71975300	2.17605400
C	-4.62789200	-0.85191700	0.01191100
H	-5.72380600	-0.74446400	-0.00584300
C	-3.92939100	-1.08155300	-1.18606000
H	-4.48813700	-1.17595400	-2.13098500
C	-2.53098400	-1.22793500	-1.20103800
C	-1.87376700	-1.11344000	2.63286100
H	-0.77611400	-1.23211400	2.56296500
C	-1.85413100	-1.64533800	-2.48410900
H	-0.75247700	-1.55646300	-2.45261700
H	-2.10635400	-0.27977500	3.33154600
H	-2.26449600	-2.02585700	3.13237600
H	-2.23542400	-1.07398800	-3.35508800
H	-2.09061900	-2.71167700	-2.69425600
C	2.05694500	2.42770800	-1.54682000
H	3.15765600	2.39337700	-1.65366800
H	0.20643800	-2.93614200	-0.84080800
H	1.69136200	3.39096300	-1.96367300
C	1.40093600	1.22549600	-2.19893000
C	0.03631500	1.23636100	-2.57112900
C	-0.41072100	2.96219100	1.34671200
H	-0.33677300	3.90325700	0.77400200
C	-1.62926600	2.34189100	1.43261400
H	-1.81038100	1.48591100	2.10205500
C	0.83657000	2.48324100	1.96719100
H	1.69675600	3.17494600	1.92316000
C	1.01574000	1.25287400	2.54065800
H	0.18100200	0.54630200	2.70140400
H	1.99040700	0.96129100	2.96165400
H	-2.50752400	2.75447700	0.91212400
H	2.06161900	0.48519000	-2.67582000
H	-0.31903800	0.40651400	-3.20340600
C	-0.91051400	2.04295200	-1.91430600
H	-1.98376200	1.92227800	-2.12967600
H	-0.61860300	3.05100600	-1.56289300
H	1.89667000	2.54117800	-0.42541200

TS_{1-2Zr} anti-S/cis-P

E: -1010.25617581 A.U.

Zr	0.04650700	0.50585100	0.42480300
N	2.01352000	-0.70621600	0.07844100
N	-0.39015900	-1.46727100	0.33857900
C	1.89752300	-2.07048800	0.12204900
C	3.02809100	-2.90360000	0.06068500
H	2.90119600	-3.99637900	0.10189300
C	4.30220300	-2.33199600	-0.05461100
H	5.19759700	-2.97086500	-0.10653600
C	4.41828600	-0.92951700	-0.10344000
H	5.39830700	-0.43776900	-0.19280500
C	3.25735900	-0.15832800	-0.03315200
H	3.31034300	0.94124800	-0.06400800
C	0.48968500	-2.61061300	0.23890300
H	0.40553800	-3.26479000	1.14015800
C	-1.77831400	-1.32805900	0.10558700
C	-2.53508100	-0.68408800	1.15700700
C	-3.83971900	-0.20835700	0.85449500
H	-4.42630800	0.29074000	1.64257200

C	-4.41230000	-0.44254800	-0.39637900
H	-5.43506000	-0.09407000	-0.60880700
C	-3.70119300	-1.16551400	-1.38222800
H	-4.18482800	-1.37436100	-2.35008700
C	-2.38793200	-1.60971700	-1.17146100
C	-2.10894700	-0.73646800	2.61588700
H	-1.03933500	-0.98254100	2.76757800
C	-1.66045100	-2.36968200	-2.25450800
H	-0.60627900	-2.04470900	-2.37973900
H	-2.36348700	0.19049100	3.16937300
H	-2.67757200	-1.55245200	3.11528600
H	-2.16828200	-2.25598300	-3.23109900
H	-1.63751100	-3.45894300	-2.03084500
C	1.44929000	3.29454400	-2.39655700
H	1.62464000	3.49042100	-3.48165300
H	0.25553600	-3.26555100	-0.63083600
H	0.60576900	3.93344000	-2.07596200
C	1.21814700	1.83228000	-2.24417900
C	0.02791200	1.18387900	-1.94541200
C	0.37347100	3.13403200	0.91218600
H	0.76029000	4.00988800	0.36841100
C	-0.98749200	2.78013700	0.70550200
H	-1.51308800	2.09319100	1.41601600
C	1.29784100	2.41378200	1.71825900
H	2.35099200	2.74185500	1.66749900
C	0.99669300	1.24905300	2.45888100
H	-0.02014300	1.12919600	2.89681900
H	1.78679600	0.74700700	3.03848700
H	-1.68771100	3.52777600	0.30899400
H	2.05843300	1.18153900	-2.54867900
H	0.01607500	0.08459000	-2.11428900
C	-1.18675800	1.77567600	-1.42403600
H	-2.11021000	1.16779300	-1.43846500
H	-1.36060800	2.83615300	-1.65127000
H	2.38523500	3.62702400	-1.90014800

1_{Zr} anti-S/cis-S

E: -1010.28662491 A.U.

Zr	0.21243100	0.77584100	-0.00235400
N	2.20143400	-0.52791400	0.01339300
N	-0.26842100	-1.16908400	-0.00727400
C	2.01127700	-1.88312600	-0.01917800
C	3.09150700	-2.78262100	-0.01201200
H	2.89683900	-3.86582600	-0.03899900
C	4.40131200	-2.28826500	0.03297400
H	5.25975400	-2.97790700	0.03939200
C	4.59807900	-0.89539000	0.07729000
H	5.60707600	-0.45922800	0.12215800
C	3.48108400	-0.05844300	0.06795400
H	3.61045900	1.03312600	0.11075200
C	0.57776500	-2.34479800	-0.04874800
H	0.37244900	-3.02281000	0.81411600
C	-1.69938700	-1.18938800	-0.01636600
C	-2.42036800	-1.25307700	1.23206900
C	-3.82253200	-1.14665100	1.19640300
H	-4.38969400	-1.17945800	2.14049300
C	-4.51146500	-1.04262200	-0.02405500
H	-5.60981100	-0.96111100	-0.02651400
C	-3.81389400	-1.09968900	-1.24141900
H	-4.37348600	-1.09650800	-2.19050300
C	-2.41067600	-1.20770300	-1.27156100

C	-1.73249300	-1.55998900	2.54192500
H	-0.64668700	-1.34312700	2.53200200
C	-1.71966700	-1.48706700	-2.58563300
H	-0.63522200	-1.26725400	-2.57319600
H	-2.20235700	-1.03069400	3.39609100
H	-1.84002900	-2.64443900	2.76660600
H	-2.19209700	-0.94308800	-3.42877600
H	-1.82646700	-2.56762100	-2.82953000
C	1.78994600	2.30251600	-1.71717700
H	2.80231600	2.00416400	-2.04548900
H	0.38344200	-2.95561500	-0.96279000
H	1.61906900	3.37284000	-1.96656300
C	0.72977400	1.39472400	-2.26386500
C	-0.64770200	1.72540000	-2.17458000
C	-0.85558300	1.70860900	2.08178700
H	-1.57986700	0.97321200	2.46394400
C	-1.33218800	2.76659900	1.31949800
H	-0.72985500	3.67002000	1.13878600
C	0.54354900	1.50110300	2.44063500
H	0.76623600	0.62983600	3.08202200
C	1.59793200	2.24359700	1.95184800
H	1.44875500	3.21842800	1.45552100
H	2.63180000	1.99195500	2.23383300
H	-2.41222600	2.85690700	1.13263700
H	1.03593200	0.57936800	-2.93858100
H	-1.36776000	1.04753700	-2.66212100
C	-1.14939100	2.74900400	-1.35610100
H	-2.23519200	2.91432500	-1.30780700
H	-0.51752200	3.61712900	-1.10712000
H	1.85452800	2.33486900	-0.56917400

TS_{1-2Zr} anti-S/cis-S

E: -1010.28027721 A.U.

Zr	0.20642700	0.72702100	0.01999900
N	2.23195800	-0.49390800	-0.00029400
N	-0.19090700	-1.23415200	-0.04796200
C	2.10572400	-1.85682600	-0.06471000
C	3.22781000	-2.70227700	-0.09177800
H	3.08539400	-3.79268700	-0.14265400
C	4.51292100	-2.14578400	-0.05143000
H	5.40343900	-2.79322400	-0.07164400
C	4.64400600	-0.74630700	0.02078000
H	5.63166000	-0.26336300	0.06037900
C	3.48879800	0.03612000	0.04691000
H	3.56512900	1.13182300	0.11243400
C	0.69298300	-2.38035400	-0.09372000
H	0.51932400	-3.07117600	0.76593200
C	-1.61932400	-1.27304300	-0.04374600
C	-2.32915900	-1.41677200	1.20668700
C	-3.73244200	-1.33367300	1.18848400
H	-4.29044700	-1.42877900	2.13375500
C	-4.43479300	-1.17097700	-0.01890200
H	-5.53455300	-1.11128800	-0.00663200
C	-3.74899300	-1.13921800	-1.24332800
H	-4.31815400	-1.08788700	-2.18542900
C	-2.34386300	-1.22223500	-1.29194900
C	-1.62072300	-1.76688600	2.49357700
H	-0.54701900	-1.49509100	2.49491700
C	-1.66195700	-1.39368400	-2.62868100
H	-0.56444400	-1.26565500	-2.58112700
H	-2.11219500	-1.30891100	3.37604900

H	-1.67387800	-2.86649000	2.65647400
H	-2.07530900	-0.71449200	-3.40263400
H	-1.85225800	-2.42361400	-3.00309100
C	1.54404300	2.29827800	-1.85072200
H	2.44262700	1.90210200	-2.35760300
H	0.52288700	-2.99278200	-1.01167400
H	1.47586200	3.39659200	-2.01795600
C	0.29877500	1.57369800	-2.26376300
C	-0.98233400	1.94575000	-1.82583600
C	-0.76802100	1.54187900	2.04501300
H	-1.35516200	0.72791100	2.49625500
C	-1.47547000	2.54880700	1.31315400
H	-1.14654800	3.59444000	1.42593100
C	0.63929400	1.60771000	2.36275400
H	1.03854700	0.82863600	3.03728000
C	1.52930900	2.45990000	1.73102200
H	1.18143000	3.36240900	1.19881600
H	2.60419300	2.41740900	1.96382400
H	-2.56638400	2.41537700	1.26235400
H	0.37883400	0.81292900	-3.05681400
H	-1.84811800	1.39826600	-2.23510900
C	-1.22737600	2.92857400	-0.80536900
H	-2.25816000	3.30971100	-0.76474000
H	-0.46440100	3.71806000	-0.68840200
H	1.77803200	2.25923900	-0.72772800

2Zr anti-P/cis-P

E: -1010.30261519 A.U.

Zr	-0.09660000	0.45020200	-0.16752600
N	-1.48397600	-1.43246700	-0.10043800
N	0.82497300	-1.05768800	0.88290800
C	-1.05162400	-2.49552800	0.64890100
C	-1.85059800	-3.63424200	0.84826600
H	-1.46923700	-4.46310800	1.46425700
C	-3.11526900	-3.70441400	0.25022000
H	-3.75197400	-4.59180100	0.39070400
C	-3.55019100	-2.62544000	-0.54263100
H	-4.52884000	-2.63936700	-1.04491900
C	-2.71311100	-1.51949200	-0.69186100
H	-3.02299900	-0.66800400	-1.31467600
C	0.33892400	-2.37517900	1.21754400
H	0.97573800	-3.19431700	0.82058800
C	2.11824300	-0.57671400	0.65772800
C	3.22067700	-1.29129700	0.06818400
C	4.31720600	-0.53212000	-0.36798800
H	5.17011500	-1.06423800	-0.81979700
C	4.36486400	0.88021000	-0.28467200
H	5.24575900	1.41970500	-0.66455900
C	3.32445500	1.57350100	0.32463000
H	3.39530800	2.66289800	0.47279500
C	2.20694200	0.86294500	0.85215600
C	3.22957900	-2.78960900	-0.12205400
H	2.41249700	-3.13087500	-0.79384100
C	1.28218800	1.56834300	1.82328200
H	1.07815300	0.96627400	2.73046200
H	4.18158900	-3.11373500	-0.58347500
H	3.13578600	-3.33647400	0.83955500
H	0.24454000	1.88892800	1.44676700
H	1.70087000	2.54961500	2.12163300
C	-1.88902900	3.27662400	2.54771400
H	-1.19893500	3.01384800	3.37694000

H	0.31584700	-2.51778400	2.32445900
H	-1.46893500	4.11614700	1.96193200
C	-2.26232400	2.08075100	1.73678900
C	-2.35961300	1.98056500	0.37145700
C	-1.34202800	1.27385500	-2.27599600
H	-2.39113200	1.09243500	-2.56706400
C	-1.06030800	2.64452800	-1.68894200
H	-0.03286200	2.70032700	-1.21871400
C	-0.37471900	0.35598800	-2.68207200
H	-0.73563100	-0.57710500	-3.15122200
C	0.99059600	0.42675000	-2.24864200
H	1.51455600	1.40228400	-2.26585500
H	1.65640400	-0.41648500	-2.49719300
H	-0.95959600	3.39326500	-2.50970100
H	-2.56775900	1.18985600	2.31959900
H	-2.86694300	1.06793800	-0.00039700
C	-2.12811000	3.07367700	-0.65822600
H	-3.08780100	3.26857900	-1.18697400
H	-1.83848700	4.03257200	-0.18520300
H	-2.80951900	3.64942200	3.05496300

2_{Zr} anti-P/cis-S

E: -1010.30165448 A.U.

Zr	-0.06370600	0.42659600	-0.22601800
N	-2.14079000	-0.63007900	-0.09432900
N	0.16700000	-1.41365800	0.53653200
C	-2.15355500	-1.87633900	0.47155300
C	-3.35431800	-2.57725900	0.67215900
H	-3.33133000	-3.57806600	1.13018700
C	-4.56700500	-1.99473200	0.27782900
H	-5.51686800	-2.53243700	0.42327300
C	-4.54976700	-0.71820200	-0.31513500
H	-5.47595900	-0.22759200	-0.64932800
C	-3.32229800	-0.07529200	-0.48647000
H	-3.27241200	0.91567400	-0.96469600
C	-0.80051700	-2.44371700	0.84275100
H	-0.61438800	-3.38365500	0.27270800
C	1.57468900	-1.35119300	0.65733800
C	2.47486000	-2.20201900	-0.06540100
C	3.83971400	-1.86552600	-0.04582100
H	4.55286700	-2.51105900	-0.58337300
C	4.31790000	-0.71509200	0.61784200
H	5.39346400	-0.48086600	0.59415500
C	3.44014400	0.10824400	1.33026200
H	3.83005100	0.97065800	1.89378000
C	2.05994500	-0.21144900	1.39928100
C	1.98154200	-3.41514700	-0.81104200
H	1.09872200	-3.18556500	-1.44480200
C	1.16349700	0.50786800	2.39733100
H	0.38891200	1.21868000	1.97966500
H	2.77143500	-3.83240100	-1.46375800
H	1.68164900	-4.22446100	-0.11009200
H	1.76545300	1.16123700	3.05850400
H	0.60078500	-0.20597900	3.03138400
C	-0.92190400	3.53064400	2.29907800
H	-1.20671500	2.90421700	3.17018000
H	-0.77466800	-2.72756600	1.92159800
H	0.17186400	3.69674900	2.28804500
C	-1.48484400	3.00511300	1.02186600
C	-0.85617800	2.89202000	-0.19374500
C	1.55987200	1.19517700	-1.89985700

H	2.62942300	0.98214400	-1.73168000
C	1.14595200	2.67180300	-1.86054200
H	0.41805800	2.88111600	-2.67483200
C	0.79407100	0.18417900	-2.51564600
H	1.29436100	-0.78474000	-2.69908600
C	-0.62086000	0.22659100	-2.56853500
H	-1.12812700	1.20149200	-2.71845000
H	-1.17388100	-0.63610600	-2.96936300
H	2.05757500	3.25422900	-2.10699000
H	-2.56476900	2.76434600	1.04330100
H	-1.51613700	2.70324400	-1.06652500
C	0.58116300	3.27606200	-0.53188500
H	0.60271200	4.38350800	-0.65262700
H	1.27385100	3.08670000	0.32310000
H	-1.40378300	4.51841900	2.49178500

2_{Zr} anti-S/cis-P

E: -1010.30277920 A.U.

Zr	0.02744500	-0.54256600	-0.02592900
N	-1.45045600	1.28456200	0.09276500
N	0.99795300	1.19236900	-0.46416500
C	-0.94392100	2.51833300	-0.21274200
C	-1.75274200	3.66726200	-0.23164100
H	-1.30696700	4.64274100	-0.47985300
C	-3.11608800	3.55443100	0.07073900
H	-3.76531800	4.44379300	0.06533200
C	-3.63712100	2.28614500	0.38801500
H	-4.69921400	2.14945100	0.64010600
C	-2.77699700	1.18659600	0.39158600
H	-3.14829300	0.18525900	0.65067600
C	0.53396200	2.55847300	-0.51062700
H	1.04982300	3.21481600	0.22600300
C	2.28186400	0.63422800	-0.51883100
C	3.41650800	1.06072700	0.24989500
C	4.51361200	0.18600800	0.31159000
H	5.39802900	0.49442800	0.89243800
C	4.51314600	-1.08596000	-0.30782200
H	5.39044400	-1.74254200	-0.20318000
C	3.42826800	-1.48683400	-1.08667900
H	3.46465000	-2.44074600	-1.63650500
C	2.31496900	-0.61648000	-1.25436800
C	3.43512600	2.37074900	0.99743500
H	2.59442200	2.44546000	1.72058200
C	1.33094700	-0.87581800	-2.38238700
H	0.28338800	-1.25129800	-2.11169200
H	4.37414800	2.48246800	1.57153100
H	3.36890900	3.24102100	0.31061700
H	1.68782300	-1.69724300	-3.03469100
H	1.15550900	0.02422800	-3.00414200
C	-3.75797500	-1.26720400	-1.88310100
H	-4.27943900	-1.88567700	-2.65009500
H	0.71872300	3.01536200	-1.51194200
H	-4.36509600	-1.30459400	-0.95971300
C	-2.37376800	-1.80165400	-1.72976500
C	-1.83698900	-2.45435000	-0.64836600
C	-1.27037100	-1.24551700	2.20048300
H	-2.11347600	-0.63208000	2.56339800
C	-1.61041900	-2.68765200	1.86262500
H	-0.69303900	-3.30203700	1.73182600
C	0.01220900	-0.75605100	2.45301100
H	0.08825500	0.23937300	2.92962600

C	1.19417100	-1.29552300	1.84976900
H	1.25180900	-2.38735400	1.65189200
H	2.17001400	-0.84336300	2.08836400
H	-2.11683900	-3.11412500	2.75844700
H	-1.75239900	-1.73876700	-2.64494000
H	-0.85910200	-2.96884700	-0.82413300
C	-2.52707200	-2.85760400	0.63664400
H	-2.82246200	-3.92783900	0.54594000
H	-3.47475000	-2.29553800	0.77337000
H	-3.75774600	-0.23607200	-2.29505600

H	2.75374600	1.95401000	1.16912600
C	1.50317700	3.39477300	0.03491000
H	2.09537300	4.30014300	0.30716800
H	0.44962500	3.74516500	0.00740600
H	-0.90657100	3.18392600	1.49741400

Zirconium - Path 2

2_{Zr} anti-S/cis-S

E: -1010.30346507 A.U.

Zr	-0.13511700	0.60635100	-0.00482000
N	-2.35188300	-0.13023700	0.02283800
N	-0.13828000	-1.34949100	-0.32590600
C	-2.52074200	-1.47145500	-0.19190700
C	-3.79945700	-2.05405800	-0.20591500
H	-3.90397700	-3.13454000	-0.38956300
C	-4.92615400	-1.25046400	0.01748800
H	-5.93498400	-1.69191100	0.01404000
C	-4.74860900	0.12874600	0.23803400
H	-5.60489500	0.79790000	0.40912400
C	-3.45343700	0.64892000	0.22278400
H	-3.28308500	1.72884500	0.36162100
C	-1.25461400	-2.27215700	-0.41214700
H	-1.29352000	-2.78123200	-1.40491200
C	1.21749100	-1.62938400	0.03118500
C	2.19996100	-1.92322300	-0.97686500
C	3.53423400	-2.09582000	-0.56336500
H	4.30418500	-2.32397500	-1.31757000
C	3.89751000	-2.00053300	0.79088200
H	4.94966400	-2.14242800	1.08392700
C	2.92906000	-1.75359700	1.77856900
H	3.22473000	-1.72414900	2.83934300
C	1.57590800	-1.58643200	1.42892100
C	1.81681200	-2.13344400	-2.41849100
H	0.85262000	-1.65737700	-2.68051800
C	0.52090700	-1.48894900	2.50952500
H	-0.34185600	-0.82135100	2.26297600
H	2.60230600	-1.76791900	-3.10938400
H	1.70631900	-3.22159800	-2.62342000
H	0.94787800	-1.14519600	3.47129200
H	0.06025500	-2.48357300	2.69879700
C	-0.59725300	2.39024700	2.20738200
H	-1.34053500	1.54751200	2.17576100
H	-1.16765800	-3.08643100	0.34457000
H	-0.75396600	2.79669100	3.23201400
C	0.83264600	1.92993200	2.04996500
C	1.73033900	2.37044000	1.11227400
C	1.45036300	1.54088700	-1.84379300
H	2.23370900	0.85243100	-2.20367300
C	1.98257400	2.89153100	-1.34632800
H	1.74439400	3.66683800	-2.10829100
C	0.16471900	1.28796000	-2.35763000
H	0.05951700	0.40346500	-3.01313000
C	-1.03710300	1.84811700	-1.85154200
H	-1.02438100	2.87076800	-1.41858300
H	-1.99496200	1.55993600	-2.31084800
H	3.08864800	2.81739600	-1.32162400
H	1.20323300	1.22848400	2.81758900

1_{Zr} syn-P/trans-P

E: -1010.28089423 A.U.

Zr	0.12009100	0.72717600	0.04916800
N	1.98814800	-0.70084700	0.16338500
N	-0.44360500	-1.08630900	-0.60785800
C	1.76104800	-1.98736200	-0.24525100
C	2.77956100	-2.95578900	-0.22835100
H	2.56415500	-3.97820500	-0.57526600
C	4.05470300	-2.60857900	0.23875300
H	4.86215900	-3.35674900	0.26653900
C	4.28396000	-1.28892100	0.66988100
H	5.26821400	-0.97046900	1.04446600
C	3.23483500	-0.36904000	0.60659700
H	3.38957500	0.67642000	0.91363400
C	0.35292800	-2.30065300	-0.69398300
H	-0.07614100	-3.11972300	-0.07156300
C	-1.83976900	-1.03273800	-0.32692300
C	-2.31490500	-1.32593500	1.01149600
C	-3.69187000	-1.21785900	1.27040700
H	-4.07204700	-1.43656800	2.28121200
C	-4.59219700	-0.85660300	0.25237000
H	-5.66802300	-0.78379600	0.47741800
C	-4.13811400	-0.62378100	-1.05623400
H	-4.86547600	-0.39403700	-1.85119100
C	-2.77379400	-0.73052300	-1.38580800
C	-1.39281600	-1.81683100	2.10625600
H	-0.32374200	-1.55419600	1.95143300
C	-2.35114600	-0.66584300	-2.83053700
H	-1.25300900	-0.67812400	-2.95998600
H	-1.70525400	-1.44779200	3.10443000
H	-1.42624800	-2.92709400	2.17121200
H	-2.77322100	0.22204500	-3.34518300
H	-2.75466500	-1.55002500	-3.37107500
C	1.72375500	1.58825800	-1.84469100
H	0.36102700	-2.69146200	-1.74000600
H	1.45632500	0.66988700	-2.41114200
C	0.69459500	2.50612300	-1.61225000
C	-0.68335400	2.13835900	-1.66123700
C	-0.78090400	2.72407800	1.58228600
H	-0.95112200	3.64063100	0.99232000
C	-1.82802300	1.85841600	1.77037700
H	-1.78156200	1.02425200	2.49010000
C	0.57551200	2.53084700	2.12307800
H	1.25616100	3.39859000	2.06909700
C	1.05891200	1.34326800	2.59784000
H	0.41565400	0.45137000	2.75208400
H	2.08424600	1.25413700	2.98825000
H	-2.80858700	2.04881700	1.30608600
H	0.97334600	3.48582300	-1.17427800
H	-0.98507300	1.39531400	-2.42165500
C	3.18484000	1.93332100	-1.80939700

H	3.82171100	1.07596100	-1.51417900
H	3.51352800	2.21351800	-2.83571600
H	3.40391500	2.79782900	-1.15030400
H	-1.44784100	2.90342400	-1.45022100

TS1-2Zr syn-P/trans-P

E: -1010.25642850 A.U.

Zr	-0.03474700	0.64154600	-0.30858900
N	-2.01978600	-0.57768500	-0.22883100
N	0.36305200	-1.23187000	0.28973700
C	-1.90756200	-1.90418000	0.09151300
C	-3.02888100	-2.75136900	0.09070900
H	-2.91026000	-3.81309100	0.35660000
C	-4.28358100	-2.23472000	-0.26276900
H	-5.17047500	-2.88728400	-0.27771300
C	-4.39148300	-0.87258500	-0.60268200
H	-5.35495200	-0.42807900	-0.89325400
C	-3.24187100	-0.08042800	-0.56724900
H	-3.28861500	0.99078300	-0.82455800
C	-0.50804800	-2.38184400	0.40834500
H	-0.21741800	-3.20056400	-0.29251200
C	1.78944700	-1.17289200	0.26752400
C	2.49168600	-1.36147100	-0.98490600
C	3.87993400	-1.11690500	-1.01208000
H	4.42920300	-1.24322800	-1.95882000
C	4.57681200	-0.76037100	0.15309800
H	5.66284500	-0.58286500	0.10706100
C	3.90753500	-0.67016800	1.38613600
H	4.47948000	-0.44375700	2.30027000
C	2.52152200	-0.89037700	1.47946300
C	1.82358400	-1.94540600	-2.20992600
H	0.72127500	-1.84042600	-2.21596900
C	1.85857700	-0.91893800	2.83491100
H	0.75395200	-0.88172300	2.77601900
H	2.22986900	-1.51487700	-3.14716400
H	2.04017800	-3.03585100	-2.25452500
H	2.21758000	-0.10341600	3.49570600
H	2.11930500	-1.86782600	3.35372700
C	-1.44489900	1.41197500	2.12436200
H	-0.46612900	-2.83330300	1.42936500
H	-0.92391900	0.54846700	2.58576000
C	-0.67752800	2.36267100	1.48212400
C	0.78023300	2.30379200	1.33891100
C	0.29211200	3.08724500	-1.53906300
H	-0.01571100	4.13905700	-1.41639800
C	1.41809700	2.64507200	-0.77206100
H	1.97108700	1.71558100	-1.07235400
C	-0.51017400	2.27192400	-2.36825800
H	-1.41396200	2.74457100	-2.79257300
C	-0.32647200	0.87780200	-2.58650300
H	0.72311400	0.48492400	-2.60179300
H	-0.98179500	0.34355100	-3.29184200
H	2.13532100	3.39856500	-0.41900500
H	-1.19359600	3.25829000	1.08761800
H	1.31635000	1.53270300	1.92723200
C	-2.90131500	1.53127100	2.40569000
H	-3.44435000	0.58571300	2.19807100
H	-3.03176900	1.70747600	3.49911800
H	-3.38206500	2.37201200	1.86897400
H	1.27614500	3.27905500	1.44643400

1Zr syn-P/trans-S

E: -1010.28213210 A.U.

Zr	0.18348100	0.76767500	0.33875400
N	2.10563200	-0.56415200	0.13284600
N	-0.38355100	-1.00953400	-0.37785000
C	1.88016200	-1.82727000	-0.33933800
C	2.92575400	-2.75872500	-0.46809400
H	2.71178700	-3.76700400	-0.85502200
C	4.22618100	-2.39270800	-0.09497900
H	5.05534000	-3.11193200	-0.18298500
C	4.45374300	-1.09252900	0.39466300
H	5.45731600	-0.76180700	0.70103000
C	3.37331800	-0.21242700	0.48685400
H	3.52081700	0.81538600	0.85643100
C	0.45030000	-2.15661000	-0.69657200
H	0.11312200	-3.06069300	-0.13606300
C	-1.81619700	-0.99785300	-0.45579600
C	-2.58779500	-1.47671300	0.66426300
C	-3.98823300	-1.36339400	0.60360400
H	-4.59381400	-1.71737400	1.45334300
C	-4.62647800	-0.83628500	-0.53216300
H	-5.72461100	-0.75644000	-0.55508000
C	-3.87523400	-0.45253600	-1.65329900
H	-4.39104700	-0.09639400	-2.55938300
C	-2.47009100	-0.54826100	-1.65628700
C	-1.95577200	-2.18418900	1.84009900
H	-0.87224200	-1.98244400	1.94762500
C	-1.72483700	-0.27586100	-2.94245000
H	-0.62447500	-0.30292900	-2.82813400
H	-2.46467000	-1.93350800	2.79318600
H	-2.06715700	-3.28452400	1.71950300
H	-2.01271800	0.69541500	-3.39758800
H	-1.98991600	-1.04967600	-3.69500700
C	1.46268000	1.78266900	-1.77178800
H	0.36998300	-2.42772600	-1.77724200
H	0.94710200	0.97981800	-2.33977800
C	0.66184200	2.76545000	-1.18335300
C	-0.74875500	2.65391700	-1.00112400
C	-1.34987300	1.36171100	2.27964200
H	-2.31531600	0.83097200	2.32407900
C	-1.31593300	2.60502300	1.65548700
H	-0.47413200	3.30924300	1.78314100
C	-0.21442400	0.70290200	2.90293900
H	-0.43276000	-0.21425600	3.47501500
C	1.11057500	1.03126100	2.68968500
H	1.41337400	2.01689000	2.26522400
H	1.92022700	0.45244600	3.15897000
H	-2.25173500	3.04289100	1.28009000
H	1.17307800	3.63549700	-0.72426100
H	-1.32510600	1.98317200	-1.66645700
C	2.92997700	1.92935100	-2.02276300
H	3.47602900	0.96807200	-1.94276300
H	3.07609000	2.26945300	-3.07434600
H	3.40683300	2.68559400	-1.36745300
H	-1.30068300	3.54913800	-0.68658900

TS1-2Zr syn-P/trans-S

E: -1010.27934047 A.U.

Zr	0.15259700	0.71273000	0.36741800
N	2.12428600	-0.54291400	0.17350600

N	-0.31439100	-1.07721200	-0.39183200
C	1.96686700	-1.80851900	-0.32064100
C	3.06333100	-2.67424600	-0.47949200
H	2.90389700	-3.68758400	-0.87916000
C	4.34564600	-2.23568500	-0.12191900
H	5.21476900	-2.90224500	-0.23545000
C	4.50386400	-0.93205000	0.38596100
H	5.49107100	-0.54712000	0.68187700
C	3.37386800	-0.12221200	0.51655100
H	3.46368400	0.90246400	0.91273200
C	0.55223400	-2.20941400	-0.66609100
H	0.25088400	-3.10358300	-0.07000500
C	-1.74488000	-1.07354900	-0.47280800
C	-2.52135000	-1.59724200	0.62524400
C	-3.92062400	-1.48309000	0.56333600
H	-4.52934200	-1.87102800	1.39573700
C	-4.55549200	-0.90480600	-0.55058600
H	-5.65378900	-0.82658700	-0.57392000
C	-3.80166400	-0.46730100	-1.64943000
H	-4.31523200	-0.07291900	-2.54089600
C	-2.39595500	-0.56706800	-1.65352100
C	-1.88564800	-2.32578600	1.78447400
H	-0.82778800	-2.04480600	1.95766400
C	-1.64493700	-0.23946100	-2.92446500
H	-0.56376300	-0.46480100	-2.85659300
H	-2.45349000	-2.17209500	2.72385700
H	-1.89857900	-3.42240400	1.59596900
H	-1.77296000	0.81969000	-3.23692900
H	-2.05056500	-0.84581900	-3.76153100
C	1.26628300	1.87224800	-1.77464700
H	0.48372000	-2.52555600	-1.73488600
H	0.66029400	1.13001200	-2.33560000
C	0.58329500	2.81858400	-1.01889400
C	-0.83290800	2.79306200	-0.72963800
C	-1.41068200	1.30977600	2.14687200
H	-2.36076800	0.75242500	2.18728200
C	-1.41166200	2.56796200	1.47823200
H	-0.67970600	3.34214100	1.76882300
C	-0.29188100	0.75746600	2.86268300
H	-0.48989000	-0.14055200	3.47264600
C	1.03503400	1.11642300	2.64550900
H	1.30078800	2.11356900	2.22033100
H	1.85157000	0.60544300	3.17689600
H	-2.39419200	2.95996700	1.17818400
H	1.17665700	3.62915300	-0.55044300
H	-1.48886500	2.17486600	-1.37466500
C	2.71273600	1.95656500	-2.14099500
H	3.21018200	0.96554100	-2.13064400
H	2.78974900	2.31952700	-3.19206600
H	3.27815400	2.66630200	-1.50537400
H	-1.28246900	3.76774900	-0.49668000

1_{Zr} syn-S/trans-P

E: -1010.28132436 A.U.

Zr	-0.16928800	0.80294600	0.01253900
N	-2.06424200	-0.55394200	-0.24871100
N	0.40977700	-1.10465800	0.12687800
C	-1.83828300	-1.89762000	-0.13047400
C	-2.87649700	-2.83280600	-0.28237700
H	-2.66201400	-3.90711400	-0.17315100
C	-4.17016600	-2.38491500	-0.58368900

H	-4.99405800	-3.10420300	-0.71152600
C	-4.39561500	-1.00322400	-0.72696400
H	-5.39207800	-0.60639400	-0.97185700
C	-3.32431500	-0.12607100	-0.54406900
H	-3.47134800	0.96177100	-0.63872400
C	-0.41023900	-2.30502400	0.14530400
H	-0.06392500	-3.03895200	-0.61997300
C	1.83735400	-1.06399900	0.10808900
C	2.52896700	-1.07892400	-1.16295800
C	3.93019000	-0.94986000	-1.16202900
H	4.47353200	-0.95656100	-2.12060000
C	4.64654100	-0.85417300	0.04187900
H	5.74358000	-0.75867100	0.01886800
C	3.97882200	-0.92254200	1.27702500
H	4.56163400	-0.90012700	2.21171400
C	2.58035200	-1.05255000	1.34455500
C	1.81985000	-1.36066700	-2.46763200
H	0.71770900	-1.26954000	-2.40189700
C	1.92085300	-1.27095100	2.68261100
H	0.81998100	-1.17706100	2.64366400
H	2.18868200	-0.71841200	-3.29488200
H	2.02967700	-2.40481500	-2.78849300
H	2.31389500	-0.57867700	3.45507900
H	2.15128900	-2.29627700	3.04653800
C	-1.64734700	1.70739200	1.85444800
H	-0.33739100	-2.83386100	1.12606500
H	-1.71990500	2.59822200	1.17624400
C	-0.38835400	1.46668000	2.42554000
C	0.81093200	1.96520800	1.85111600
C	0.67768400	2.93431900	-1.41395600
H	0.71504500	3.84945100	-0.79702200
C	1.82455600	2.20140400	-1.57066300
H	1.90239200	1.37442900	-2.29581200
C	-0.62418000	2.61999500	-2.02818400
H	-1.38862600	3.41659600	-1.98322900
C	-0.96741600	1.41072700	-2.56678800
H	-0.23543400	0.58699700	-2.70134200
H	-1.96410500	1.23680700	-3.00081400
H	2.75291700	2.49167500	-1.05387500
H	-0.32987600	0.68156000	3.20223000
H	0.79940200	2.99485300	1.44510400
C	-2.94147200	1.25408900	2.46934400
H	-3.33539500	2.05645600	3.13245600
H	-3.73503700	1.05111800	1.72412800
H	-2.80321300	0.34948200	3.09486900
H	1.78211800	1.65469200	2.26674700

TS_{1-2Zr} syn-S/trans-P

E: -1010.25955656 A.U.

Zr	0.02701200	0.68405200	-0.29468600
N	-2.01729500	-0.47106400	-0.29587100
N	0.35602800	-1.30237700	-0.58242400
C	-1.95917700	-1.81371100	-0.56109100
C	-3.12365400	-2.58870700	-0.69944300
H	-3.03718800	-3.66466000	-0.91595100
C	-4.37861400	-1.98079200	-0.56542500
H	-5.30086400	-2.57254300	-0.67367800
C	-4.43808600	-0.60049900	-0.29572900
H	-5.40021900	-0.07770000	-0.18937700
C	-3.24395700	0.11092100	-0.16797700
H	-3.25710100	1.19240000	0.03405400

C	-0.57484600	-2.39819500	-0.70996500
H	-0.47835300	-2.89577200	-1.70518300
C	1.75027200	-1.27080500	-0.38825300
C	2.46000100	-0.34901500	-1.25102100
C	3.79386900	0.00951000	-0.91406100
H	4.34650000	0.70823500	-1.56249600
C	4.43223200	-0.58165300	0.17655800
H	5.47533700	-0.32078800	0.41382900
C	3.75865700	-1.55008700	0.95733100
H	4.29326400	-2.03094100	1.79246100
C	2.42270200	-1.90487300	0.71704400
C	1.93974300	0.02015800	-2.63342000
H	0.83301200	-0.01936300	-2.74716100
C	1.73830200	-2.92914000	1.58968200
H	0.72464800	-2.61134100	1.91297500
H	2.31329600	1.00606100	-2.97512000
H	2.31217200	-0.72841400	-3.36883400
H	2.33227300	-3.13505200	2.50033600
H	1.62090100	-3.89775100	1.05663300
C	-1.01453800	1.26763900	2.51355300
H	-0.41458500	-3.20186200	0.04439400
H	-1.04645600	2.37201700	2.55902700
C	0.19466500	0.67214500	2.18084300
C	1.38133800	1.40043000	1.78209500
C	-0.21302600	3.35780200	0.01333100
H	-0.52379200	4.04358100	0.81840500
C	1.13909300	2.92244600	0.00481100
H	1.58003100	2.44951700	-0.90804200
C	-1.21534800	2.92524800	-0.89813700
H	-2.25069800	3.23215500	-0.66747300
C	-0.99294500	2.05303000	-1.98601800
H	-0.02343600	2.10157700	-2.52359500
H	-1.83911500	1.74856900	-2.62157100
H	1.90318000	3.50411000	0.53815600
H	0.26189500	-0.43370700	2.22324100
H	1.53298900	2.37885900	2.25799300
C	-2.21031400	0.54948400	3.03302500
H	-2.28580100	0.75434600	4.12739300
H	-3.15786100	0.93816200	2.60623200
H	-2.15965000	-0.54790300	2.89597600
H	2.31581400	0.83221900	1.62649700

1_{Zr} syn-S/trans-S

E: -1010.28237476 A.U.

Zr	0.18038600	0.85517200	0.15242300
N	2.15924800	-0.39715600	0.22891700
N	-0.31411900	-1.06959800	-0.05539600
C	1.98810800	-1.74768700	0.10821600
C	3.08049600	-2.63232500	0.15876500
H	2.90879700	-3.71518900	0.05848700
C	4.37365300	-2.12322500	0.33692700
H	5.23978500	-2.80183300	0.38023500
C	4.54650000	-0.73093400	0.45836600
H	5.54286800	-0.28599200	0.59879200
C	3.42033600	0.09187000	0.39688300
H	3.52622500	1.18579400	0.48397300
C	0.56743500	-2.22463200	-0.07828800
H	0.29616500	-2.95181600	0.72369900
C	-1.74316300	-1.12690700	-0.16312200
C	-2.53855300	-1.33032800	1.02207800
C	-3.93762200	-1.25780400	0.90367700

H	-4.56149400	-1.40010400	1.80063500
C	-4.55126800	-1.03859900	-0.34214000
H	-5.64908100	-0.98164700	-0.40838100
C	-3.77607200	-0.94480000	-1.50731400
H	-4.27246400	-0.84593100	-2.48590600
C	-2.36987900	-1.02054600	-1.45566700
C	-1.92584800	-1.72037100	2.34668900
H	-0.85597800	-1.44873900	2.43494200
C	-1.59619400	-1.13883800	-2.74771500
H	-0.50636100	-0.99079700	-2.62675600
H	-2.47981100	-1.28647800	3.20389500
H	-1.98722200	-2.82382200	2.47529700
H	-1.97498000	-0.44182300	-3.52312500
H	-1.73892900	-2.16025500	-3.16463900
C	1.36284300	1.66494500	-1.92469900
H	0.46942300	-2.78673900	-1.03783800
H	1.87620000	2.39905900	-1.25122300
C	-0.00687600	1.87951500	-2.14446800
C	-0.80794400	2.73496600	-1.34706300
C	-1.26505000	1.69629300	2.04984500
H	-2.13900700	1.04728100	2.22141600
C	-1.42465800	2.82572000	1.25554200
H	-0.69270400	3.64997100	1.27257100
C	-0.02349300	1.32460900	2.71497700
H	-0.08178300	0.51179400	3.45876500
C	1.22254300	1.79729800	2.36358600
H	1.35604900	2.70154600	1.72981400
H	2.12908500	1.43197100	2.86933000
H	-2.41207100	3.06487300	0.83494100
H	-0.51465100	1.22391100	-2.87404700
H	-0.34635400	3.65526300	-0.94986700
C	2.25668100	0.88821700	-2.84602900
H	2.71900300	1.58609500	-3.58084500
H	3.09492700	0.39257900	-2.31770000
H	1.69585000	0.12969300	-3.42851400
H	-1.88468900	2.80313000	-1.56380100

TS_{1-2Zr} syn-S/trans-S

E: -1010.27631252 A.U.

Zr	-0.16458200	0.78887000	-0.23999800
N	-2.18482600	-0.39425500	-0.22876900
N	0.24989200	-1.14591900	0.01850800
C	-2.06619300	-1.74998400	-0.09554700
C	-3.19591400	-2.58714100	-0.08882400
H	-3.06644200	-3.67546000	0.01538400
C	-4.47271200	-2.02403700	-0.21574800
H	-5.36800800	-2.66512500	-0.21376000
C	-4.59171300	-0.62701400	-0.34786100
H	-5.57356500	-0.14176600	-0.45209100
C	-3.42973500	0.14669000	-0.35210700
H	-3.48987400	1.24169400	-0.46472300
C	-0.65783000	-2.27922900	0.03674500
H	-0.43438500	-2.99261700	-0.79250100
C	1.67265000	-1.19907500	0.16634400
C	2.50957500	-1.36249900	-0.99722700
C	3.90427900	-1.28146000	-0.82935800
H	4.55924600	-1.39203700	-1.70842900
C	4.47298200	-1.09684500	0.44169900
H	5.56764200	-1.03683700	0.54717200
C	3.65834200	-1.03895400	1.58440700
H	4.12233700	-0.96424800	2.58089900

C	2.25676600	-1.11838000	1.48260200
C	1.94702200	-1.71984200	-2.35167000
H	0.86945800	-1.48966700	-2.45697800
C	1.43072100	-1.25799800	2.73964600
H	0.35533000	-1.04486400	2.58527800
H	2.50379500	-1.22775300	-3.17501300
H	2.05899200	-2.81363900	-2.52177900
H	1.81533700	-0.62077900	3.56204500
H	1.50093100	-2.30453900	3.11105700
C	-1.19098600	1.92885700	1.90792400
H	-0.55090700	-2.86832400	0.97842400
H	-1.67512500	2.68963400	1.24959800
C	0.19797900	1.91838800	1.95236300
C	1.07161000	2.73236200	1.12548300
C	1.30466300	1.72001600	-1.94232200
H	2.24741300	1.18789800	-2.14681700
C	1.34192500	2.84225000	-1.05305700
H	0.58213600	3.63167300	-1.18976100
C	0.14234400	1.33786600	-2.69520300
H	0.28451300	0.57069600	-3.47543000
C	-1.16084100	1.67965500	-2.34645900
H	-1.37656200	2.58174000	-1.72866200
H	-2.01752300	1.28835200	-2.91491600
H	2.33884000	3.23173300	-0.80223500
H	0.68237200	1.19231700	2.63051300
H	0.75013300	3.77932300	0.99948300
C	-2.09060300	1.23664000	2.88254400
H	-2.48305100	1.99298200	3.60097500
H	-2.98213000	0.78735900	2.39937500
H	-1.56194300	0.46378300	3.47478400
H	2.14289200	2.62328100	1.35362700

2_{Zr} syn-P/trans-P

E: -1010.30564380 A.U.

Zr	-0.02414800	0.57696100	-0.06206200
N	-1.55916000	-1.17288700	-0.26538700
N	0.74527000	-1.13136300	0.80060200
C	-1.23939200	-2.35857900	0.34275600
C	-2.13190700	-3.44401400	0.36245800
H	-1.84006300	-4.37783900	0.86723900
C	-3.37406400	-3.32801400	-0.27444200
H	-4.08194300	-4.17154900	-0.27722600
C	-3.69383700	-2.11924000	-0.92174700
H	-4.65054700	-1.98533200	-1.44811800
C	-2.76840500	-1.07581200	-0.89391100
H	-2.98128300	-0.12364900	-1.39977100
C	0.13436500	-2.42985200	0.95837200
H	0.71407700	-3.25004700	0.48509400
C	2.07861400	-0.75777400	0.62163200
C	3.11447600	-1.50418000	-0.04535400
C	4.27780400	-0.80565800	-0.40246100
H	5.08005100	-1.36224900	-0.91374800
C	4.45735100	0.57927500	-0.16724600
H	5.38674000	1.07172200	-0.49135800
C	3.48476200	1.29561800	0.52092000
H	3.65662300	2.35058000	0.78831400
C	2.30345700	0.63779600	0.97444700
C	2.99152200	-2.96843700	-0.39626000
H	2.15583600	-3.16176600	-1.10313000
C	1.45444900	1.30610900	2.03350700
H	0.43416700	1.73901100	1.71881900

H	3.91638200	-3.32479700	-0.88820200
H	2.83927500	-3.60516700	0.50037200
H	1.94812700	2.21921800	2.42077500
H	1.21689600	0.63027200	2.87829400
C	-1.94212600	2.09134500	1.82882800
H	0.05630200	-2.69892400	2.03903700
H	-1.30800700	2.86705600	2.30530800
C	-2.25494800	2.26080200	0.50576700
C	-1.81724300	3.44122200	-0.34800000
C	-1.14657600	1.73173700	-2.09022600
H	-2.20139600	1.67960000	-2.40951100
C	-0.74727300	3.00442300	-1.36954300
H	0.25103300	2.89590400	-0.84480800
C	-0.25827900	0.77354600	-2.57815400
H	-0.69154100	-0.07373300	-3.13980900
C	1.09873500	0.67896000	-2.12902200
H	1.70705300	1.59893600	-2.03230200
H	1.69202300	-0.19359900	-2.44876600
H	-0.51138300	3.81049600	-2.10389900
H	-3.01427300	1.58175700	0.07460900
H	-1.43539300	4.27004500	0.28273100
C	-2.51258600	1.05768000	2.74938400
H	-1.73212500	0.55487800	3.35914800
H	-3.16942900	1.57120100	3.48816700
H	-3.12411500	0.29721100	2.22573100
H	-2.70332500	3.84038500	-0.88726300

2_{Zr} syn-P/trans-S

E: -1010.30551365 A.U.

Zr	-0.09169900	0.56369000	-0.34080800
N	-2.18134900	-0.45660900	-0.24702200
N	0.10386600	-1.22230100	0.52780400
C	-2.21241800	-1.70674500	0.31387700
C	-3.42247400	-2.39566100	0.49948000
H	-3.41365000	-3.40133500	0.94722600
C	-4.62643200	-1.79314200	0.10817500
H	-5.58329400	-2.32162600	0.24139900
C	-4.59217200	-0.50609200	-0.46105400
H	-5.51194100	0.00329900	-0.78484500
C	-3.35646600	0.12181200	-0.62806100
H	-3.29380900	1.11891100	-1.09165600
C	-0.86901700	-2.28174100	0.69948500
H	-0.63499600	-3.17167100	0.06782200
C	1.52973000	-1.30527800	0.48923700
C	2.19144200	-1.81814300	-0.68931300
C	3.59584200	-1.75987800	-0.74172400
H	4.11719900	-2.14039900	-1.63442200
C	4.34119400	-1.23927300	0.33003900
H	5.44014500	-1.20523800	0.26440400
C	3.69982000	-0.79480700	1.49748000
H	4.30293700	-0.44046500	2.34879600
C	2.29719800	-0.84258400	1.62105500
C	1.42733400	-2.47393000	-1.81397900
H	0.40150400	-2.07261500	-1.95228500
C	1.66098900	-0.54273900	2.95767100
H	0.55644100	-0.50698400	2.91145100
H	1.96820200	-2.38651300	-2.77649200
H	1.31603600	-3.56357900	-1.61654600
H	2.04571300	0.39827500	3.40283500
H	1.92743800	-1.34721400	3.67755300
C	-0.62325700	2.22372400	1.93909600

H	-0.88801500	-2.65292200	1.75166000
H	0.13305200	1.68989900	2.54985100
C	-0.20638300	2.81354500	0.76930600
C	1.23530700	2.90625300	0.28410200
C	1.52391000	1.46990900	-1.94434200
H	2.53362300	1.03684500	-2.04395800
C	1.45356800	2.84633100	-1.27614700
H	0.68793700	3.48675500	-1.76593500
C	0.50615200	0.90416100	-2.73390500
H	0.77750800	0.03039500	-3.35315900
C	-0.87288900	1.14806600	-2.51129200
H	-1.18590400	2.16154800	-2.16635300
H	-1.62724700	0.62363900	-3.11645000
H	2.43017200	3.33497100	-1.46981100
H	-0.94196400	3.42581500	0.20609000
H	1.90051100	2.18548000	0.82379300
C	-1.98794200	2.33824800	2.53203600
H	-2.37657300	1.35865600	2.87944000
H	-1.91392400	2.96612200	3.45033400
H	-2.71988000	2.81911400	1.85429400
H	1.60492200	3.90339700	0.61446000

2_{Zr} syn-S/trans-P

E: -1010.30630252 A.U.

Zr	-0.01167000	0.57059400	-0.01155300
N	-1.58712900	-1.14640300	-0.22655500
N	0.73035600	-1.17737300	0.81079700
C	-1.27699900	-2.35850500	0.33223800
C	-2.18762200	-3.42924300	0.33002500
H	-1.90280300	-4.38501000	0.79624700
C	-3.43841700	-3.27026500	-0.27971600
H	-4.16024600	-4.10164200	-0.30041600
C	-3.74955200	-2.03298600	-0.87575000
H	-4.71368200	-1.86395900	-1.37796500
C	-2.80652500	-1.00643100	-0.82720900
H	-3.01631000	-0.03097100	-1.28798600
C	0.10594000	-2.47404800	0.91736600
H	0.66601500	-3.27735300	0.39391300
C	2.06274800	-0.81580200	0.61603500
C	3.08305000	-1.55113700	-0.08842600
C	4.24408300	-0.84944700	-0.44639700
H	5.03435600	-1.39635900	-0.98594600
C	4.43702400	0.52677100	-0.17480500
H	5.36362200	1.02247800	-0.50203600
C	3.48424800	1.22878700	0.55644600
H	3.67230000	2.27196600	0.85718900
C	2.30706300	0.56591500	1.01060600
C	2.94885900	-3.00653800	-0.46983400
H	2.11033500	-3.18001800	-1.17860400
C	1.48412900	1.19584900	2.11649800
H	0.46532300	1.64161600	1.83638600
H	3.87009600	-3.35893200	-0.97136500
H	2.79364100	-3.66035500	0.41381200
H	1.99371100	2.08905500	2.52871300
H	1.26312500	0.48509800	2.93671600
C	-2.46854600	1.77023200	1.18841400
H	0.04499000	-2.79309700	1.98552000
H	-3.22496600	1.53320800	0.41619100
C	-1.60066900	2.79956100	0.93466500
C	-1.56289400	3.64307600	-0.32595200
C	-1.12495400	1.76039900	-1.98221600

H	-2.19604500	1.76878900	-2.24658800
C	-0.59848900	3.04666300	-1.37277500
H	0.42879000	2.91922800	-0.91967400
C	-0.31843400	0.74736300	-2.50564800
H	-0.82675000	-0.08294000	-3.02820500
C	1.04973400	0.57792700	-2.12114000
H	1.71630600	1.45947500	-2.05783100
H	1.57366300	-0.33267800	-2.45484500
H	-0.38874600	3.77515700	-2.19190400
H	-0.94688600	3.13495800	1.76492500
H	-2.57765000	3.72415800	-0.76927100
C	-2.61611500	1.06040000	2.50182600
H	-3.57899300	1.37219400	2.96678500
H	-2.68887900	-0.04096700	2.38588300
H	-1.81028200	1.30538100	3.22277400
H	-1.24576700	4.67293200	-0.06550700

2_{Zr} syn-S/trans-S

E: -1010.30614016 A.U.

Zr	-0.15829800	0.56412800	-0.18892600
N	-2.39357700	-0.01211100	0.02308200
N	-0.28980900	-1.41092400	0.07113100
C	-2.66351600	-1.34229600	0.19482300
C	-3.97992000	-1.80187500	0.36396300
H	-4.17075700	-2.87881500	0.48937700
C	-5.03527900	-0.87787100	0.37639000
H	-6.07293000	-1.22082000	0.51179700
C	-4.75117600	0.49076200	0.20786500
H	-5.54978200	1.24732600	0.20591000
C	-3.42331500	0.88062400	0.02195600
H	-3.16797200	1.94039600	-0.14810400
C	-1.45856400	-2.26086000	0.19166100
H	-1.53699800	-2.98925100	-0.65050200
C	1.06644200	-1.64959300	0.40973300
C	1.93713300	-2.43771800	-0.41436000
C	3.29785500	-2.48041200	-0.06626500
H	3.98631900	-3.08883800	-0.67437400
C	3.80324300	-1.75811700	1.03492700
H	4.87678800	-1.81317300	1.27407000
C	2.95009900	-0.99430000	1.84176300
H	3.34916000	-0.47634100	2.72833400
C	1.56343900	-0.94388000	1.56555400
C	1.39771700	-3.22246200	-1.58050900
H	0.61627500	-2.66186700	-2.13397600
C	0.60694900	-0.34574800	2.58113100
H	-0.18639500	0.35508000	2.19172100
H	2.20061100	-3.50210700	-2.28892900
H	0.92996300	-4.17088100	-1.23507100
H	1.15059000	0.23125300	3.35262100
H	0.02534000	-1.14014200	3.09541200
C	0.61428600	2.91340300	0.80966000
H	-1.42472600	-2.87006100	1.12483500
H	0.15449100	3.28925900	-0.13422900
C	1.89697000	2.43361400	0.74257200
C	2.75925900	2.33665300	-0.49146400
C	1.43343600	0.79280100	-2.07910100
H	2.19388800	0.00042600	-2.19726600
C	2.01444100	2.18384000	-1.83174500
H	1.25543600	2.98353700	-1.96715300
C	0.16291700	0.52680500	-2.63517200
H	0.00772400	-0.47040200	-3.08617800

C	-0.99213200	1.28519400	-2.32810600
H	-0.90028100	2.37845500	-2.15024000
H	-1.96780700	0.97125500	-2.72809300
H	2.74744800	2.35685600	-2.65227900
H	2.39649100	2.18706500	1.69889000
H	3.38415600	3.26158400	-0.50839100
C	-0.13889700	3.24708800	2.07255800
H	-0.23548400	4.35365300	2.14990300
H	-1.18510800	2.86669200	2.08236600
H	0.38023500	2.89216000	2.98368200
H	3.49063500	1.50991500	-0.36356000

H	1.25923300	1.07494600	3.10971200
H	0.97069600	-0.77116400	3.31369400
H	-2.85009300	2.80365600	1.32910700
H	0.69646700	3.71142100	0.34008500
H	-1.54734000	3.26016600	-0.61512700
C	2.02395900	1.73991700	-2.28060900
H	2.46345800	2.50278400	-2.96403500
H	2.76304000	0.91641800	-2.22481400
H	1.10332100	1.36816900	-2.77111500
H	-0.82703100	2.19688400	-1.94703700

Zirconium - Path 3

1_{Zr} anti-P/trans-P

E: -1010.28331424 A.U.

Zr	0.13397100	0.77511800	0.35468200
N	2.16287400	-0.37496500	0.18306500
N	-0.17615000	-0.83160300	-0.79327500
C	2.13556100	-1.47970000	-0.62231100
C	3.28384600	-2.26676600	-0.82402100
H	3.23207300	-3.14595300	-1.48465300
C	4.47695500	-1.92576500	-0.17301600
H	5.38342700	-2.53478400	-0.31432600
C	4.49820500	-0.79216700	0.66290900
H	5.41286200	-0.48582800	1.19195400
C	3.32932400	-0.04334400	0.80565500
H	3.32017100	0.86292000	1.43361800
C	0.80318900	-1.79896300	-1.26313100
H	0.49538000	-2.83990400	-1.01288400
C	-1.58417300	-1.03470200	-0.65927000
C	-2.09509200	-1.85418900	0.41636500
C	-3.48713400	-1.91292900	0.60275500
H	-3.89590000	-2.52573700	1.42246200
C	-4.36853500	-1.22904000	-0.25816800
H	-5.45507500	-1.29245500	-0.08868800
C	-3.87415600	-0.51367600	-1.35715900
H	-4.57640500	-0.04227800	-2.06313000
C	-2.48767400	-0.42908000	-1.60738600
C	-1.19681400	-2.72184900	1.26898900
H	-0.16894500	-2.32513200	1.38949400
C	-2.01312300	0.15059600	-2.91522800
H	-0.91349100	0.25345300	-2.96721500
H	-1.62959800	-2.89440100	2.27481200
H	-1.09852100	-3.72890800	0.80590100
H	-2.48643800	1.12882800	-3.13758400
H	-2.31709900	-0.52959800	-3.74094900
C	1.79535200	2.39567200	-0.94396500
H	0.89693000	-1.77149700	-2.37582800
H	2.71285300	2.67768900	-0.39613300
C	0.61332500	3.02813600	-0.52998100
C	-0.69384600	2.65533700	-0.95278700
C	-1.31612000	1.69007700	2.35325500
H	-0.75307300	2.60192700	2.63682200
C	-2.46389600	1.81329600	1.61538800
H	-3.07606600	0.93462600	1.34299200
C	-0.76700300	0.39953400	2.76749200
H	-1.45281600	-0.46563900	2.78131100
C	0.56647700	0.21304700	3.03017700

TS_{1-2Zr} anti-P/trans-P

E: -1010.25641046 A.U.

Zr	0.21168500	0.68879200	0.54062400
N	2.18687700	-0.46781600	0.21601300
N	-0.21403000	-0.81395000	-0.72331200
C	2.11352700	-1.48342500	-0.69875600
C	3.24676100	-2.24769600	-1.02757000
H	3.16238000	-3.05838300	-1.76777400
C	4.46827400	-1.97885800	-0.39384100
H	5.36229700	-2.57587000	-0.63270300
C	4.53403200	-0.94212000	0.55749100
H	5.47062600	-0.70330700	1.08285000
C	3.37697200	-0.21088600	0.82994200
H	3.39279200	0.61080600	1.56602900
C	0.74805300	-1.74697400	-1.29611600
H	0.44730400	-2.80196000	-1.09910600
C	-1.62650600	-1.03380800	-0.64153200
C	-2.15994700	-1.93652300	0.35149700
C	-3.55689700	-2.01179300	0.49809000
H	-3.98168800	-2.68149300	1.26288200
C	-4.41801700	-1.26633600	-0.32651900
H	-5.50808400	-1.34021200	-0.18768800
C	-3.89714500	-0.46730900	-1.35668500
H	-4.58383300	0.05300800	-2.04356400
C	-2.50780500	-0.35774400	-1.55958600
C	-1.28294100	-2.85125800	1.17341000
H	-0.24865900	-2.47901200	1.30272400
C	-2.00311300	0.34396000	-2.79746300
H	-0.90389300	0.46705600	-2.80573500
H	-1.71794400	-3.04046300	2.17514300
H	-1.21208200	-3.84584400	0.67936600
H	-2.48677400	1.33086500	-2.95052800
H	-2.26289700	-0.26176500	-3.69303100
C	1.79023800	2.55271200	-0.99583100
H	0.78963400	-1.65131200	-2.40828500
H	2.78652100	2.79109600	-0.57899700
C	0.71112200	2.99856200	-0.25416900
C	-0.72573500	2.78180200	-0.53113700
C	-1.12760100	1.77453600	2.20318400
H	-0.41483900	2.47931600	2.68183200
C	-1.91441900	2.30543000	1.12251100
H	-2.69328100	1.66592300	0.66479300
C	-1.01287500	0.40617300	2.60264400
H	-1.85429200	-0.28451500	2.40727600
C	0.24480400	-0.11758000	2.93651800
H	1.05506400	0.57430600	3.25226400
H	0.37344600	-1.16530200	3.24619000
H	-2.22011700	3.35613200	1.22272700
H	0.94999600	3.60143400	0.64487000
H	-1.29719400	3.72226600	-0.51197400

C	1.79708500	1.96968400	-2.37148300
H	2.20414800	2.74765300	-3.05955500
H	2.49686100	1.11294700	-2.45776700
H	0.79997900	1.68305600	-2.75464700
H	-0.96999400	2.23093700	-1.45902700

1_{Zr} anti-P/trans-S

E: -1010.28247989 A.U.

Zr	-0.12907300	0.82931900	-0.14644600
N	-2.13956300	-0.36723700	-0.21604500
N	0.24922400	-1.03025400	0.47462400
C	-2.05990400	-1.65755800	0.22982500
C	-3.19166700	-2.49266100	0.25661800
H	-3.09796700	-3.52530900	0.62679100
C	-4.42310200	-2.00045200	-0.19552800
H	-5.31784400	-2.64229500	-0.18543400
C	-4.49835300	-0.67353200	-0.66225400
H	-5.44453500	-0.24556900	-1.02551800
C	-3.34187200	0.10750300	-0.64900000
H	-3.36922700	1.15603100	-0.98884600
C	-0.69086700	-2.12184200	0.67336100
H	-0.38602100	-3.02694200	0.09798400
C	1.66783100	-1.15323800	0.31554700
C	2.20762500	-1.55824900	-0.96132100
C	3.60341600	-1.55209400	-1.12787800
H	4.03269500	-1.85022900	-2.09796200
C	4.45910000	-1.20132100	-0.06772100
H	5.54955100	-1.20374900	-0.22256000
C	3.93467600	-0.89268100	1.19574500
H	4.61826200	-0.67985100	2.03307600
C	2.54430500	-0.88867800	1.42729700
C	1.33391800	-2.07787800	-2.08107800
H	0.26755500	-1.79182700	-1.97986700
C	2.03723000	-0.73498300	2.83889500
H	0.93638800	-0.64623400	2.89531100
H	1.69981300	-1.75460500	-3.07716100
H	1.36129900	-3.18986900	-2.09631100
H	2.50119900	0.12954500	3.35720700
H	2.32162700	-1.63230000	3.43071700
C	-1.72532100	1.92204700	1.70705000
H	-0.72078300	-2.44198800	1.74308500
H	-2.69148200	2.30816600	1.33411400
C	-0.59909900	2.69780300	1.40325100
C	0.75556400	2.28619600	1.58145200
C	1.35489700	1.74447200	-2.02569400
H	1.91415200	0.84031700	-2.33149800
C	1.95037400	2.64962900	-1.18115200
H	1.47565600	3.61827800	-0.95008900
C	-0.01275200	1.91744700	-2.52460300
H	-0.46940200	2.92107600	-2.40382100
C	-0.76570400	0.90317700	-3.05204100
H	-1.80284300	1.07452600	-3.38094600
H	-0.33441300	-0.09227000	-3.25414000
H	2.97332300	2.48961400	-0.80553000
H	-0.77789200	3.60522600	0.79049000
H	1.55536000	3.02307300	1.41834500
C	-1.83012400	0.89337900	2.80046100
H	-2.27400100	1.39299400	3.69230200
H	-2.52033700	0.06634000	2.54025800
H	-0.85909500	0.47118400	3.12232100
H	0.99322500	1.53742900	2.35808100

TS_{1-2Zr} anti-P/trans-S

E: -1010.26860777 A.U.

Zr	0.09826900	0.70877000	0.40934600
N	2.14984700	-0.39845000	0.23557300
N	-0.14482500	-0.80317000	-0.88979300
C	2.19734200	-1.37334200	-0.72339800
C	3.39115000	-2.06086000	-1.00551900
H	3.40132900	-2.84010100	-1.78329400
C	4.55146600	-1.75409100	-0.28103300
H	5.49199400	-2.29020100	-0.48269800
C	4.49497300	-0.75621200	0.71117500
H	5.38052200	-0.48706800	1.30590200
C	3.28148300	-0.10322600	0.93505400
H	3.20169300	0.68574800	1.70156100
C	0.89244500	-1.66950300	-1.43306200
H	0.62757800	-2.74447200	-1.31685500
C	-1.52092500	-1.13769300	-0.69362400
C	-1.90225500	-2.13778900	0.27630400
C	-3.26659900	-2.27853600	0.57841400
H	-3.57650600	-3.02401800	1.32821700
C	-4.24493400	-1.49147500	-0.06200600
H	-5.30619300	-1.61684200	0.20442100
C	-3.87829800	-0.58670200	-1.06653600
H	-4.65728600	-0.02987500	-1.61166300
C	-2.52518000	-0.41452600	-1.43172500
C	-0.90497000	-3.06945900	0.92874000
H	0.11496000	-2.64714900	1.02725800
C	-2.19990700	0.39000800	-2.66701000
H	-1.11382800	0.54325400	-2.80461400
H	-1.24859500	-3.38510500	1.93392700
H	-0.80751000	-4.00331700	0.33139100
H	-2.72100400	1.36946700	-2.68443000
H	-2.56262800	-0.16115800	-3.56196400
C	1.63405700	2.48848600	-0.99889100
H	1.00891300	-1.50930600	-2.53254000
H	2.65443900	2.62816600	-0.59745600
C	0.61214100	3.04855900	-0.24515100
C	-0.83118000	2.91609300	-0.45485400
C	-1.64650800	1.10133000	1.92991600
H	-2.28962900	0.21704200	1.76143300
C	-1.94873000	2.34202700	1.28085500
H	-1.62334700	3.26294800	1.79381300
C	-0.50802300	0.99336900	2.81588400
H	-0.09147500	1.93261700	3.23473000
C	0.24477700	-0.16230500	2.92532800
H	1.15918100	-0.19518600	3.53757600
H	-0.15748700	-1.13710500	2.59025600
H	-2.91621100	2.42740100	0.76198300
H	0.91941200	3.60360400	0.66470100
H	-1.39656300	3.84220200	-0.27155400
C	1.56814500	1.97442600	-2.40575500
H	2.05821700	2.73739500	-3.05500200
H	2.16100100	1.04750200	-2.54625400
H	0.54363500	1.82800900	-2.79580400
H	-1.16333600	2.45459900	-1.40599400

1_{Zr} anti-S/trans-A

E: -1010.29331385 A.U.

Zr	0.20840100	0.81967400	0.06615500
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N	2.19662700	-0.47554200	0.03964200
N	-0.22908300	-1.01892700	-0.58860100
C	2.06509400	-1.71467500	-0.52254600
C	3.16237900	-2.58297600	-0.65931800
H	3.01992300	-3.57033200	-1.12504300
C	4.42086300	-2.18360100	-0.19054100
H	5.29068700	-2.85209200	-0.28530300
C	4.54955200	-0.91828900	0.41211400
H	5.51395900	-0.56600800	0.80726700
C	3.42208000	-0.09960000	0.50244800
H	3.49752300	0.89640400	0.96513800
C	0.67041100	-2.09755300	-0.95866400
H	0.36701100	-3.05677600	-0.47974400
C	-1.63558000	-1.14950100	-0.36321400
C	-2.10514800	-1.71682200	0.88010500
C	-3.48756800	-1.71399300	1.13061700
H	-3.86486400	-2.13398700	2.07684500
C	-4.39964900	-1.21063700	0.18153500
H	-5.47827800	-1.21704100	0.40447500
C	-3.94648700	-0.75148900	-1.06248700
H	-4.67479100	-0.42752000	-1.82313900
C	-2.57139600	-0.74248800	-1.38063000
C	-1.17642200	-2.39490800	1.86200700
H	-0.13310600	-2.02379300	1.82142800
C	-2.15341500	-0.43890000	-2.79747500
H	-1.05796500	-0.45382500	-2.94048700
H	-1.54621400	-2.30609100	2.90354100
H	-1.13610000	-3.48645900	1.64938800
H	-2.55441200	0.53176700	-3.15594600
H	-2.58419700	-1.20985000	-3.47232400
C	1.59206500	1.98747600	-1.54695900
H	0.64363600	-2.28986400	-2.05854800
H	2.39987100	1.47756900	-2.09410600
C	0.30957600	2.02537100	-2.13750800
C	-0.81954700	2.52063000	-1.45902300
C	-1.16163600	2.10936500	1.94595500
H	-0.69413200	3.11058300	2.02080600
C	-2.33407100	1.96667200	1.25002800
H	-2.86571500	0.99939000	1.19922400
C	-0.46026400	0.98616100	2.56447700
H	-1.03023900	0.05048200	2.70784600
C	0.87043800	1.01795300	2.89886600
H	1.44516400	1.96116900	2.88657300
H	1.37318000	0.13335900	3.32067000
H	-2.82384200	2.83510600	0.78271400
H	0.16357600	1.43323400	-3.05713500
H	-0.70162700	3.36493400	-0.75424500
C	1.98737800	2.87909500	-0.39340900
H	1.78304300	2.46124600	0.65240300
H	3.08226100	3.04251600	-0.37025600
H	1.48091200	3.86698100	-0.40509800
H	-1.81606100	2.43949600	-1.91869600

TS_{1-2Zr} anti-S/trans-P

E: -1010.26158638 A.U.

Zr	0.23267500	0.73715100	0.14198100
N	2.27563800	-0.41508500	0.03052200
N	-0.12974500	-1.15105200	-0.42675000
C	2.20224100	-1.69235900	-0.45567100
C	3.35316600	-2.47523000	-0.64885200
H	3.25514500	-3.49713000	-1.04648700

C	4.60938300	-1.94868700	-0.32052100
H	5.52122300	-2.54978100	-0.46081200
C	4.68215400	-0.64496600	0.20476300
H	5.64358300	-0.19500000	0.49348200
C	3.50131800	0.08160100	0.36482100
H	3.52930000	1.09766400	0.78684000
C	0.81294800	-2.21030100	-0.73525100
H	0.61523600	-3.12036500	-0.12087500
C	-1.54150600	-1.30677800	-0.27612800
C	-2.07898000	-1.76925800	0.98149700
C	-3.47479200	-1.74894800	1.15466100
H	-3.90421200	-2.07856600	2.11425400
C	-4.32971000	-1.34064500	0.11477200
H	-5.41921200	-1.32996000	0.27623400
C	-3.80693800	-0.99848800	-1.14330800
H	-4.49320400	-0.75582200	-1.97058400
C	-2.41802900	-1.00399800	-1.37956600
C	-1.20186300	-2.34867700	2.06694700
H	-0.15623400	-1.98274500	2.03709100
C	-1.90966500	-0.82053500	-2.78955500
H	-0.81029400	-0.71283500	-2.84916600
H	-1.61842900	-2.16166600	3.07729900
H	-1.15717600	-3.45528100	1.95743200
H	-2.39255800	0.03765900	-3.30135400
H	-2.17828900	-1.71684700	-3.39064900
C	1.12033000	2.21704500	-1.60014700
H	0.72351000	-2.53961500	-1.79831500
H	1.81418700	1.75505600	-2.32191900
C	-0.25068400	2.11412800	-1.86372000
C	-1.33006500	2.72196100	-1.09380400
C	-1.12298100	2.18592800	1.69143900
H	-0.60787200	3.15765800	1.83248200
C	-2.13701200	2.15305000	0.67736500
H	-2.69082200	1.20737900	0.51574500
C	-0.56918700	1.07252900	2.39029300
H	-1.18716700	0.16017700	2.48862600
C	0.79358100	1.01091100	2.71526400
H	1.39208600	1.93689800	2.77875100
H	1.21199700	0.12908300	3.22402400
H	-2.78286700	3.04062500	0.58771400
H	-0.54693000	1.49330000	-2.72616100
H	-1.09759600	3.72820600	-0.70247400
C	1.70291500	3.00502100	-0.46066700
H	1.80739200	2.41970600	0.52034500
H	2.74863500	3.30735800	-0.66566800
H	1.11193200	3.90551400	-0.19199600
H	-2.29937500	2.67643900	-1.61729700

1_{Zr} anti-S/trans-S

E: -1010.29055005 A.U.

Zr	0.23002000	0.80773700	-0.02034100
N	2.19533800	-0.51649900	0.01992600
N	-0.30069600	-1.12385600	-0.08270700
C	1.98218100	-1.86408400	-0.07301900
C	3.04869500	-2.78052100	-0.06570500
H	2.83944100	-3.85841300	-0.14600100
C	4.36334300	-2.30991500	0.04725200
H	5.21034100	-3.01352300	0.05378300
C	4.58015600	-0.92365100	0.15860400
H	5.59349400	-0.50710300	0.25858400
C	3.47727800	-0.06806100	0.14008600

H	3.61906400	1.01968800	0.22953700
C	0.54219900	-2.30291600	-0.17082400
H	0.30222800	-3.02842100	0.64278500
C	-1.73574300	-1.15221300	-0.06996200
C	-2.42957800	-1.23336900	1.19141700
C	-3.83178600	-1.12430500	1.19029200
H	-4.37701700	-1.17292600	2.14661300
C	-4.54824600	-0.99564700	-0.01219700
H	-5.64602800	-0.91049400	0.01086100
C	-3.87628900	-1.03201900	-1.24337200
H	-4.45464400	-1.00654900	-2.18083400
C	-2.47339600	-1.14333500	-1.30696000
C	-1.71820800	-1.55655300	2.48594900
H	-0.62420800	-1.39099200	2.43948600
C	-1.82506500	-1.38678100	-2.64934200
H	-0.72272000	-1.30186600	-2.63422500
H	-2.13431000	-0.99366200	3.34713900
H	-1.86717400	-2.63127100	2.73129200
H	-2.22937400	-0.71368900	-3.43314000
H	-2.06593600	-2.41907700	-2.98617000
C	1.26733400	1.52258100	-2.08216300
H	0.36945200	-2.85750000	-1.12436700
H	1.89636600	0.82548900	-2.65755100
C	-0.11355900	1.57392500	-2.36895200
C	-1.00870300	2.37943500	-1.63730500
C	-0.97101300	1.84891500	1.95613200
H	-1.41761900	0.92880800	2.37250400
C	-1.73591500	2.67173300	1.16161500
H	-1.38216300	3.66974400	0.85700100
C	0.43235600	2.11922000	2.26747400
H	0.81356700	3.14212000	2.08228500
C	1.29727300	1.15015800	2.70351900
H	2.36022400	1.37307300	2.88741800
H	0.94395600	0.14074100	2.97859300
H	-2.78179200	2.41791000	0.92803200
H	-0.52186700	0.79521100	-3.03315500
H	-0.65974600	3.35574500	-1.25882100
C	1.95989500	2.63070700	-1.31735000
H	1.77238300	2.65441900	-0.19470500
H	3.05940500	2.56829900	-1.41588300
H	1.63214200	3.64011000	-1.64931100
H	-2.09002400	2.30731000	-1.82977400

TS_{1-2Zr} anti-S/trans-S

E: -1010.27668718

Zr	0.21815500	0.76260000	0.04313800
N	2.26090500	-0.43169000	0.01169400
N	-0.17260300	-1.20092300	0.06870700
C	2.14195900	-1.79478800	-0.01354300
C	3.26970600	-2.63325100	-0.04905600
H	3.13429800	-3.72564500	-0.06707500
C	4.55108400	-2.06713400	-0.06043100
H	5.44542900	-2.70883200	-0.09045800
C	4.67357700	-0.66551800	-0.02479200
H	5.65835200	-0.17514600	-0.02224200
C	3.51324400	0.10933600	0.01537600
H	3.58342200	1.20673100	0.06185900
C	0.73327300	-2.33252000	0.00913200
H	0.59375700	-3.01340500	0.88320000
C	-1.59874400	-1.27920400	-0.01317700
C	-2.38031200	-1.35698100	1.19683600

C	-3.78263800	-1.31836900	1.08876400
H	-4.39506100	-1.36296600	2.00366500
C	-4.41191100	-1.26425700	-0.16655000
H	-5.51140800	-1.23764500	-0.22612300
C	-3.65016200	-1.29379300	-1.34648400
H	-4.16031100	-1.31970600	-2.32274200
C	-2.24374800	-1.33057800	-1.30387300
C	-1.75185300	-1.58454600	2.55155700
H	-0.66031600	-1.40069400	2.56605200
C	-1.47274800	-1.54929700	-2.58474400
H	-0.40817500	-1.25213600	-2.52159600
H	-2.23350200	-0.97434200	3.34391600
H	-1.90404600	-2.64346400	2.85612000
H	-1.94161200	-1.02872500	-3.44439100
H	-1.49008500	-2.63138100	-2.84396100
C	0.59550900	1.60021200	-2.19977200
H	0.54368200	-2.95975300	-0.89423900
H	0.91023700	0.86609700	-2.95928000
C	-0.77624700	1.79450700	-1.98960200
C	-1.32545500	2.75314200	-1.05417800
C	-0.95961200	1.73147600	1.81032700
H	-1.30431400	0.80709900	2.30543900
C	-1.85381100	2.45167900	0.94865700
H	-1.84867100	3.55158300	1.01938800
C	0.35550600	2.25134000	2.13488000
H	0.56159400	3.31846200	1.92072000
C	1.40773600	1.44141300	2.49859900
H	2.41776700	1.85079700	2.65559700
H	1.24974100	0.38749400	2.79392900
H	-2.85493700	2.01335300	0.81017600
H	-1.47966900	1.12661700	-2.51475900
H	-0.70817100	3.65291800	-0.88039600
C	1.63983400	2.53130700	-1.63411800
H	1.72688600	2.53438400	-0.49796100
H	2.65113900	2.28791100	-2.00757700
H	1.41946400	3.59774400	-1.86190200
H	-2.38493200	2.99186700	-1.23653100

2_{Zr} anti-P/trans-A

E: -1010.29626338 A.U.

Zr	-0.12283800	0.43119000	-0.02822000
N	-1.14887600	-1.66885300	-0.12660200
N	1.09094700	-0.98683200	0.86921900
C	-0.51302500	-2.70665800	0.50478300
C	-1.08039100	-3.99055300	0.56790800
H	-0.54422100	-4.79531300	1.09407800
C	-2.31246100	-4.23362500	-0.05322200
H	-2.76653900	-5.23638500	-0.02093800
C	-2.95316000	-3.17679300	-0.72695100
H	-3.91521300	-3.32115500	-1.24061600
C	-2.34667300	-1.92062300	-0.73513000
H	-2.82695900	-1.07855800	-1.25491300
C	0.83794700	-2.39035900	1.09812400
H	1.60752500	-3.05843200	0.65823400
C	2.26209900	-0.30237700	0.54721300
C	3.39189300	-0.78704400	-0.20667900
C	4.29186500	0.17129600	-0.69751900
H	5.16134300	-0.18174300	-1.27553200
C	4.12056900	1.56527500	-0.51299300
H	4.85454800	2.26548700	-0.94035400
C	3.05981000	2.03967800	0.25205600

H	2.96947800	3.11552700	0.47105800
C	2.14399700	1.12021200	0.84281500
C	3.62906500	-2.24890000	-0.50159700
H	2.80915000	-2.69447800	-1.10499600
C	1.22777100	1.60375400	1.94633700
H	0.10824200	1.72328300	1.70611300
H	4.56214500	-2.37827400	-1.08195400
H	3.74052600	-2.85045800	0.42511800
H	1.48575800	2.63779400	2.24882200
H	1.24237200	0.94274100	2.83508500
C	-2.30914900	1.30952400	1.83520300
H	0.83285100	-2.61193100	2.19231900
H	-2.37673100	0.30351400	2.29433900
C	-2.68867500	1.41933600	0.51595800
C	-2.86670700	2.69670300	-0.28209100
C	-1.70295700	1.42820600	-2.10378600
H	-1.97402000	0.39927100	-2.41335400
C	-2.83060500	2.39261600	-1.79747100
H	-2.71931100	3.33312600	-2.37680000
C	-0.36149300	1.76634600	-2.19392600
H	-0.07275200	2.83026300	-2.06907400
C	0.68518000	0.77723500	-2.15370200
H	0.43584300	-0.22930400	-2.56558900
H	1.73221400	1.07709100	-2.32410600
H	-3.79480600	1.94620600	-2.11526700
H	-3.11798500	0.50580600	0.06465900
H	-3.82392700	3.18679300	0.01084200
C	-2.04477800	2.44271900	2.78133500
H	-2.99124100	2.63532700	3.33901200
H	-1.29430500	2.19238100	3.55731400
H	-1.77175300	3.39313900	2.28245600
H	-2.07394600	3.43466200	-0.02545700

2_{Zr} anti-P/trans-S

E: -1010.29594960 A.U.

Zr	0.05628300	0.54114900	0.04737200
N	2.28116400	-0.11160100	0.13873800
N	0.20605900	-1.32237700	-0.69382200
C	2.57561400	-1.31376000	-0.45156700
C	3.90095400	-1.76887000	-0.55147900
H	4.10995300	-2.73580300	-1.03462000
C	4.94044500	-0.99219100	-0.01947200
H	5.98315900	-1.34103100	-0.08072500
C	4.63083500	0.23158100	0.60408200
H	5.41414300	0.86608100	1.04462200
C	3.29530200	0.63376500	0.66312100
H	3.01406300	1.57928300	1.15470200
C	1.39113200	-2.11139900	-0.95805500
H	1.35845400	-3.10666000	-0.45919900
C	-1.15401200	-1.67790800	-0.51128300
C	-1.58709200	-2.50692100	0.59238400
C	-2.96418500	-2.59051800	0.85188800
H	-3.31262300	-3.21431800	1.69056800
C	-3.90815900	-1.89030000	0.07121600
H	-4.97969800	-1.96815500	0.31345000
C	-3.49400900	-1.13353200	-1.03039100
H	-4.24456900	-0.64615700	-1.67320900
C	-2.12396400	-1.04232800	-1.37503200
C	-0.61304100	-3.30654200	1.42179700
H	0.34425500	-2.77859800	1.60628300
C	-1.75262900	-0.44601300	-2.71851800

H	-0.66103200	-0.37950900	-2.88421400
H	-1.05116600	-3.58137200	2.40054200
H	-0.36214200	-4.26144200	0.90808800
H	-2.21955700	0.54618500	-2.89044700
H	-2.15076100	-1.10491100	-3.52117700
C	0.77045800	2.98184100	-0.75510000
H	1.50834100	-2.32534300	-2.04803700
H	1.78393000	3.28691200	-0.43769300
C	-0.28616200	3.43282200	-0.00724000
C	-1.75966400	3.21614400	-0.23733800
C	-1.85637200	1.32590300	1.46862100
H	-2.41745200	0.38313300	1.29915400
C	-2.48427500	2.63495600	1.01658600
H	-2.43834200	3.38060900	1.83994100
C	-0.73071000	1.30701700	2.30636300
H	-0.35343900	2.27844400	2.68238900
C	0.15732800	0.19874100	2.38492000
H	1.05402600	0.25509600	3.02110700
H	-0.26897400	-0.82234100	2.29289600
H	-3.55702300	2.50077900	0.77549900
H	-0.03271000	4.04046800	0.88161600
H	-2.21094400	4.20452800	-0.49034000
C	0.69027600	2.24799800	-2.07651600
H	1.31345100	2.77770600	-2.83064300
H	1.16797300	1.22608600	-2.07347000
H	-0.33048000	2.17087700	-2.49904200
H	-1.95114500	2.57840900	-1.13124200

2_{Zr} anti-S/trans-P

E: -1010.30394177 A.U.

Zr	0.24747000	0.67888000	0.09322800
N	2.49751900	0.18896800	-0.03170000
N	0.42398100	-1.29826800	0.14522200
C	2.80964100	-1.14600100	0.02552700
C	4.14384200	-1.57986500	-0.02532000
H	4.37006800	-2.65610500	0.02444900
C	5.17435400	-0.63415600	-0.13701600
H	6.22536600	-0.96070000	-0.17827700
C	4.84984800	0.73498200	-0.19030200
H	5.62855600	1.50765700	-0.27194500
C	3.50543100	1.10388000	-0.13007600
H	3.21608100	2.16856000	-0.15405900
C	1.63831300	-2.09632900	0.15396000
H	1.72968600	-2.69093500	1.09469800
C	-0.92772100	-1.74418200	0.01215200
C	-1.74064000	-1.92460300	1.19007100
C	-3.10618300	-2.23083100	1.01211700
H	-3.74701500	-2.36115000	1.89874100
C	-3.64653600	-2.41573000	-0.26869700
H	-4.71346000	-2.66526900	-0.38119800
C	-2.82768400	-2.32647500	-1.41103600
H	-3.25733700	-2.52833700	-2.40536000
C	-1.46227300	-2.01165600	-1.30233400
C	-1.15417100	-1.93874500	2.58060600
H	-0.17547700	-1.42949400	2.65197300
C	-0.58384600	-2.05481200	-2.53105700
H	0.32898700	-1.42993500	-2.44696100
H	-1.84825200	-1.50302600	3.32717800
H	-0.99398000	-2.99422400	2.89449300
H	-1.13763700	-1.75516900	-3.44297300
H	-0.23659800	-3.09653700	-2.71151500

C	-1.00273100	1.51861100	-1.96237800
H	1.64660400	-2.83841700	-0.67862600
H	-0.81076200	0.58057100	-2.52034300
C	-2.20876400	1.59920500	-1.30334800
C	-2.85390300	2.78673600	-0.63693600
C	-1.34938200	2.39311500	1.26393200
H	-0.65905700	3.15705600	0.83020300
C	-2.79669100	2.60618400	0.89684000
H	-3.41966200	1.74750900	1.22527500
C	-0.78920800	1.55119900	2.21738900
H	-1.44771300	0.85537200	2.76896700
C	0.63708700	1.36740400	2.27006700
H	1.26310900	2.26855800	2.07912100
H	1.07545500	0.68738200	3.01822700
H	-3.20309100	3.50774400	1.40809300
H	-2.80625700	0.66612900	-1.28561800
H	-2.35581000	3.73563300	-0.92556200
C	0.01052700	2.61915400	-2.16257600
H	1.03280600	2.35667500	-1.75750300
H	0.22093900	2.76799500	-3.24419800
H	-0.28437300	3.59089200	-1.72329500
H	-3.90633400	2.85893700	-0.98725700

C	1.43724100	1.26784600	-1.78485400
H	1.39655600	0.29461900	-2.31220500
C	2.81995500	1.77923400	-1.40862400
H	3.27327000	2.32621900	-2.26628200
C	0.31074500	2.10519400	-1.91492700
H	0.41709200	3.17158000	-1.63539700
C	-1.00429600	1.60339500	-2.03761500
H	-1.85704200	2.30140000	-2.05040800
H	-1.17778000	0.64441300	-2.56339900
H	3.48882600	0.91405200	-1.21861900
H	2.89618000	1.11723400	1.38289300
H	2.21687400	3.62372200	-0.35974400
C	0.05416300	3.22095400	1.49362600
H	-0.97338200	2.81368800	1.26765700
H	-0.11428900	3.79544600	2.43007600
H	0.31559800	3.93407800	0.68973600
H	3.82728000	3.01699100	0.08050300

Zirconium - Path 4

2Zr anti-S/trans-S

E: -1010.30928468 A.U.

Zr	-0.17470600	0.61997700	0.01751200
N	-2.44365400	0.07383700	0.08475200
N	-0.34286000	-1.31903500	-0.39933700
C	-2.73486600	-1.23185100	-0.20521300
C	-4.05966300	-1.69904600	-0.21635300
H	-4.26511600	-2.75181300	-0.46457500
C	-5.10482900	-0.81696600	0.09464000
H	-6.14846600	-1.16832700	0.09480300
C	-4.80072900	0.52262500	0.40115000
H	-5.58922800	1.24915400	0.64725800
C	-3.46500200	0.92849600	0.37510400
H	-3.19681000	1.97796000	0.58120600
C	-1.54779500	-2.12821400	-0.49970300
H	-1.65273300	-2.57964800	-1.51524800
C	0.94545500	-1.72417400	0.06225800
C	1.94421500	-2.21261600	-0.84418100
C	3.21876600	-2.49646600	-0.31866100
H	4.00093200	-2.88454600	-0.99066400
C	3.51156000	-2.30416000	1.04470800
H	4.51903300	-2.53876500	1.42277000
C	2.52965600	-1.83432500	1.93158400
H	2.76484600	-1.71848800	3.00155600
C	1.22756500	-1.55730500	1.46622900
C	1.62154900	-2.48533800	-2.28935900
H	0.76882200	-1.87941100	-2.65516900
C	0.12112200	-1.22114700	2.44725300
H	-0.57919000	-0.38658800	2.15437800
H	2.49794600	-2.31092100	-2.94403000
H	1.33726500	-3.55283600	-2.42395400
H	0.52701600	-0.93680100	3.43683800
H	-0.56149100	-2.08482900	2.59913300
C	1.08665800	2.14243300	1.72026900
H	-1.51900600	-2.98594900	0.21191200
H	0.95264000	1.53736900	2.63781300
C	2.25317700	1.94269000	1.02185700
C	2.79005200	2.69512400	-0.16206300

1Zr syn-P/trans-P

E: -1010.28400095 A.U.

Zr	0.17057200	0.76208000	0.26565300
N	2.09943800	-0.55157000	0.10296900
N	-0.30765200	-0.90198400	-0.73230300
C	1.95517400	-1.71100700	-0.60794900
C	3.02451400	-2.60863700	-0.77048100
H	2.87920200	-3.52786900	-1.35866200
C	4.25898400	-2.32799500	-0.16801100
H	5.10408700	-3.02558200	-0.27598400
C	4.39839700	-1.14342300	0.57940100
H	5.34649300	-0.88439200	1.07379300
C	3.30408100	-0.28129900	0.68002000
H	3.38951900	0.66381400	1.24054200
C	0.57830700	-1.96741300	-1.17728000
H	0.20559000	-2.96359000	-0.84511600
C	-1.72723100	-0.98808700	-0.58692700
C	-2.28799800	-1.66126300	0.56179300
C	-3.68149300	-1.61416500	0.74480100
H	-4.12771200	-2.11397600	1.61963300
C	-4.51686400	-0.97165200	-0.18917400
H	-5.60543500	-0.94893900	-0.02261000
C	-3.97758400	-0.40826700	-1.35478900
H	-4.64928800	0.02783900	-2.11133800
C	-2.58933800	-0.43257500	-1.60063700
C	-1.44803500	-2.50304000	1.49632800
H	-0.38187100	-2.20329000	1.53763300
C	-2.07434600	-0.01174900	-2.95369500
H	-0.97068700	0.04302500	-3.00313600
H	-1.85708900	-2.50662400	2.52704200
H	-1.46895600	-3.56422900	1.16204600
H	-2.50517900	0.95609800	-3.28324900
H	-2.39663200	-0.75972000	-3.71128800
C	1.75711500	2.06172700	-1.39358200
H	0.62350300	-2.01893600	-2.29214200
H	1.51200900	1.29601000	-2.16082600
C	0.70820400	2.88202600	-0.96060300
C	-0.66300600	2.54078300	-1.13888800
C	-1.14854700	1.90209100	2.24637900

H	-0.54619200	2.81520800	2.42695500
C	-2.32856500	2.00353300	1.55759700
H	-2.97619000	1.12444200	1.38541400
C	-0.61698500	0.63123000	2.73540900
H	-1.32423900	-0.20964100	2.84426500
C	0.72102000	0.42335600	2.95811200
H	1.43937800	1.26758900	2.94746400
H	1.10751600	-0.54941300	3.30010800
H	-2.70015500	2.97952100	1.20914500
H	0.96237800	3.73731400	-0.30130800
H	-1.42990000	3.25501600	-0.80740300
C	3.20949700	2.40585100	-1.24985900
H	3.85467700	1.51065900	-1.14446600
H	3.55107200	2.91252500	-2.18144800
H	3.40552400	3.10391700	-0.41066400
H	-0.93861300	1.95474700	-2.03295900

TS_{1-2Zr} syn-P/trans-P

E: -1010.25920927 A.U.

Zr	0.23040500	0.67111600	0.46740700
N	2.13479500	-0.60038000	0.15789600
N	-0.31632100	-0.92608600	-0.61843400
C	1.96928900	-1.71480600	-0.61844800
C	3.04945300	-2.56654400	-0.90645100
H	2.89067400	-3.45556300	-1.53617700
C	4.31520800	-2.28000100	-0.37492700
H	5.16936400	-2.94317200	-0.58300500
C	4.47689700	-1.13816900	0.43325900
H	5.45054200	-0.88121500	0.87629500
C	3.36692200	-0.32526800	0.67165800
H	3.45638500	0.57751700	1.29928800
C	0.56384700	-1.97860400	-1.11047300
H	0.22225000	-2.98069900	-0.75934800
C	-1.74477700	-1.00240600	-0.57986000
C	-2.40009300	-1.70864000	0.49439500
C	-3.80395600	-1.64177500	0.57312400
H	-4.32162200	-2.15988600	1.39622400
C	-4.55434000	-0.95201400	-0.39383200
H	-5.65171700	-0.91282800	-0.30890100
C	-3.91724800	-0.35388900	-1.49463400
H	-4.52336900	0.12174900	-2.28227900
C	-2.51720500	-0.38787100	-1.63015400
C	-1.64886800	-2.59030900	1.46423600
H	-0.57433400	-2.34064500	1.55185000
C	-1.88844000	0.09918700	-2.91482900
H	-0.79371200	0.24904800	-2.84137100
H	-2.10276600	-2.56998200	2.47577200
H	-1.71064500	-3.64882000	1.12688400
H	-2.35982100	1.03320200	-3.28295000
H	-2.05105300	-0.65765700	-3.71394000
C	1.57711500	2.20140200	-1.40038600
H	0.54741900	-2.03031100	-2.22587400
H	1.21694200	1.43937800	-2.12465900
C	0.63272900	2.90782200	-0.67882900
C	-0.81960900	2.65835200	-0.71374800
C	-0.94099000	1.92421200	2.13798100
H	-0.15838600	2.63249800	2.48741900
C	-1.80898800	2.41031900	1.09951500
H	-2.66291400	1.78433400	0.77803300
C	-0.83389700	0.58767700	2.63244600
H	-1.71063900	-0.08257900	2.56440300

C	0.43071000	0.04722000	2.90842000
H	1.27951000	0.73188300	3.12023300
H	0.55267000	-0.98151000	3.27967900
H	-2.04763400	3.48234000	1.14358500
H	0.98875800	3.73444100	-0.03232800
H	-1.40147300	3.59085000	-0.76150100
C	3.03546800	2.52143100	-1.44961600
H	3.66592500	1.60987700	-1.38826600
H	3.26691600	2.97433500	-2.44096500
H	3.34551800	3.24516900	-0.67028500
H	-1.16366100	1.97489100	-1.51340900

1_{Zr} syn-P/trans-S

E: -1010.28308970 A.U.

Zr	0.20294400	0.81410500	0.21445200
N	2.10771900	-0.53822200	0.11838400
N	-0.41040500	-1.04963300	-0.17300900
C	1.86372700	-1.85585900	-0.15228100
C	2.90640600	-2.79828400	-0.19024000
H	2.68043500	-3.85157600	-0.41735400
C	4.22067300	-2.38455200	0.06823400
H	5.04813500	-3.11077400	0.04610500
C	4.46509900	-1.02883200	0.35895400
H	5.47981700	-0.66103100	0.57222000
C	3.38736700	-0.14067500	0.36685000
H	3.54547500	0.92971300	0.57935900
C	0.41930300	-2.22641700	-0.39339900
H	0.11535000	-3.05711600	0.28686700
C	-1.84292300	-1.04542300	-0.28892400
C	-2.64790800	-1.27689100	0.88248300
C	-4.04616600	-1.16897200	0.76247700
H	-4.67665700	-1.33450200	1.65076500
C	-4.64854800	-0.89153900	-0.47499700
H	-5.74474500	-0.81299600	-0.54522500
C	-3.86322700	-0.75566800	-1.63110300
H	-4.35141000	-0.59185300	-2.60512500
C	-2.46039000	-0.84912700	-1.57402900
C	-2.06113500	-1.74655800	2.19402600
H	-0.96000100	-1.64323200	2.24072100
C	-1.67430200	-0.82214500	-2.86433600
H	-0.57904700	-0.77281600	-2.71299300
H	-2.51139000	-1.22715400	3.06584700
H	-2.28808100	-2.82535500	2.33950600
H	-1.97839900	0.02051400	-3.52032200
H	-1.87902600	-1.74649600	-3.44719400
C	1.39849900	1.60518500	-1.95568000
H	0.28879500	-2.62562400	-1.42826800
H	0.94603700	0.70455300	-2.42568200
C	0.51390300	2.61203900	-1.54976900
C	-0.87294800	2.38819000	-1.32342700
C	-1.01972100	1.70933600	2.21472900
H	-1.64721100	0.84974400	2.51091100
C	-1.56544100	2.72713700	1.46356200
H	-1.01237900	3.66283500	1.27576900
C	0.38956000	1.70557500	2.61554100
H	0.93914100	2.66709500	2.54827100
C	1.07350100	0.57347300	2.97589500
H	2.14594600	0.61056900	3.22411000
H	0.55794600	-0.39087900	3.12786100
H	-2.62378600	2.70217600	1.16032100
H	0.94812600	3.57886400	-1.22340700

H	-1.51738600	3.24628300	-1.08748800
C	2.85416000	1.82975100	-2.24455500
H	3.47228800	0.92940600	-2.05727300
H	2.97381900	2.05891100	-3.32790600
H	3.27446000	2.68908400	-1.68382000
H	-1.38217300	1.59395900	-1.90235000

TS_{1-2Zr} syn-P/trans-S

E: -1010.27153053 A.U.

Zr	-0.19581400	0.74538700	-0.30180800
N	-2.16879400	-0.48076000	-0.13254500
N	0.29985100	-1.15211900	0.09192600
C	-2.01310900	-1.81483900	0.12226800
C	-3.12354600	-2.67062800	0.22627600
H	-2.96989400	-3.74160100	0.42969200
C	-4.41456100	-2.14688400	0.06912300
H	-5.29503900	-2.80368100	0.14646600
C	-4.56901300	-0.77131400	-0.19036500
H	-5.56354900	-0.31981900	-0.32215900
C	-3.42516300	0.02386600	-0.28458300
H	-3.50686000	1.10382900	-0.49452500
C	-0.58773200	-2.29107200	0.28144200
H	-0.36467300	-3.09862900	-0.45659500
C	1.72171500	-1.16935100	0.27697200
C	2.58245600	-1.42595900	-0.84980700
C	3.97335600	-1.32283000	-0.66341100
H	4.64560800	-1.50724400	-1.51663700
C	4.51645900	-1.02135000	0.59636800
H	5.60856300	-0.94781700	0.71817500
C	3.67745700	-0.85565300	1.71048500
H	4.12014400	-0.67776900	2.70372600
C	2.27824300	-0.94931700	1.58846900
C	2.05237700	-1.89358300	-2.18430300
H	0.95646100	-1.77678800	-2.28369900
C	1.43523000	-0.90503100	2.84343000
H	0.34748300	-0.95490500	2.64626000
H	2.54794400	-1.37976100	-3.03443100
H	2.27544300	-2.97508700	-2.31559300
H	1.64552000	-0.00360300	3.45726700
H	1.68400700	-1.77364500	3.49027800
C	-0.97018500	1.79773300	1.93494000
H	-0.44558000	-2.75605200	1.28626800
H	-0.43391600	0.91332700	2.34710400
C	-0.20682600	2.75753500	1.28392300
C	1.17745100	2.58428500	0.86147200
C	1.09064500	1.58973500	-2.05211000
H	1.71405600	0.73234300	-2.36062200
C	1.63352000	2.60669500	-1.19654700
H	1.23308100	3.62761800	-1.31728600
C	-0.25141000	1.72518100	-2.58847500
H	-0.70978200	2.73593800	-2.57206600
C	-1.06337900	0.64924400	-2.88486500
H	-2.10656000	0.79382600	-3.20605400
H	-0.65159500	-0.37206500	-2.98441400
H	2.71612200	2.56792400	-0.99777500
H	-0.70770300	3.69980900	0.98442800
H	1.75390500	3.52118300	0.84035300
C	-2.36935400	2.00814300	2.43326200
H	-3.00006600	1.10393600	2.31598900
H	-2.33516300	2.21633600	3.52648400
H	-2.86746900	2.87209600	1.94980300

H	1.75690400	1.78734800	1.37245200
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1_{Zr} syn-S/trans-P

E: -1010.28687615 A.U.

Zr	-0.16029400	0.76249900	-0.37060400
N	-2.12156800	-0.48570500	-0.09934700
N	0.27180500	-0.79870200	0.78445900
C	-2.00784600	-1.55512000	0.74522100
C	-3.09462800	-2.41124700	0.99434000
H	-2.97305100	-3.25849100	1.68684200
C	-4.31602900	-2.18344900	0.34497600
H	-5.17449000	-2.85024100	0.52088800
C	-4.42447400	-1.09304500	-0.53818600
H	-5.36082700	-0.87921200	-1.07477200
C	-3.31347900	-0.26672900	-0.72239100
H	-3.37380600	0.60458700	-1.39512500
C	-0.64445900	-1.76758200	1.36538900
H	-0.29516000	-2.80903400	1.18113500
C	1.69448500	-0.92606600	0.68849100
C	2.26127000	-1.77241400	-0.33576400
C	3.65918400	-1.79013200	-0.48204100
H	4.11183200	-2.42647900	-1.25939100
C	4.49084300	-1.03477800	0.36802600
H	5.58330200	-1.06572800	0.23103800
C	3.94012600	-0.28333200	1.41512500
H	4.60485600	0.25225000	2.11160200
C	2.54549200	-0.23624900	1.62412400
C	1.41713600	-2.71129800	-1.16783500
H	0.37364000	-2.36739300	-1.31269400
C	2.01232500	0.41775100	2.87315100
H	0.91034400	0.49922200	2.88377400
H	1.87154200	-2.89727700	-2.16182300
H	1.35938100	-3.70568100	-0.67159600
H	2.45435800	1.42106600	3.04178400
H	2.30510000	-0.19413300	3.75446900
C	-1.73961900	2.42254600	0.73438200
H	-0.70100100	-1.65878400	2.47536300
H	-1.80538000	2.84380800	-0.30424500
C	-0.50138300	2.55619500	1.37723800
C	0.70436500	2.76740500	0.66047500
C	1.22807400	1.55266400	-2.48610600
H	0.69916400	2.48586700	-2.76701900
C	2.41434100	1.63391200	-1.80633700
H	2.99911700	0.73206500	-1.54981400
C	0.58842500	0.28531800	-2.83903600
H	1.21578800	-0.62357200	-2.83358100
C	-0.75644900	0.17463400	-3.07797500
H	-1.39590000	1.07377700	-3.17907800
H	-1.22385500	-0.79553500	-3.30793800
H	2.85294100	2.61015000	-1.54627500
H	-0.45053100	2.27288400	2.44518700
H	0.65991400	3.42676900	-0.22883700
C	-3.04761500	2.26391300	1.45386500
H	-3.50647900	3.26595800	1.61009300
H	-3.78925700	1.66899800	0.88510500
H	-2.91268900	1.80471900	2.45362900
H	1.66075900	2.80293600	1.20484400

TS_{1-2Zr} syn-S/trans-P

E: -1010.25684139 A.U.

Zr	-0.19280300	0.65378400	-0.45632600
N	-2.19662600	-0.45136300	-0.14068900
N	0.18875300	-0.95008700	0.67482900
C	-2.13756200	-1.55962700	0.65929300
C	-3.28869600	-2.31209200	0.94887700
H	-3.21219700	-3.19796200	1.59806100
C	-4.51922600	-1.93052300	0.39552800
H	-5.42904000	-2.51463300	0.60446400
C	-4.57316300	-0.79498800	-0.43564400
H	-5.51625400	-0.46454800	-0.89569200
C	-3.39584800	-0.08382700	-0.67431300
H	-3.40244200	0.80830800	-1.32323300
C	-0.76557800	-1.92578000	1.17948300
H	-0.49738700	-2.95854500	0.85523000
C	1.61143000	-1.08886500	0.63389500
C	2.22432600	-1.87038400	-0.41471600
C	3.62557300	-1.84122600	-0.53075500
H	4.11177500	-2.41668300	-1.33467800
C	4.41547600	-1.11291800	0.37746400
H	5.51086800	-1.10286400	0.26264100
C	3.82064500	-0.44349800	1.45925700
H	4.45696000	0.05865600	2.20569100
C	2.42260000	-0.44139900	1.63366600
C	1.42236600	-2.77777200	-1.31778200
H	0.36951700	-2.45924300	-1.44789100
C	1.84127100	0.12888800	2.90542300
H	0.73562100	0.11831900	2.92223000
H	1.89018000	-2.88041200	-2.31758700
H	1.39804600	-3.80391400	-0.88770800
H	2.20201800	1.15873700	3.10931600
H	2.18384600	-0.48364900	3.76748900
C	-1.38986700	2.67386700	0.76601200
H	-0.76773600	-1.95067000	2.29559700
H	-1.59007200	3.21153500	-0.18956700
C	-0.06145000	2.53574100	1.15632200
C	1.10127200	2.93267800	0.36391900
C	1.14317700	1.69235900	-2.24208200
H	0.51653000	2.51904200	-2.63944700
C	2.09084100	2.03985600	-1.22519700
H	2.73379300	1.23848900	-0.80977400
C	0.79042000	0.37038500	-2.65455000
H	1.54212500	-0.43219200	-2.54471800
C	-0.54171900	0.02975900	-2.92061900
H	-1.28033900	0.82737100	-3.14465600
H	-0.82487200	-0.98621200	-3.23530000
H	2.61298000	3.00410800	-1.31686400
H	0.13808000	2.07744000	2.14256600
H	0.91750800	3.82484100	-0.25917300
C	-2.56767200	2.46805400	1.67004700
H	-2.93779300	3.46328400	2.00705200
H	-3.42437800	1.98621100	1.15637600
H	-2.31094800	1.88450100	2.57637000
H	2.02916100	2.99734900	0.95612100

1Zr syn-S/trans-S

E: -1010.28607245 A.U.

Zr	0.16874600	0.85672300	0.06825100
N	2.15523900	-0.37363500	0.21149200
N	-0.31030300	-1.07685800	-0.03965000
C	1.99723700	-1.72972800	0.13725700
C	3.09615400	-2.60066200	0.24471300

H	2.93742400	-3.68809000	0.17828400
C	4.37979000	-2.07248500	0.43829500
H	5.25045600	-2.74089700	0.52652100
C	4.53777600	-0.67547000	0.51769000
H	5.52622500	-0.21692100	0.66978300
C	3.40720000	0.13427400	0.39376500
H	3.49892200	1.23219500	0.44284700
C	0.58306200	-2.22418500	-0.05975000
H	0.31370100	-2.95706800	0.73721500
C	-1.74144100	-1.13934800	-0.12470100
C	-2.51518900	-1.27365300	1.08423800
C	-3.91613800	-1.20436600	0.98893900
H	-4.52354200	-1.29656800	1.90359200
C	-4.55245600	-1.05480800	-0.25623200
H	-5.65134100	-1.00074000	-0.30570800
C	-3.79837900	-1.02393500	-1.43842800
H	-4.31209700	-0.97270200	-2.41171000
C	-2.39123200	-1.09612200	-1.40845500
C	-1.88091800	-1.60249600	2.41655700
H	-0.80083000	-1.36007900	2.46307600
C	-1.63980600	-1.25590000	-2.70825800
H	-0.54560000	-1.13083700	-2.60402000
H	-2.39985900	-1.10283700	3.26026900
H	-1.96917500	-2.69402500	2.61292200
H	-2.01132900	-0.56086600	-3.48884800
H	-1.81357200	-2.27975400	-3.10646500
C	1.42364600	1.63892000	-1.94805200
H	0.50037400	-2.78384500	-1.02247300
H	1.82638500	2.42953300	-1.26067000
C	0.06360200	1.75234600	-2.27980500
C	-0.85434400	2.49088800	-1.49343400
C	-1.14175400	1.84480800	2.00315700
H	-1.52938800	0.90426700	2.43358200
C	-1.95809700	2.60638000	1.20034100
H	-1.67223600	3.62005000	0.87919600
C	0.24428600	2.20325500	2.30972800
H	0.57484400	3.23476900	2.07381700
C	1.15488000	1.30166400	2.79519800
H	2.20287700	1.58826900	2.97669700
H	0.85206700	0.28827300	3.11377100
H	-2.98213900	2.27568800	0.96431100
H	-0.32881400	1.07660700	-3.06067900
H	-0.48082600	3.41997800	-1.02062600
C	2.44189700	0.94231900	-2.80679500
H	2.89310900	1.67341300	-3.51426700
H	3.27952700	0.51197000	-2.22341300
H	1.98175700	0.13923200	-3.41670900
H	-1.91994700	2.50533600	-1.76902700

TS1-Zr syn-S/trans-S

E: -1010.27145155 A.U.

Zr	0.18866300	0.79486400	0.23560100
N	2.22714100	-0.33282600	0.16176900
N	-0.19321100	-1.14730900	-0.02507500
C	2.14569300	-1.68551100	-0.02195300
C	3.30167000	-2.48223100	-0.09389500
H	3.20672300	-3.56952800	-0.23798500
C	4.56247600	-1.87942700	0.01675600
H	5.47802600	-2.48881000	-0.03852400
C	4.64120100	-0.48521300	0.20043000
H	5.60976000	0.02819900	0.29308800

C	3.45521400	0.24784700	0.27067900
H	3.48001800	1.33963600	0.42753500
C	0.74874800	-2.24887200	-0.14326600
H	0.57207900	-3.02091500	0.64367700
C	-1.61438100	-1.23300900	-0.17871500
C	-2.44244700	-1.51935100	0.96630600
C	-3.83823700	-1.47883400	0.80496200
H	-4.48675700	-1.68512800	1.67144200
C	-4.41762500	-1.20814500	-0.44774000
H	-5.51407600	-1.17943000	-0.54771400
C	-3.60913200	-1.02068800	-1.57912200
H	-4.07727600	-0.87499700	-2.56574600
C	-2.20387400	-1.05999200	-1.48335400
C	-1.86110900	-1.94884100	2.29260200
H	-0.79007500	-1.69155500	2.40606400
C	-1.38113600	-1.06614300	-2.74953800
H	-0.31436400	-0.82081100	-2.58632200
H	-2.42516800	-1.52775900	3.15003400
H	-1.93751100	-3.05420700	2.39304000
H	-1.79699000	-0.38265300	-3.51752600
H	-1.41339800	-2.08254700	-3.20108200
C	0.95814200	1.95625400	-1.84112400
H	0.63088700	-2.77934700	-1.11804500
H	1.59424500	2.56689900	-1.14853000
C	-0.41743000	2.16591300	-1.75870900
C	-1.05432300	2.95306600	-0.71010700
C	-1.15337500	1.52544700	1.98089400
H	-1.61068600	0.57549400	2.30610400
C	-1.88507000	2.41247600	1.11482500
H	-1.84665200	3.48888200	1.34975700
C	0.14112700	1.90933700	2.51401300
H	0.42787800	2.97913900	2.45678700
C	1.10506100	0.99550500	2.88035800
H	2.11072100	1.31965300	3.19096100
H	0.86202600	-0.07327700	3.02504300
H	-2.88192000	2.06654100	0.79612100
H	-1.06886900	1.66744200	-2.49937300
H	-0.41497300	3.76502000	-0.31406800
C	1.68647800	1.33436100	-2.99709400
H	2.14449800	2.14190300	-3.61142100
H	2.51942400	0.67765400	-2.67454800
H	1.00870500	0.76364100	-3.66101500
H	-2.05632900	3.31355900	-0.99192400

2_{Zr} syn-P/trans-P

E: -1010.30040403 A.U.

Zr	-0.31437600	0.80031000	0.00406300
N	-2.51421000	0.11550400	0.00655800
N	-0.28250300	-1.18532500	-0.15197300
C	-2.69597900	-1.23403400	-0.13672000
C	-3.98545400	-1.79004400	-0.16724100
H	-4.10861200	-2.87753800	-0.28635400
C	-5.10261200	-0.94999100	-0.04595200
H	-6.11969900	-1.37174900	-0.06814800
C	-4.90840800	0.43698300	0.10093500
H	-5.75765700	1.12974400	0.19574500
C	-3.60250700	0.92934700	0.11804500
H	-3.41195500	2.01185900	0.21841500
C	-1.43881400	-2.06590700	-0.26393900
H	-1.43614500	-2.60886500	-1.23943800
C	1.08032200	-1.62631700	-0.08045700

C	1.85588400	-1.74161600	-1.28779400
C	3.22084700	-2.07488000	-1.16902600
H	3.83330600	-2.15927400	-2.08097200
C	3.79668600	-2.34102900	0.08166700
H	4.86378000	-2.60503500	0.14863000
C	3.00924500	-2.31668400	1.24734900
H	3.46197300	-2.58400500	2.21556700
C	1.64397900	-1.98497100	1.19586800
C	1.23550100	-1.66522800	-2.66288100
H	0.24242000	-1.17829200	-2.67590800
C	0.80325900	-2.10564600	2.44645700
H	-0.11969300	-1.49198100	2.42456300
H	1.90006100	-1.15340200	-3.38852900
H	1.09631500	-2.69572200	-3.05837100
H	1.38098600	-1.84480900	3.35599100
H	0.47976400	-3.16132400	2.58363500
C	0.98499700	1.40761600	2.04646600
H	-1.41502400	-2.85598500	0.52324900
H	1.49400500	0.43394700	2.18391300
C	1.64019900	2.39540600	1.34795300
C	2.94731900	2.25534300	0.60711600
C	1.26197300	2.59635600	-1.21362200
H	0.63063200	3.43401200	-0.84792000
C	2.73702700	2.69286200	-0.87341900
H	3.34861200	2.06466700	-1.55143300
C	0.64306100	1.72454700	-2.11014700
H	1.26961800	0.98464400	-2.64154800
C	-0.78259400	1.57769800	-2.14376700
H	-1.39297100	2.47967500	-1.91136900
H	-1.24921600	0.90713200	-2.88333700
H	3.06944300	3.74147600	-1.03128400
H	1.19415700	3.40957300	1.36308500
H	3.72443700	2.87067100	1.11299500
C	-0.33714100	1.62086200	2.74501600
H	-1.19927300	1.04172600	2.28595900
H	-0.32383500	1.22151000	3.78149900
H	-0.63875300	2.68756900	2.78150500
H	3.29459300	1.20210100	0.65378800

2_{Zr} syn-P/trans-S

E: -1010.30263665 A.U.

Zr	-0.26116500	0.73086900	0.02803700
N	-2.48504200	0.08839700	0.02228800
N	-0.30090800	-1.23929100	-0.27922800
C	-2.70795400	-1.24274200	-0.20370600
C	-4.01216800	-1.76383400	-0.24240100
H	-4.16619000	-2.83675800	-0.43499700
C	-5.10270800	-0.90798400	-0.03014000
H	-6.13100500	-1.30130700	-0.05436400
C	-4.86656000	0.45935700	0.20993000
H	-5.69400400	1.16448300	0.37803400
C	-3.54828100	0.91828000	0.21863500
H	-3.32679000	1.98753400	0.37749100
C	-1.47359100	-2.09526400	-0.39851200
H	-1.50810800	-2.60068500	-1.39348200
C	1.04265500	-1.67550500	-0.05544300
C	1.91670500	-1.89698700	-1.17833200
C	3.26211000	-2.21446500	-0.91905100
H	3.94741700	-2.38440400	-1.76478600
C	3.73712300	-2.34704900	0.39739600
H	4.79528100	-2.59654700	0.57387400

C	2.86370600	-2.20620200	1.48803500
H	3.23851500	-2.36885200	2.51130900
C	1.50282300	-1.89968500	1.29279300
C	1.40779000	-1.89810000	-2.59898200
H	0.44414400	-1.36652300	-2.71877200
C	0.56706900	-1.92088100	2.48058800
H	0.34835400	-2.97378400	2.76481000
H	2.14823300	-1.46802200	-3.30352000
H	1.24046900	-2.94580600	-2.93444900
H	-0.41407700	-1.44090300	2.28899700
H	1.02424000	-1.45382400	3.37604200
C	1.23317200	1.74104800	1.81384600
H	-1.44612600	-2.91539200	0.35731700
H	1.98993300	0.93287900	1.86739900
C	1.47099700	2.84931500	1.03851200
C	2.62811200	3.08270200	0.09577700
C	1.48876600	1.53175300	-1.58683300
H	1.52089800	0.59406900	-2.17459800
C	2.79438500	1.94445000	-0.93530400
H	3.54023600	2.23204100	-1.71169700
C	0.34986900	2.33930700	-1.75685400
H	0.38351600	3.38743500	-1.39897800
C	-0.93190400	1.77932600	-2.00981400
H	-1.81067600	2.44058100	-2.08691100
H	-1.00741700	0.85024600	-2.61149400
H	3.23600500	1.04784800	-0.44634200
H	0.73949200	3.67902800	1.13191500
H	2.48124100	4.05520500	-0.41537200
C	0.01474800	1.62600900	2.70201200
H	0.26729700	1.23380100	3.70917300
H	-0.51983700	2.59079700	2.81883800
H	-0.76159800	0.86692800	2.35626800
H	3.56763100	3.19431200	0.68248900

2_{Zr} syn-S/trans-P

E: -1010.30290238 A.U.

Zr	-0.31863800	0.81265200	0.00033300
N	-2.52297900	0.13018600	0.03775400
N	-0.30058000	-1.17345900	-0.18645200
C	-2.71248300	-1.21393700	-0.13623200
C	-4.00346900	-1.76733200	-0.14592400
H	-4.13249900	-2.85073800	-0.29289300
C	-5.11485300	-0.92972500	0.03253700
H	-6.13314000	-1.34902900	0.02767500
C	-4.91264300	0.45184600	0.21291800
H	-5.75681400	1.14338500	0.35185500
C	-3.60549900	0.94195500	0.20201700
H	-3.41008000	2.02181000	0.31922900
C	-1.46106400	-2.04543000	-0.32103300
H	-1.47784900	-2.54650300	-1.31871900
C	1.05953200	-1.60611700	-0.06793800
C	1.87080200	-1.75147300	-1.24938100
C	3.23945500	-2.04408000	-1.08060200
H	3.87986000	-2.14729600	-1.97124800
C	3.78663800	-2.24824300	0.19564400
H	4.85783300	-2.48160900	0.30104500
C	2.96559200	-2.20860900	1.33662500
H	3.39494700	-2.43954500	2.32482000
C	1.59308700	-1.91581400	1.23447500
C	1.28407500	-1.74093400	-2.64054000
H	0.26886300	-1.30481100	-2.68816500

C	0.71522300	-2.05332700	2.45698500
H	-0.26524600	-1.54698700	2.36147100
H	1.93996500	-1.21528400	-3.36427600
H	1.20610800	-2.78744000	-3.00987000
H	1.22176600	-1.68868300	3.37363600
H	0.50020100	-3.12955600	2.63952400
C	0.87076500	2.22784100	1.85002100
H	-1.42591700	-2.86878600	0.43055200
H	0.62723600	3.29013900	1.64440800
C	2.05658100	1.74067900	1.35842500
C	2.98806700	2.53176300	0.47117800
C	1.25172400	2.33627000	-1.30806100
H	0.75866800	3.21521700	-0.83193300
C	2.72923600	2.22574900	-1.03325600
H	3.10588000	1.21643300	-1.30264100
C	0.46024100	1.62641700	-2.20989700
H	0.92981400	0.84457900	-2.83299000
C	-0.96779600	1.64803800	-2.08436300
H	-1.43790500	2.60994900	-1.77612900
H	-1.58785100	1.05951000	-2.77931800
H	3.30146800	2.95287200	-1.65318100
H	2.35934800	0.70461000	1.61605300
H	2.83963400	3.61705600	0.65396200
C	-0.08387800	1.49802000	2.76155800
H	-0.39053900	2.14755300	3.60965300
H	-1.09003200	1.25546000	2.29251200
H	0.32871800	0.55391800	3.16409700
H	4.04199000	2.29926000	0.72749600

2_{Zr} syn-S/trans-S

E: -1010.30482684 A.U.

Zr	-0.21337500	0.65291400	-0.09270100
N	-2.45135100	0.07272200	0.00556100
N	-0.33100100	-1.32957600	-0.27576400
C	-2.72508200	-1.26353400	-0.10526600
C	-4.04517300	-1.74103900	-0.05573000
H	-4.24061800	-2.81958200	-0.15844300
C	-5.09898800	-0.83388200	0.13013300
H	-6.13929900	-1.19226000	0.17539600
C	-4.81053000	0.53880700	0.25279800
H	-5.60799300	1.28305700	0.39532800
C	-3.47916800	0.95161800	0.17376000
H	-3.21940000	2.02238600	0.23521900
C	-1.52161700	-2.16798000	-0.27289500
H	-1.61049800	-2.75278100	-1.21955300
C	0.97854800	-1.67899100	0.16820900
C	1.94886100	-2.23119700	-0.73290600
C	3.24658200	-2.45635700	-0.23725300
H	4.00742500	-2.89105100	-0.90519700
C	3.58800200	-2.15100700	1.09386700
H	4.61251800	-2.34165600	1.45015200
C	2.63178400	-1.62688300	1.97810400
H	2.90478800	-1.42572900	3.02625100
C	1.30975000	-1.40213000	1.54346000
C	1.57744000	-2.63215500	-2.13662300
H	0.68993900	-2.08700400	-2.51492100
C	0.23706100	-1.00178400	2.53512100
H	-0.49687900	-0.22596800	2.18126400
H	2.42017900	-2.48508000	-2.84059700
H	1.32702600	-3.71591600	-2.17128100
H	0.67381300	-0.60930700	3.47268500
H	-0.40614000	-1.86757000	2.80439400

C	0.86006100	2.79936300	1.20302300
H	-1.48134300	-2.92227500	0.54731200
H	0.44435400	3.59957900	0.55346800
C	2.04829600	2.23792400	0.81627100
C	2.81361400	2.62283200	-0.42565400
C	1.42700900	1.06558400	-1.90666700
H	1.34111300	0.05092600	-2.34291100
C	2.81922000	1.50151000	-1.49022400
H	3.39466100	1.84028100	-2.38246700
C	0.34610100	1.93952000	-2.13354600
H	0.49063900	3.02084400	-1.94404900
C	-0.98774700	1.46942700	-2.22036000
H	-1.81674100	2.19077000	-2.31209100
H	-1.18691900	0.47829800	-2.67463400
H	3.37129100	0.61749200	-1.10562200
H	2.52203400	1.48578200	1.47993900
H	2.40710400	3.56654000	-0.84636700
C	0.15262600	2.60189300	2.51912500
H	0.10605100	3.57896900	3.05115700
H	-0.92174300	2.30890200	2.41449700
H	0.66350800	1.87858700	3.18251700
H	3.86268400	2.84593800	-0.13247600

Zirconium - Second insertion

3_{Zr} anti -S/cis-S

E: -1166.23713701 A.U.

Zr	0.24131500	-0.10927600	0.62054100
N	-0.61869500	2.00404600	-0.07580300
N	1.48105100	0.72041700	-0.72626700
C	0.12461500	2.66270900	-1.01750400
C	-0.26031300	3.91741100	-1.52115400
H	0.36534600	4.41378400	-2.27877100
C	-1.43344900	4.51965700	-1.04915700
H	-1.75073900	5.50228400	-1.43164800
C	-2.19452700	3.84778500	-0.07449900
H	-3.12007000	4.28275400	0.33082400
C	-1.75468700	2.60388100	0.38115900
H	-2.33046000	2.05892400	1.14376300
C	1.37851400	1.96115300	-1.46670200
H	2.26808800	2.61386000	-1.29588300
C	2.54318100	-0.22675200	-0.88242100
C	3.73364000	-0.10970100	-0.07553100
C	4.70046600	-1.12855900	-0.16279200
H	5.60847000	-1.06319600	0.45797200
C	4.54764500	-2.19958400	-1.05886200
H	5.31861600	-2.98442200	-1.10962800
C	3.44694700	-2.24458000	-1.92944500
H	3.37922200	-3.04757400	-2.68075600
C	2.44457400	-1.25715400	-1.88645000
C	4.03797100	1.12547100	0.74104900
H	3.14478300	1.73692600	0.97291400
C	1.38796700	-1.23210900	-2.96629900
H	0.49320000	-0.63992800	-2.69602700
H	4.56698400	0.88118400	1.68525600
H	4.73384300	1.77909500	0.16957100
H	1.07129100	-2.25293700	-3.26215600
H	1.81512400	-0.77170900	-3.88477700
C	-2.44552200	-0.87733500	0.41718300
H	1.34806400	1.77902300	-2.56796700
H	-2.72411100	-1.70756100	1.10654000
C	-1.43918900	-1.33446500	-0.59339700
C	-0.47833600	-2.34077900	-0.31021000
C	1.59026300	-0.20552000	2.70595500
H	2.60603200	0.11610600	2.43005200
C	1.32889300	-1.56867200	2.79765800
H	0.46634300	-1.95605800	3.35886500
C	0.61888700	0.85085500	2.96130800
H	0.98960900	1.89030700	2.91595200
C	-0.73373900	0.63796400	3.14401800
H	-1.14562300	-0.36262600	3.36171500
H	-1.41479400	1.48801200	3.30304400
H	2.13580800	-2.28583100	2.58578600
H	-1.58345200	-1.02783600	-1.64324200
H	0.16782300	-2.67881100	-1.13725400
C	-0.18266200	-2.78757700	0.98771000
H	0.58027500	-3.56623900	1.12865200
H	-0.94689000	-2.71231000	1.77941200
H	-1.98751500	-0.11962300	1.17573100
C	-3.72078500	-0.21929400	-0.17290000
H	-4.26220800	0.31674800	0.63439300
H	-3.41254800	0.54235200	-0.92496900
C	-4.62708000	-1.25562000	-0.78795600
H	-4.23836400	-1.79966900	-1.67005600

C	-5.86694800	-1.54714200	-0.33005500
H	-6.24116500	-0.99518500	0.55523600
C	-6.80662600	-2.54390900	-0.93124700
H	-7.10867600	-3.30449000	-0.17833400
H	-7.74904800	-2.04858100	-1.25233400
H	-6.37055100	-3.06576100	-1.80580000

3_{Zr} anti -S/trans-S

E: -1166.24117000 A.U.

Zr	0.08516000	-0.22055600	0.36150400
N	-0.42179300	2.07077800	-0.04892900
N	1.61804200	0.61077600	-0.63505700
C	0.50001100	2.73259000	-0.80992500
C	0.33568400	4.08463800	-1.16056400
H	1.09728600	4.58142500	-1.78121000
C	-0.79151400	4.78247300	-0.70901900
H	-0.93578600	5.84200300	-0.97168400
C	-1.73021500	4.10619700	0.09241300
H	-2.62574100	4.61404000	0.48006600
C	-1.51051500	2.76077400	0.39384400
H	-2.23135100	2.20813000	1.01569300
C	1.70668800	1.93290200	-1.23056800
H	2.64198700	2.45046700	-0.91167900
C	2.73036600	-0.30007400	-0.60665800
C	3.69573600	-0.19287000	0.45710100
C	4.72028900	-1.15278200	0.52865500
H	5.46146100	-1.09066000	1.34161600
C	4.83174100	-2.16885700	-0.43702900
H	5.64155600	-2.91120800	-0.36030100
C	3.94629000	-2.20995800	-1.52312400
H	4.08370900	-2.96884900	-2.31012100
C	2.90158300	-1.27163600	-1.65090000
C	3.70312700	0.96291900	1.43315600
H	2.74249800	1.51369500	1.46686300
C	2.08581200	-1.26219200	-2.92153900
H	1.31473300	-0.47046200	-2.93533100
H	3.96691700	0.63899400	2.46119600
H	4.48345200	1.69940800	1.14042700
H	1.59768100	-2.24093000	-3.11271600
H	2.75687700	-1.08541400	-3.78883300
C	-1.94663800	-0.39377500	-0.98996500
H	1.76604100	1.87377000	-2.34454100
H	-2.25824500	0.43198000	-1.65102800
C	-1.08741600	-1.37433700	-1.51555700
C	-0.50882900	-2.39663800	-0.72069600
C	1.06359500	-1.35040000	2.42455700
H	2.09236100	-0.95083600	2.36420300
C	0.80083400	-2.60441600	1.92470300
H	-0.17284100	-3.09446800	2.08739300
C	0.03139900	-0.48691800	2.99546200
H	-0.93012300	-0.95912100	3.27559500
C	0.16815300	0.87138100	3.10981200
H	-0.64937400	1.49698100	3.50159600
H	1.13040900	1.37306900	2.90846300
H	1.59891800	-3.20955800	1.46781200
H	-0.68288300	-1.19478900	-2.52598300
H	-1.13247700	-2.86939600	0.05722200
C	-2.67340600	-0.52552800	0.33018800
H	-2.15760400	0.06739800	1.16278900
H	-2.67988600	-1.57760100	0.69051500
H	0.24273300	-3.06372700	-1.16976900

C	-4.14358300	0.00870700	0.30867900
H	-4.50952200	0.07055600	1.35492000
H	-4.12848600	1.04671200	-0.09513200
C	-5.05456500	-0.87037800	-0.50578800
H	-4.86235100	-0.92042600	-1.59449100
C	-6.09073400	-1.56787900	0.01477900
H	-6.27278000	-1.49639600	1.10588600
C	-7.05079800	-2.41605200	-0.75820700
H	-8.08854900	-2.03354800	-0.64239400
H	-6.81145400	-2.45207600	-1.83928600
H	-7.06788300	-3.45515700	-0.36285200

TS_{3Zr} *anti* -S/*cis*-S

E: -1166.23167911 A.U.

Zr	0.26275600	-0.04253400	0.62899100
N	-0.57970200	2.07141300	-0.04940600
N	1.44238100	0.73946600	-0.79466100
C	0.13374600	2.71318300	-1.02641500
C	-0.25294400	3.97108600	-1.51993300
H	0.34863700	4.45467000	-2.30480300
C	-1.39753200	4.59250200	-1.00433600
H	-1.71529100	5.57816000	-1.37852200
C	-2.13001600	3.93563500	0.00198600
H	-3.03335200	4.38513600	0.44019500
C	-1.68938700	2.68903200	0.44879700
H	-2.23959500	2.15724400	1.23937700
C	1.35424000	1.98523600	-1.52632700
H	2.26490100	2.61509000	-1.38285100
C	2.45391500	-0.25549200	-0.96433200
C	3.69016700	-0.15877500	-0.22386000
C	4.60851700	-1.21981100	-0.31946300
H	5.55132200	-1.16914000	0.24846600
C	4.36074000	-2.32173100	-1.15632700
H	5.09684000	-3.13893300	-1.21516600
C	3.20831100	-2.36215200	-1.95685900
H	3.06437400	-3.19621200	-2.66239000
C	2.25185600	-1.32953500	-1.90700900
C	4.07470500	1.08689500	0.53929800
H	3.21023400	1.71463200	0.83065500
C	1.13226800	-1.31375600	-2.92099000
H	0.33238100	-0.58832000	-2.68075600
H	4.67111100	0.85104600	1.44422300
H	4.73140300	1.72082900	-0.09733300
H	0.68148400	-2.31754700	-3.06371500
H	1.54414200	-1.02657000	-3.91342700
C	-2.41692800	-0.86458600	0.48642400
H	1.27900600	1.81118500	-2.62680200
H	-2.75167300	-1.58453400	1.26916800
C	-1.39575500	-1.49699800	-0.41148800
C	-0.40632100	-2.38536800	0.04171800
C	1.62830900	-0.22825300	2.57537700
H	2.65750400	0.03827500	2.29198400
C	1.30210200	-1.61723700	2.68622400
H	0.63775600	-1.92655300	3.50891900
C	0.73830100	0.84534300	2.94975900
H	1.15211300	1.86977500	2.93352600
C	-0.62502100	0.68220400	3.13761800
H	-1.06614800	-0.30873500	3.34171900
H	-1.26492200	1.55024700	3.35693500
H	2.12633400	-2.31443600	2.47534800
H	-1.51116200	-1.36283700	-1.50028800

H	0.25622400	-2.85118700	-0.70753900
C	-0.13894800	-2.65024300	1.42854900
H	0.46352200	-3.54872900	1.62585800
H	-0.98660700	-2.52573500	2.12471800
H	-1.95086300	-0.03570200	1.15479400
C	-3.63843700	-0.24791800	-0.24045400
H	-4.21393100	0.36717100	0.48213100
H	-3.26912800	0.44177700	-1.03420800
C	-4.53207200	-1.31485200	-0.82304700
H	-4.10682800	-1.93603900	-1.63492400
C	-5.80409900	-1.54305300	-0.42384900
H	-6.21981900	-0.91220800	0.38701700
C	-6.72790400	-2.56975700	-1.00005900
H	-7.09148300	-3.26200300	-0.20956500
H	-7.63749500	-2.08621000	-1.41862500
H	-6.25084700	-3.16800700	-1.80129500

TS_{3Zr} *anti* -S/*trans*-S

E: -1166.22740809 A.U.

Zr	0.18347200	-0.10159200	0.54940400
N	-0.52841700	2.09712700	-0.01078300
N	1.58695400	0.78651300	-0.57831900
C	0.32499100	2.80454100	-0.81189100
C	0.03196100	4.11439800	-1.23067900
H	0.74507300	4.65088500	-1.87525900
C	-1.16296600	4.71914200	-0.82039200
H	-1.40985000	5.74366300	-1.13947500
C	-2.03676200	3.99556700	0.01235600
H	-2.98246300	4.43046500	0.36823300
C	-1.68254200	2.70048500	0.39391500
H	-2.34194100	2.11954400	1.05628000
C	1.59557000	2.09514400	-1.20351100
H	2.48420300	2.69240300	-0.88633500
C	2.60004600	-0.20645200	-0.76879200
C	3.72500900	-0.26297400	0.13053600
C	4.64534500	-1.31681800	-0.01744200
H	5.50422500	-1.38279300	0.66957500
C	4.50685400	-2.26219000	-1.04810600
H	5.24122100	-3.07729200	-1.14480700
C	3.46654100	-2.14537300	-1.98384800
H	3.40956900	-2.85369000	-2.82583900
C	2.51466000	-1.11229100	-1.88803500
C	4.00335600	0.82032400	1.14663300
H	3.12340100	1.45538200	1.36695500
C	1.53411000	-0.90993300	-3.02031000
H	0.64811500	-0.30647200	-2.74345100
H	4.39718400	0.40692700	2.09800900
H	4.79761000	1.49663300	0.76010500
H	1.19272000	-1.87408300	-3.44918500
H	2.04086100	-0.37416900	-3.85362500
C	-1.59086900	-1.11772900	-0.74536500
H	1.66778700	2.01658100	-2.31469300
H	-1.76688400	-0.68485600	-1.74531300
C	-0.63423500	-2.13538200	-0.62250300
C	-0.31702200	-2.81162600	0.61568100
C	1.25209600	-0.90261500	2.46647700
H	2.22863100	-0.40991100	2.31925200
C	1.09437400	-2.27860400	2.09789300
H	0.49252300	-2.91902200	2.76205200
C	0.18984000	-0.16247200	3.11906300
H	-0.65613300	-0.73521600	3.54719700

C	0.08036200	1.20788600	3.04348100
H	-0.78315100	1.73680200	3.47532000
H	0.91975000	1.83542000	2.69097800
H	1.98112500	-2.77350800	1.67204700
H	-0.03225400	-2.38632400	-1.51207800
H	-1.15482300	-2.90575600	1.32807800
C	-2.54263000	-0.74126600	0.36443800
H	-2.07022100	0.00244400	1.10705300
H	-2.76161800	-1.61801100	1.01451100
H	0.24828100	-3.74701400	0.48416000
C	-3.87623600	-0.10540700	-0.11706200
H	-4.39324000	0.34410000	0.75652800
H	-3.63914500	0.72539700	-0.82053200
C	-4.77580200	-1.12634900	-0.76776900
H	-4.42317400	-1.57353400	-1.71683900
C	-5.97251000	-1.50681600	-0.26575600
H	-6.31376700	-1.04191400	0.68086600
C	-6.90892900	-2.49441500	-0.88863100
H	-7.88653600	-2.01592300	-1.11596800
H	-6.50737600	-2.92854300	-1.82560400
H	-7.13599400	-3.32306800	-0.18294100

4_{Zr} anti -S/cis-S

E: -1166.25622171 A.U.

Zr	0.22375500	0.10540000	0.55179500
N	0.26629900	2.40278800	0.12895100
N	1.83864400	0.49779400	-0.53741100
C	1.33111400	2.83584700	-0.61270200
C	1.48656900	4.19345700	-0.94151400
H	2.35700200	4.51420800	-1.53436100
C	0.52926400	5.12177000	-0.50941500
H	0.63573800	6.18878800	-0.75977900
C	-0.56465200	4.67102300	0.25396400
H	-1.33459900	5.36622600	0.61995200
C	-0.65519100	3.31116700	0.55636500
H	-1.48561600	2.92759200	1.17185700
C	2.31680500	1.77152800	-1.04246100
H	3.33460600	2.01295300	-0.65213900
C	2.28124800	-0.81062400	-0.91997800
C	3.30500500	-1.47532100	-0.15690200
C	3.61574900	-2.80986700	-0.48410900
H	4.39095700	-3.33712800	0.09468100
C	2.98144800	-3.46306900	-1.55139300
H	3.24423300	-4.50597600	-1.78845100
C	2.04388600	-2.78241100	-2.34709300
H	1.59728100	-3.29008500	-3.21687400
C	1.69118500	-1.44887200	-2.07174700
C	4.12720800	-0.76299500	0.88955200
H	3.73524500	0.23835600	1.14754500
C	0.80798200	-0.69884100	-3.04235800
H	0.25551900	0.14669000	-2.58326300
H	4.22827800	-1.36327000	1.81726800
H	5.16162000	-0.61884000	0.50813100
H	0.07966100	-1.37023200	-3.53887600
H	1.42739200	-0.26031600	-3.85593300
C	-2.21054300	-0.04038300	-0.63705700
H	2.41454100	1.75532500	-2.15368900
H	-2.57563000	0.36449800	0.33544600
C	-1.55367800	-1.39196700	-0.49282700
C	-1.39956900	-2.10556900	0.67068700
C	0.67774400	-1.55089000	2.64311400

H	1.42508900	-2.34924200	2.49295200
C	-0.71815500	-2.00756200	3.07909600
H	-0.97359100	-1.54695100	4.05836600
C	1.18742300	-0.25772500	2.80617800
H	2.28263600	-0.14177100	2.72220500
C	0.40769300	0.93556300	2.77117500
H	-0.64646000	0.89883500	3.12122100
H	0.90654800	1.90218400	2.94284600
H	-0.67380600	-3.10175900	3.25436400
H	-1.22423800	-1.86698700	-1.43367900
H	-0.93219600	-3.10406000	0.58588000
C	-1.83692200	-1.71067700	2.06001000
H	-2.76168100	-2.27846800	2.31725500
H	-2.15599900	-0.64342300	2.10846700
H	-1.49242100	0.71277700	-1.08255400
C	-3.43271400	-0.03632400	-1.64102700
H	-3.73928800	1.02016400	-1.78595100
H	-3.05027400	-0.40213900	-2.61971200
C	-4.58816500	-0.86548100	-1.15978800
H	-4.44191800	-1.96204700	-1.12938200
C	-5.79254000	-0.34985900	-0.81781300
H	-5.92454800	0.74941100	-0.87356300
C	-6.99587800	-1.13641400	-0.40437200
H	-7.37409400	-0.79507900	0.58393800
H	-7.83187500	-0.96826500	-1.11835200
H	-6.79681600	-2.22505000	-0.35390300

4_{Zr} anti -S/trans-S

E: -1166.26116677 A.U.

Zr	0.28739300	0.21869400	0.31920400
N	1.45993900	2.22213400	0.01660000
N	2.20449700	-0.23982400	0.00776400
C	2.80232000	2.07847000	-0.20811800
C	3.63488000	3.19430000	-0.39845000
H	4.71294600	3.04780200	-0.56692300
C	3.07959300	4.48161300	-0.37533500
H	3.71743600	5.36627300	-0.52715800
C	1.69761900	4.62514400	-0.15109300
H	1.22026700	5.61575100	-0.12137800
C	0.92872000	3.47693100	0.04845800
H	-0.15164200	3.55647300	0.25195100
C	3.32248800	0.65513400	-0.24751300
H	4.13050600	0.52402700	0.51155100
C	1.99172200	-1.53302000	-0.56135200
C	2.38987400	-2.72489200	0.13098000
C	2.06261900	-3.96258200	-0.45555400
H	2.36602800	-4.89255300	0.05145600
C	1.37187900	-4.03520100	-1.67885200
H	1.13661200	-5.01963700	-2.11302700
C	0.99305300	-2.86717200	-2.36102400
H	0.47616400	-2.94025700	-3.33107800
C	1.30935400	-1.60105100	-1.82998700
C	3.19910400	-2.66039600	1.39927800
H	3.10018000	-1.68539600	1.91564300
C	1.03497900	-0.34446400	-2.63173500
H	0.63797200	0.53563800	-2.05167700
H	2.92688600	-3.47429300	2.10019400
H	4.27953100	-2.79479900	1.16965700
H	0.30827800	-0.52892400	-3.44580000
H	1.96405500	0.05113800	-3.09613000
C	-1.97954200	-0.39705900	-0.76537600

H	3.79722200	0.44211200	-1.23366700
H	-1.70617300	-0.40248400	-1.83898400
C	-1.97332100	-1.61541300	-0.12855800
C	-2.42822700	-1.97042000	1.25919700
C	-0.19260600	-1.28155900	2.26396200
H	0.86014000	-1.59182800	2.41496400
C	-1.21862600	-2.39649600	2.12402200
H	-1.56859100	-2.72654500	3.12836400
C	-0.52820900	0.02888700	2.65928700
H	-1.60081200	0.28118400	2.77369500
C	0.37808800	1.10900700	2.57355900
H	0.03800600	2.12936100	2.81302300
H	1.46035300	0.92898900	2.72298900
H	-0.73125600	-3.28379100	1.66903400
H	-1.58556200	-2.46593300	-0.72158000
H	-2.99448400	-1.14375600	1.73431600
C	-2.47979800	0.92743500	-0.23904800
H	-1.64660700	1.70169000	-0.28981000
H	-2.78182600	0.86109500	0.82675600
H	-3.13815000	-2.82309200	1.17587900
C	-3.65440700	1.53713000	-1.07763300
H	-3.84074200	2.56568300	-0.70436300
H	-3.31448600	1.63337300	-2.13381900
C	-4.90895000	0.71064800	-0.98403100
H	-4.89553900	-0.28029800	-1.47693600
C	-6.04202600	1.12498500	-0.37116600
H	-6.04316900	2.12758600	0.10145700
C	-7.32782100	0.36257300	-0.29902800
H	-8.14576500	0.93313200	-0.79100100
H	-7.26064700	-0.63252300	-0.78181800
H	-7.65048000	0.22567800	0.75618800

Titanium - Path 1

1Ti anti-P/cis-P

E: -1021.78940879 A.U.

Ti	-0.05952200	0.67360100	-0.15604200
N	-1.76606800	-0.67113700	-0.18308400
N	0.47285000	-0.76486000	0.89784900
C	-1.66225500	-1.75984800	0.64123800
C	-2.70770500	-2.68869300	0.77125900
H	-2.59714700	-3.54339500	1.45621400
C	-3.86881100	-2.52401400	0.00299800
H	-4.69259800	-3.25144300	0.07466200
C	-3.96170800	-1.41934900	-0.86647200
H	-4.85114200	-1.25759500	-1.49365100
C	-2.90215500	-0.51233000	-0.91996700
H	-2.95012400	0.37823800	-1.56492400
C	-0.33633800	-1.88034600	1.35074800
H	0.14058300	-2.86306500	1.13815300
C	1.85426600	-0.74627400	0.59974400
C	2.38919300	-1.56870000	-0.47220800
C	3.74898500	-1.43520900	-0.78793300
H	4.17482700	-2.04178800	-1.60324000
C	4.58768000	-0.55757000	-0.06693400
H	5.65252500	-0.47945200	-0.33843600
C	4.08831700	0.18202900	1.01313900
H	4.76998000	0.81590900	1.60266100
C	2.73339600	0.08952700	1.39521800
C	1.55632200	-2.59520900	-1.20384500
H	0.48333000	-2.33095300	-1.27836700
C	2.28635200	0.74618300	2.67611100
H	1.21164500	0.60418500	2.88382800
H	1.94412600	-2.77068200	-2.22681000
H	1.61656300	-3.57690500	-0.68301000
H	2.51927200	1.83105100	2.69035400
H	2.85642500	0.30421500	3.52200900
C	-3.63227100	1.74570900	1.48999200
H	-4.41710200	1.10101500	1.03976000
H	-0.47731500	-1.84249400	2.45794100
H	-3.00542500	1.14582900	2.17631600
C	-2.87509600	2.49134700	0.45146300
C	-1.50929200	2.69842200	0.38852800
C	0.88392000	2.37298800	-1.77971900
H	0.63396600	3.42325000	-1.55364500
C	2.09106800	1.89386500	-1.33897800
H	2.49873000	0.90909900	-1.62460800
C	-0.13506900	1.60704400	-2.51166600
H	-1.03221500	2.16461400	-2.82965600
C	-0.06512700	0.25995100	-2.75185800
H	0.85099700	-0.32736500	-2.56436600
H	-0.87982500	-0.26863200	-3.27016600
H	2.75960000	2.54721000	-0.75713300
H	-3.48730000	3.01627800	-0.30565000
H	-1.17804800	3.42860100	-0.36886000
C	-0.49252000	2.13234700	1.27130900
H	0.41993700	2.74978100	1.40482100
H	-0.83038100	1.69066500	2.22741900
H	-4.19881500	2.48535800	2.10494300

TS1-2Ti anti-P/cis-P

E: -1021.77311323 A.U.

Ti	-0.10950900	0.66627900	-0.42232800
N	-2.01165700	-0.40150000	-0.22898900
N	0.31009000	-0.86561600	0.55063000
C	-1.95385700	-1.57755000	0.46113300
C	-3.09184000	-2.38588400	0.62875100
H	-3.01551400	-3.32723300	1.19444900
C	-4.30626900	-1.98545900	0.05444300
H	-5.20737900	-2.60862300	0.16525000
C	-4.35493200	-0.77938700	-0.67248300
H	-5.28543300	-0.43237900	-1.14596400
C	-3.19139900	-0.01547700	-0.78611100
H	-3.19107900	0.93771000	-1.33966700
C	-0.58124000	-1.92793400	0.98050300
H	-0.25531100	-2.92135400	0.59438400
C	1.73001100	-0.93992900	0.41037700
C	2.30160300	-1.61235600	-0.73840000
C	3.68943300	-1.50839800	-0.94265400
H	4.13965200	-1.99648600	-1.82185500
C	4.51267500	-0.82531200	-0.03020800
H	5.59582300	-0.75558300	-0.21724500
C	3.96964700	-0.28102100	1.14473400
H	4.63640100	0.18113100	1.89024000
C	2.58920000	-0.35180800	1.40888200
C	1.49721600	-2.51321000	-1.64897700
H	0.40675100	-2.33197900	-1.62071900
C	2.07863000	0.07100900	2.76368100
H	2.45897400	1.06874100	3.06638700
H	1.83956200	-2.44378200	-2.70129000
H	1.65975700	-3.57163700	-1.34626400
H	2.45223400	-0.64047100	3.53228500
H	0.97489400	0.06219900	2.82791600
C	-1.74701600	1.33510800	2.82913400
H	-2.30656900	0.37599300	2.87661100
H	-0.58456600	-2.02506700	2.09357700
H	-0.69596900	1.18349100	3.13381000
C	-1.92256500	1.99783900	1.51369800
C	-0.96844000	2.57698800	0.69686600
C	0.46609600	2.59443800	-2.14112800
H	0.24667000	3.65790200	-2.33563400
C	1.44921600	2.28952800	-1.15427100
H	1.93767900	1.28239600	-1.14313700
C	-0.35063500	1.62824900	-2.76875600
H	-1.19086700	1.99927500	-3.38220400
C	-0.24087400	0.23476800	-2.53936700
H	0.77659200	-0.18150300	-2.34027500
H	-0.90506100	-0.47249300	-3.05824700
H	2.17790300	3.06409000	-0.87889300
H	-2.97241100	2.13471600	1.19459900
H	-1.36120800	3.19545700	-0.13350100
C	0.48201200	2.53093700	0.84806300
H	0.98139300	3.50429900	0.73426600
H	0.90266900	1.96191800	1.69540800
H	-2.23543700	1.98012000	3.59798400

1Ti anti-P/cis-S

E: -1021.78588905 A.U.

Ti	0.16746800	-0.62112000	-0.24666900
N	1.77918000	0.85186600	-0.16224100
N	-0.69168700	1.02133000	-0.12864400
C	1.37676800	2.16027600	-0.12746800
C	2.30010900	3.21692200	-0.08699900

H	1.93811000	4.25631500	-0.06748300
C	3.67223300	2.92956400	-0.06775700
H	4.41286700	3.74390600	-0.03529300
C	4.08594900	1.58440800	-0.09120600
H	5.15197000	1.31274700	-0.07701500
C	3.11562600	0.58193200	-0.14327300
H	3.40346000	-0.47803500	-0.17450300
C	-0.11592000	2.35083400	-0.12855200
H	-0.44126900	2.94093400	-1.01935500
C	-2.05035000	0.70463900	0.17244200
C	-2.98997400	0.52200100	-0.90935100
C	-4.29044400	0.08783600	-0.59314400
H	-5.01845900	-0.06821600	-1.40533500
C	-4.68733400	-0.09523900	0.74103200
H	-5.71091700	-0.43407700	0.96585000
C	-3.80484300	0.20376700	1.79512200
H	-4.15470400	0.12137000	2.83657600
C	-2.49025800	0.63141500	1.54584300
C	-2.67292100	0.92234900	-2.32901600
H	-1.59903900	1.12580000	-2.49511200
C	-1.62822500	1.07219600	2.70420400
H	-0.56038000	1.19448700	2.44306200
H	-3.02349800	0.17200600	-3.06772500
H	-3.22054900	1.85947800	-2.57204800
H	-1.70346400	0.37163800	3.56075300
H	-1.99033600	2.05387700	3.08159600
C	2.98160000	-1.86612700	2.28597500
H	3.99428200	-1.68253900	1.87091600
H	-0.44522300	2.93756400	0.76095700
H	2.51207400	-0.90607600	2.57237700
C	2.15726500	-2.73193000	1.40060800
C	0.77936800	-2.66822600	1.20187700
C	-0.10679800	-1.30131100	-2.57024400
H	-0.46765700	-0.56030200	-3.30219400
C	-1.02734100	-2.03681900	-1.85772600
H	-0.72495100	-2.87075900	-1.19443000
C	1.32719000	-1.31748900	-2.30791300
H	1.91822100	-0.47834400	-2.71040300
C	1.97677400	-2.35113800	-1.66148500
H	1.47875800	-3.31200000	-1.46128900
H	3.06841500	-2.32996200	-1.51899800
H	-2.10635500	-1.94522200	-2.04604900
H	2.66905800	-3.62115400	0.98892200
H	0.33188900	-3.53364100	0.67893900
C	-0.11254700	-1.61743200	1.61661800
H	-1.18859700	-1.86778200	1.69666200
H	0.23405900	-0.90491900	2.38910700
H	3.16992600	-2.43938600	3.22691100

TS_{1-2Ti} anti-P/cis-S

E: -1021.78462678 A.U.

Ti	0.18774200	-0.74738400	-0.11535500
N	1.92097700	0.56177300	-0.27827600
N	-0.55984500	0.94197600	-0.30211100
C	1.61740600	1.87711800	-0.50465400
C	2.61524300	2.83849000	-0.73402700
H	2.33152500	3.88773400	-0.90859700
C	3.96049500	2.44428800	-0.73914600
H	4.75818600	3.18198700	-0.91897700
C	4.27341200	1.09110000	-0.50798900
H	5.31510300	0.73686100	-0.50090500

C	3.23374000	0.18843400	-0.27654700
H	3.44052300	-0.87323900	-0.07781400
C	0.14648300	2.19814400	-0.48208600
H	-0.16517700	2.70207300	-1.42813200
C	-1.94135900	0.84504000	0.05692100
C	-2.92269600	0.65482000	-0.98175000
C	-4.26310700	0.46696800	-0.59925300
H	-5.02833000	0.31452700	-1.37715700
C	-4.64560700	0.51600300	0.75140600
H	-5.70053200	0.36213500	1.02756200
C	-3.69964100	0.80864100	1.74810900
H	-4.02512200	0.90327000	2.79635200
C	-2.34429200	1.00633000	1.43042900
C	-2.58961300	0.81147600	-2.44743600
H	-1.50537100	0.75680300	-2.66355700
C	-1.39574000	1.45648200	2.51661800
H	-0.32693000	1.38862200	2.23445300
H	-3.12722800	0.07477000	-3.07988500
H	-2.93401900	1.81006200	-2.79677800
H	-1.54725200	0.88380400	3.45505500
H	-1.59962900	2.51896100	2.77458400
C	2.46614400	-0.74533300	3.01785300
H	3.31824700	-0.11960200	2.67478100
H	-0.09191700	2.91834300	0.33634300
H	1.58291100	-0.10170800	3.18809200
C	2.22732900	-1.89802300	2.10733800
C	1.02142900	-2.34546300	1.59942300
C	-0.86292500	-2.05277800	-1.94052700
H	-1.69978500	-1.48380500	-2.37326200
C	-1.15249200	-3.04355300	-1.04225400
H	-0.39227500	-3.73106100	-0.63460600
C	0.48360400	-1.67590900	-2.41737400
H	0.52186900	-0.86808600	-3.16849700
C	1.65983900	-2.24263300	-2.01149600
H	1.70779800	-3.10388700	-1.32309200
H	2.61701900	-1.89560600	-2.43112100
H	-2.19620100	-3.23525200	-0.74540800
H	3.11189000	-2.52668200	1.89144500
H	1.05485100	-3.32348700	1.08384600
C	-0.27468900	-1.68312100	1.69574800
H	-1.17358700	-2.33051600	1.66832100
H	-0.37454000	-0.88349200	2.45515000
H	2.79193300	-1.14644800	4.00649000

1Ti anti-S/cis-P

E: -1021.79596015 A.U.

Ti	-0.25571900	0.90804200	-0.10486200
N	-2.05288200	-0.38904000	-0.06549800
N	0.30374600	-0.59904000	0.84484600
C	-1.95482600	-1.40612800	0.84087200
C	-3.02676700	-2.27710000	1.09181700
H	-2.91624200	-3.08250600	1.83426500
C	-4.22389000	-2.11353600	0.37829300
H	-5.07554800	-2.78872200	0.55547100
C	-4.31190500	-1.08391600	-0.57625100
H	-5.22443600	-0.92908400	-1.17108500
C	-3.21042100	-0.24351900	-0.76473800
H	-3.25148900	0.57488400	-1.49967700
C	-0.60844700	-1.51547200	1.52004800
H	-0.22533300	-2.55868600	1.49269700
C	1.64654100	-0.90317100	0.47502800

C	1.89466700	-1.86451700	-0.57771600
C	3.21542400	-2.02645600	-1.02335300
H	3.42479800	-2.74375000	-1.83318400
C	4.28245100	-1.31313400	-0.43598200
H	5.30717500	-1.45502700	-0.81400100
C	4.05083600	-0.47689700	0.66265300
H	4.90091300	0.00574100	1.17101500
C	2.74817700	-0.28073000	1.16987000
C	0.81577400	-2.76573000	-1.13762400
H	-0.20552500	-2.34558300	-1.06968600
C	2.58499100	0.42389700	2.49086800
H	1.52888500	0.56871600	2.77335200
H	1.01626600	-3.02899000	-2.19550600
H	0.80905500	-3.72934400	-0.58119900
H	3.11342200	1.39895000	2.51901400
H	3.05678900	-0.19629600	3.28429000
C	-2.17336400	2.76385600	0.10545800
H	-3.26342500	2.64310300	-0.03456300
H	-0.69721200	-1.25274800	2.60255900
H	-1.93306300	3.84672000	0.17356700
C	-1.67925400	1.98744000	1.30218000
C	-0.40125000	2.21377500	1.85285700
C	0.89033300	2.15852500	-2.01547300
H	0.77878200	3.25259600	-1.92782700
C	2.04950300	1.58275300	-1.55940200
H	2.31079600	0.52746800	-1.74420800
C	-0.22362900	1.44572700	-2.65211000
H	-1.01175100	2.07167800	-3.10705500
C	-0.36771600	0.08644900	-2.66285000
H	0.43194200	-0.58634300	-2.30953100
H	-1.24431000	-0.39237500	-3.12520100
H	2.81898000	2.20225100	-1.07390600
H	-2.42311800	1.44367000	1.90366300
H	-0.15687800	1.71421500	2.80553600
C	0.61887200	2.77406900	1.07430100
H	1.65560300	2.79210600	1.44146700
H	0.37273800	3.53892000	0.31835100
H	-1.72463200	2.45096300	-0.88955200

TS_{1-2Ti} anti-S/cis-P

E: -1021.77654504 A.U.

Ti	0.21823400	0.49066900	0.33747600
N	1.89077700	-0.89234500	0.03129300
N	-0.58809700	-1.10923500	-0.14641900
C	1.52741100	-2.16691300	-0.30236900
C	2.48235300	-3.18349900	-0.47193300
H	2.15624800	-4.19852800	-0.74620200
C	3.83913800	-2.88915800	-0.27977600
H	4.60319100	-3.67208500	-0.40561200
C	4.20811700	-1.57950000	0.08332200
H	5.26020400	-1.30707600	0.25454200
C	3.20922200	-0.61403400	0.22506800
H	3.45942500	0.41867000	0.51315400
C	0.04226300	-2.38081200	-0.44729200
H	-0.31046500	-3.18362300	0.24343900
C	-1.98767200	-0.82774200	-0.17935700
C	-2.75413500	-0.88234700	1.04220800
C	-4.09945800	-0.46312700	0.99946400
H	-4.69791500	-0.48757400	1.92428900
C	-4.69846200	-0.06721100	-0.20511900
H	-5.75258300	0.25166100	-0.21395300

C	-3.97485600	-0.11970600	-1.41156800
H	-4.47662700	0.13705700	-2.35816800
C	-2.62757500	-0.51327400	-1.43435900
C	-2.22556800	-1.48943200	2.32378700
H	-1.17599300	-1.82895100	2.25159200
C	-1.91656100	-0.67285300	-2.75714300
H	-0.81518500	-0.58721300	-2.67956500
H	-2.32585700	-0.80181900	3.19070700
H	-2.83781000	-2.38000400	2.58153000
H	-2.27702700	0.05712200	-3.50898300
H	-2.13078000	-1.67992300	-3.17989700
C	2.37144800	3.72931900	-1.13451300
H	2.82683100	4.18044500	-2.04952500
H	-0.21544600	-2.73183100	-1.47501700
H	1.45856600	4.30496300	-0.89495500
C	2.14891300	2.28888400	-1.41286400
C	0.93891800	1.62757500	-1.58388000
C	0.48082200	2.70806400	1.64612400
H	0.96948000	3.68943400	1.53492400
C	-0.77253800	2.51255300	1.01686500
H	-1.44893600	1.67799000	1.33220600
C	1.20688400	1.68133800	2.30732100
H	2.24168500	1.90995900	2.61667800
C	0.72512500	0.36606700	2.45603200
H	-0.37341500	0.19596100	2.54327100
H	1.32961700	-0.40928500	2.94974900
H	-1.35648500	3.38229600	0.68641300
H	3.05875800	1.69961400	-1.63090900
H	1.00361900	0.60253700	-2.00565400
C	-0.37274600	2.14069700	-1.28089500
H	-1.25004300	1.63085100	-1.71143800
H	-0.48725900	3.23172900	-1.23083200
H	3.13803100	3.88464000	-0.34511900

1Ti anti-S/cis-S

E: -1021.79210853 A.U.

Ti	-0.16700900	0.33967900	0.63427800
N	-1.71077300	-1.05917900	-0.08414000
N	0.78688300	-0.97541100	-0.24816700
C	-1.21196800	-2.17430700	-0.69964600
C	-2.05352500	-3.16292400	-1.23458300
H	-1.61498300	-4.05127000	-1.71464500
C	-3.44340700	-2.99705600	-1.15652700
H	-4.12105300	-3.76057100	-1.56935900
C	-3.95571500	-1.83587900	-0.54842100
H	-5.03884100	-1.65768100	-0.47441900
C	-3.06288200	-0.90024300	-0.02077700
H	-3.43760200	0.01064700	0.46885000
C	0.29220600	-2.23224100	-0.77864300
H	0.63058600	-2.38154600	-1.83050300
C	2.09697100	-0.44015900	-0.44528700
C	2.36099800	0.35702900	-1.61983200
C	3.62656800	0.95676400	-1.74278500
H	3.84301900	1.58171300	-2.62385900
C	4.62719500	0.74178700	-0.77958100
H	5.61092200	1.22285700	-0.89680500
C	4.39580200	-0.11737600	0.30706100
H	5.21006000	-0.32631400	1.01927200
C	3.14927000	-0.74197100	0.49064100
C	1.37558900	0.47150500	-2.76022400
H	0.34205500	0.18406600	-2.48189800

C	2.99102000	-1.75903300	1.59308900
H	1.95918300	-2.14302500	1.68964800
H	1.36291600	1.49137100	-3.19596000
H	1.68273800	-0.20688200	-3.58666400
H	3.31840100	-1.35894600	2.57555600
H	3.64933200	-2.63106200	1.38860300
H	0.69021800	-3.10344100	-0.20407900
C	0.97826300	0.98964100	2.46815700
C	0.23140200	-0.12592600	2.89358700
C	-2.68845900	3.05858500	-1.17241800
H	-3.50125200	2.67082700	-1.81052100
C	-2.92037900	4.16815600	-0.41727900
H	-2.12664900	4.66866700	0.16353200
C	-1.39572700	2.40637300	-1.30962700
H	-1.27604400	1.79308700	-2.22245200
C	-0.32197500	2.46493600	-0.43606700
H	-0.35362500	3.15233900	0.42991100
H	0.68473400	2.19650900	-0.81895200
H	-3.91428100	4.64444200	-0.40347100
H	2.07668000	0.99488100	2.52690700
H	0.75684000	-1.05349900	3.17441200
C	-1.14666800	-0.20307900	2.62252000
H	-1.66423300	-1.15779200	2.80365200
C	-1.99491600	1.04125600	2.45908400
H	-1.70900300	1.83743600	3.17975300
H	-1.93651400	1.54760200	1.44671200
H	-3.06903800	0.81372000	2.59358600
H	0.50888100	1.99603400	2.47058000

TS_{1-2Ti} anti-S/cis-S

E: -1021.78973137 A.U.

Ti	-0.18593700	0.52313800	0.52436100
N	-1.91989300	-0.67188400	-0.04193200
N	0.52074500	-1.15943900	0.27397000
C	-1.66861000	-2.01705800	-0.10037200
C	-2.67699400	-2.93990200	-0.41547800
H	-2.44547900	-4.01580300	-0.44386700
C	-3.96854000	-2.47225500	-0.70468300
H	-4.77320900	-3.18023500	-0.95788700
C	-4.21643700	-1.08728900	-0.67649900
H	-5.20989300	-0.67760200	-0.91229500
C	-3.17357900	-0.22351300	-0.33261000
H	-3.33576400	0.86453000	-0.29273100
C	-0.22890000	-2.40099400	0.16351100
H	0.17223200	-3.04083200	-0.65409100
C	1.83791500	-0.89241800	-0.20855200
C	2.03719300	-0.69561400	-1.62658800
C	3.31487000	-0.31632500	-2.06688000
H	3.48789500	-0.14987500	-3.14209500
C	4.38291700	-0.17224800	-1.15977200
H	5.37479500	0.13172500	-1.52966800
C	4.20499000	-0.46086700	0.20100500
H	5.06664100	-0.41298000	0.88591900
C	2.95064500	-0.85939300	0.70527800
C	0.95045000	-0.98643100	-2.63815500
H	-0.07681800	-0.78171600	-2.26986700
C	2.85255400	-1.35853200	2.12351100
H	1.81598600	-1.57920000	2.43420600
H	1.10501200	-0.41632500	-3.57573300
H	0.97478300	-2.06110200	-2.92626000
H	3.31085800	-0.65628700	2.85020800

H	3.42955500	-2.30474400	2.21362400
H	-0.14406800	-3.00691700	1.09777600
C	0.92666700	1.45674100	2.38570300
C	0.00151700	0.51690000	2.86381600
C	-1.20886700	2.70867000	-1.91150500
H	-1.73279300	2.07601700	-2.64910600
C	-1.77491400	3.89375800	-1.55355000
H	-1.27117400	4.61729900	-0.88984200
C	0.11772300	2.24217200	-1.49322200
H	0.56476100	1.46184700	-2.13534600
C	0.87173400	2.68068400	-0.43120200
H	0.55031500	3.52298900	0.20404000
H	1.91011100	2.32828800	-0.30600600
H	-2.75194700	4.19975600	-1.96126300
H	2.00656000	1.30793500	2.53185800
H	0.35675000	-0.41912600	3.32547000
C	-1.34873400	0.58252800	2.46159300
H	-2.02806400	-0.23367600	2.75209500
C	-1.96559600	1.87797900	1.98500200
H	-1.72601900	2.72361500	2.66663000
H	-1.60048600	2.25330500	0.97755600
H	-3.06370000	1.79706300	1.88985400
H	0.60979900	2.50270700	2.23450400

2Ti anti-P/cis-P

E: -1021.81076945 A.U.

Ti	-0.02268800	-0.37707700	0.25028000
N	-1.57976400	1.16207200	0.18558100
N	0.63378900	0.98067700	-0.88880800
C	-1.35292000	2.21490800	-0.66008700
C	-2.30538600	3.22619900	-0.86268800
H	-2.08489300	4.05156300	-1.55688200
C	-3.52010700	3.17322500	-0.16589300
H	-4.27871900	3.95938300	-0.30441700
C	-3.74729300	2.10417500	0.72099100
H	-4.68003600	2.02613200	1.29918500
C	-2.76111800	1.12722300	0.86827600
H	-2.90866900	0.28644000	1.56086000
C	-0.00201800	2.20115400	-1.32227400
H	0.57240200	3.11314300	-1.05383200
C	1.97489600	0.64890500	-0.67874900
C	3.00801300	1.51547000	-0.17009300
C	4.20011600	0.90551100	0.24717600
H	5.00777100	1.54795800	0.63357100
C	4.39788900	-0.49575500	0.22086300
H	5.35021200	-0.91737900	0.57752100
C	3.40953800	-1.33256400	-0.29478600
H	3.58875600	-2.41578600	-0.38221100
C	2.20321500	-0.77668300	-0.79459400
C	2.85021200	3.01169000	-0.05385200
H	1.99001700	3.29414100	0.59071500
C	1.26384900	-1.62874000	-1.61206600
H	1.07029800	-1.19103200	-2.61188300
H	3.75469200	3.46236300	0.39657000
H	2.70971300	3.49536600	-1.04391000
H	0.21869400	-1.81778200	-1.19594100
H	1.66087300	-2.65598500	-1.72765800
C	-1.78428800	-3.20843300	-2.60086300
H	-1.26262800	-2.76225400	-3.47461600
H	-0.10339900	2.21698600	-2.43379700
H	-1.17470800	-4.03017800	-2.17926100

C	-2.18814100	-2.16732000	-1.61390100
C	-2.03541300	-2.18754500	-0.25129700
C	-1.00862300	-1.48783700	2.33805400
H	-2.04958500	-1.58679600	2.69449200
C	-0.44875700	-2.70386600	1.63693600
H	0.54231400	-2.48648100	1.14233600
C	-0.31420000	-0.33197200	2.65016600
H	-0.87242800	0.47702700	3.15344600
C	0.99753900	-0.04757700	2.12684000
H	1.77211700	-0.83793000	2.16043900
H	1.40965200	0.95808000	2.31486700
H	-0.15033900	-3.46808600	2.39367200
H	-2.72308200	-1.29453300	-2.03457100
H	-2.60306600	-1.41334300	0.29622900
C	-1.45052900	-3.29002000	0.61383900
H	-2.28095600	-3.78739200	1.16409900
H	-0.96453500	-4.08467500	0.01350600
H	-2.70834300	-3.66336200	-3.02808400

2Ti anti-P/cis-S

E: -1021.82217638 A.U.

Ti	0.14347600	0.38308100	0.44182100
N	2.12163100	-0.49667800	0.19668500
N	-0.13300700	-1.01565300	-0.72119200
C	2.17473700	-1.52079400	-0.71168700
C	3.39027100	-2.12431800	-1.07077500
H	3.39655600	-2.94395400	-1.80571100
C	4.57993900	-1.67902300	-0.47650800
H	5.54275200	-2.14476900	-0.73862100
C	4.52198600	-0.63625600	0.46760900
H	5.42855100	-0.26225700	0.96633500
C	3.28048800	-0.07777700	0.77891900
H	3.20457300	0.72619900	1.52825100
C	0.83489600	-1.94643900	-1.26132300
H	0.60700200	-2.99742000	-0.96668000
C	-1.54934400	-1.09067700	-0.65032000
C	-2.18152500	-2.02865300	0.24947700
C	-3.57794100	-1.97335500	0.38234100
H	-4.08088300	-2.67701200	1.06466600
C	-4.34462800	-1.03795300	-0.33989100
H	-5.43782500	-1.01217300	-0.20765200
C	-3.73191700	-0.16031700	-1.24615700
H	-4.35089100	0.53083900	-1.84013900
C	-2.33668800	-0.18324300	-1.44903500
C	-1.39237800	-3.07503400	0.99675500
H	-0.38639400	-2.72576900	1.30531500
C	-1.74012800	0.63529600	-2.56745700
H	-0.63595700	0.68687500	-2.52589900
H	-1.93467600	-3.41866200	1.89907000
H	-1.24635500	-3.97716600	0.36141100
H	-2.15612400	1.66223900	-2.59452600
H	-2.00413200	0.16967400	-3.54260300
C	0.61463700	3.27432100	-2.38369700
H	0.66080000	2.65727500	-3.30464500
H	0.83114100	-1.93152600	-2.37708100
H	-0.42060200	3.61508300	-2.19715800
C	1.26493700	2.60806500	-1.22633000
C	0.83365700	2.59646600	0.08140000
C	-1.44713700	1.30047300	1.97923400
H	-2.51525000	1.25395000	1.70050900
C	-0.82956800	2.69072100	2.03140300

H	0.02564100	2.71284000	2.74116200
C	-0.88528200	0.13549000	2.51687300
H	-1.54533800	-0.74458200	2.60464200
C	0.51684400	-0.07713600	2.58197400
H	1.18011200	0.79154600	2.78045300
H	0.91834100	-1.04055200	2.93162700
H	-1.60183200	3.36306400	2.46387600
H	2.24857000	2.14225900	-1.42842700
H	1.60504000	2.28363700	0.82629700
C	-0.38011800	3.29884800	0.67227600
H	-0.10610600	4.36419500	0.84772600
H	-1.22370800	3.32283900	-0.05142800
H	1.22571300	4.17962600	-2.61975100

2Ti anti-S/cis-P

E: -1021.81940785 A.U.

Ti	0.08515400	0.43947500	0.28052600
N	1.66102000	-1.00281000	0.22516600
N	-0.63644200	-0.97638000	-0.67309800
C	1.40500800	-2.14091500	-0.50065300
C	2.38422200	-3.12733200	-0.68374000
H	2.15003700	-4.02897000	-1.27037600
C	3.65126300	-2.95261900	-0.10425800
H	4.42976400	-3.72191700	-0.22813300
C	3.91131500	-1.78619700	0.63972200
H	4.88983100	-1.61323700	1.11194600
C	2.89550700	-0.83882100	0.78370200
H	3.05444700	0.08456300	1.35937900
C	0.00021600	-2.22308300	-1.04755500
H	-0.53624900	-3.10861000	-0.63632300
C	-2.01599600	-0.73061900	-0.41334600
C	-2.67578600	-1.36626000	0.70796200
C	-4.00724500	-1.01744300	0.97233700
H	-4.52344000	-1.47648500	1.83034900
C	-4.69317000	-0.08591500	0.16771600
H	-5.73642100	0.17476600	0.40613100
C	-4.06955700	0.48971900	-0.94797900
H	-4.63715600	1.17496000	-1.59756500
C	-2.74184500	0.16136900	-1.28802900
C	-1.97999200	-2.38390800	1.57795800
H	-0.89275400	-2.19357400	1.69321400
C	-2.18710700	0.64328000	-2.60866300
H	-1.17103500	0.25715400	-2.81172500
H	-2.42810800	-2.41660800	2.59039200
H	-2.09394600	-3.40789000	1.15737800
H	-2.18319600	1.75078400	-2.69024200
H	-2.83977900	0.28439000	-3.43268500
C	2.78392600	1.59123900	-2.26325700
H	2.92644800	2.14147400	-3.22369600
H	0.00928200	-2.36132200	-2.15534800
H	3.43044600	2.07184700	-1.50557800
C	1.33100100	1.61336600	-1.93771000
C	0.70030800	2.37232800	-0.97670300
C	1.37552500	2.18456400	2.05058200
H	2.45102700	2.16351100	2.30659000
C	0.89237300	3.42750600	1.34474900
H	-0.21051400	3.53395200	1.42919700
C	0.58304900	1.15630800	2.53121700
H	1.07328800	0.37495800	3.14090100
C	-0.79019800	0.93180700	2.13296500
H	-1.40475500	1.81394600	1.83884900

H	-1.37315300	0.17647300	2.68428200
H	1.32583800	4.30825600	1.86750400
H	0.68864800	0.99252000	-2.58897800
H	-0.42238500	2.37927100	-1.03064600
C	1.31641000	3.47708100	-0.13914000
H	1.00074500	4.44993600	-0.57966400
H	2.42199000	3.44818800	-0.22059600
H	3.14029800	0.56079500	-2.46788900

H	-0.92723300	4.22697500	-0.28114900
H	-1.58522000	2.78001700	-1.01666400
H	-3.09076500	3.15989700	2.45047000

Titanium – Path 2

1_{Ti} syn-P/cis-P

E: -1021.79082153 A.U.

Ti	0.20594700	-0.78129100	-0.14939000
N	1.94801600	0.55457200	-0.22078000
N	-0.52582900	0.90710000	0.14037100
C	1.65723400	1.87224200	-0.01362300
C	2.64715600	2.86650000	-0.09076400
H	2.37943500	3.91910300	0.08880100
C	3.96224700	2.50107800	-0.41083200
H	4.75160100	3.26523500	-0.48483600
C	4.25501700	1.14338000	-0.64131700
H	5.27134800	0.81187500	-0.90186000
C	3.22747100	0.20380700	-0.52745000
H	3.42209600	-0.86851400	-0.68609800
C	0.20651700	2.15936300	0.27273500
H	-0.19068700	2.92675000	-0.43284400
C	-1.94401100	0.79892200	0.23574100
C	-2.74063100	0.90351500	-0.96658700
C	-4.13202900	0.72315800	-0.86092200
H	-4.75523100	0.79457100	-1.76676200
C	-4.73896200	0.49823000	0.38433500
H	-5.82985900	0.35906000	0.44442700
C	-3.97017200	0.49836200	1.56305200
H	-4.47082200	0.38183900	2.53751000
C	-2.57712500	0.67189600	1.52523000
C	-2.15916600	1.34090000	-2.29097800
H	-1.05258400	1.37101200	-2.29802100
C	-1.81508900	0.80497200	2.82084500
H	-0.71727000	0.79555600	2.68608300
H	-2.51086000	0.71237100	-3.13691600
H	-2.50753700	2.37015200	-2.52661500
H	-2.09005800	0.00964300	3.54470300
H	-2.07927600	1.76672800	3.31274200
C	1.90563600	-1.39290500	2.08495100
H	0.07728200	2.59397900	1.29332000
H	1.49165600	-0.51747900	2.62419500
C	1.00808100	-2.28541900	1.52278600
C	-0.41697300	-2.05216300	1.45600500
C	-0.44042900	-2.72178900	-1.58247000
H	-0.36161500	-3.66356100	-1.01316900
C	-1.66619800	-2.11694000	-1.68547800
H	-1.84976100	-1.27053900	-2.36591500
C	0.80267500	-2.21811100	-2.18445000
H	1.66856200	-2.90372300	-2.16552600
C	0.97254400	-0.95165200	-2.67215100
H	0.13686400	-0.23148000	-2.76740600
H	1.93760000	-0.62212200	-3.08591500
H	-2.54449600	-2.53266900	-1.16742900
H	1.42541800	-3.19243400	1.04070800
C	-0.83599200	-1.38436200	2.22988600
C	3.37421400	-1.59622000	2.19609500
H	3.94683600	-0.67629500	1.95233900
H	3.61584700	-1.80726900	3.26477200
H	3.74734800	-2.44795200	1.59421300

2_{Ti} anti-S/cis-S

E: -1021.82148896 A.U.

Ti	-0.08339000	0.44398700	-0.30243500
N	-1.94236700	-0.66855100	-0.25411800
N	0.36406800	-1.11004600	0.56799000
C	-1.86600700	-1.86753900	0.40708800
C	-3.00009100	-2.67022800	0.60466100
H	-2.90443000	-3.62826400	1.13845300
C	-4.24001400	-2.24216300	0.10736800
H	-5.13924000	-2.86316200	0.24343300
C	-4.31476000	-1.01390400	-0.57693300
H	-5.26472900	-0.64529800	-0.99185100
C	-3.14846300	-0.26364500	-0.74184700
H	-3.16981100	0.68945400	-1.29338700
C	-0.48008600	-2.24514900	0.87379800
H	-0.13177900	-3.17142200	0.35931000
C	1.77821900	-0.97179200	0.54382000
C	2.54645100	-1.58922500	-0.51402700
C	3.91860500	-1.30039400	-0.58446900
H	4.52320700	-1.75505400	-1.38530700
C	4.53375600	-0.44566800	0.35070400
H	5.61031500	-0.22922300	0.26449800
C	3.79591000	0.10486000	1.40951800
H	4.30502400	0.72539500	2.16416800
C	2.42031500	-0.16729400	1.55595600
C	1.92711000	-2.56160900	-1.48736800
H	1.92750000	-3.58837900	-1.05737200
C	1.71292000	0.27109900	2.81665800
H	0.61955500	0.10651300	2.77940000
H	0.87681300	-2.31721400	-1.74508600
H	2.51226100	-2.62029800	-2.42576900
H	1.92025000	1.33190800	3.06720500
H	2.09850400	-0.32286700	3.67400900
C	-2.86329500	2.38059500	1.68378900
H	-3.21436100	2.76251100	0.70698200
H	-0.46953900	-2.47667700	1.96535800
H	-3.46512300	1.50024200	1.99362700
C	-1.40570400	2.10102400	1.75307700
C	-0.45122700	2.42592500	0.81673700
C	1.31622300	1.82086400	-1.63650700
H	2.39729500	1.84064700	-1.41492700
C	0.57293700	3.14518500	-1.42606700
H	0.27237800	3.54297500	-2.42084100
C	0.87109200	0.73374900	-2.40550800
H	1.62288500	-0.03288200	-2.66362100
C	-0.49331500	0.38877400	-2.53041600
H	-1.25586700	1.19245100	-2.55823400
H	-0.78770900	-0.54101100	-3.04098400
H	1.30793800	3.86457900	-1.01263800
H	-1.04749200	1.63862600	2.69190800
H	0.61250000	2.32429300	1.14315000
C	-0.67565000	3.16448900	-0.49964100

H -1.07003500 -2.90954300 1.22653700

TS_{1-2Ti} syn-P/cis-P

E: -1021.77621387 A.U.

Ti	-0.13739600	0.74075900	-0.30676600
N	-1.96003000	-0.46973400	-0.27660200
N	0.46824700	-0.98521600	0.04999800
C	-1.75872800	-1.80988900	-0.11587700
C	-2.82366700	-2.72466900	-0.18241600
H	-2.63021600	-3.79986100	-0.04632700
C	-4.11876300	-2.25103700	-0.43657700
H	-4.96570400	-2.95172400	-0.50198200
C	-4.31809800	-0.86801500	-0.61200100
H	-5.31608000	-0.45420300	-0.82015100
C	-3.21761700	-0.01226000	-0.51821400
H	-3.33460500	1.07660300	-0.64459300
C	-0.31985200	-2.20467700	0.10044400
H	0.00946700	-2.93419000	-0.67754700
C	1.89675900	-0.91940700	0.12826600
C	2.67908500	-0.96051100	-1.08352800
C	4.06870400	-0.74773000	-0.98266500
H	4.68074400	-0.76671400	-1.89875500
C	4.68749900	-0.55897000	0.26176400
H	5.77534400	-0.39582700	0.31415900
C	3.93267000	-0.62648400	1.44639000
H	4.43996000	-0.54018400	2.42063600
C	2.54262100	-0.82659200	1.41305600
C	2.10601100	-1.34281400	-2.43229900
H	1.01942900	-1.54640400	-2.41325800
C	1.79449900	-1.02138900	2.71071900
H	0.69556900	-0.97591300	2.58986100
H	2.31505600	-0.57893100	-3.21158400
H	2.60202400	-2.27086100	-2.78813400
H	2.10130200	-0.28678800	3.48358800
H	2.03115300	-2.02310900	3.13199200
C	-1.53487300	1.10362200	2.22242700
H	-0.18527000	-2.73047800	1.07646500
H	-0.94527000	0.26635500	2.64295700
C	-0.85258700	2.09604500	1.54645800
C	0.59694100	2.12739900	1.38375700
C	0.05479500	3.10978300	-1.42557000
H	-0.24840300	4.15628000	-1.25418200
C	1.20173600	2.62950300	-0.73479800
H	1.73791000	1.71423000	-1.09573700
C	-0.79721400	2.29309600	-2.20646800
H	-1.73924900	2.74356500	-2.56580000
C	-0.57920100	0.91486700	-2.42215900
H	0.47204600	0.53672300	-2.46109100
H	-1.27105700	0.32167100	-3.03833500
H	1.91998400	3.35520200	-0.32966300
H	-1.43262000	2.97052500	1.19412300
H	1.18813900	1.35136900	1.90363700
C	-2.97838400	1.12750800	2.56009500
H	-3.46549800	0.14947200	2.35985600
H	-3.07085700	1.26793900	3.66376800
H	-3.53666300	1.94557100	2.06606500
H	1.04452500	3.12335500	1.51027800

1_{Ti} syn-P/cis-S

E: -1021.78852315 A.U.

Ti	0.02791600	0.31421400	0.59589600
N	-1.63505800	-0.74991500	-0.26191700
N	0.70578400	-0.27860900	-1.02242400
C	-1.40485000	-1.24384800	-1.52014500
C	-2.43092200	-1.84108700	-2.26838200
H	-2.21648800	-2.23479900	-3.27386600
C	-3.72019400	-1.92751600	-1.72014600
H	-4.53599800	-2.39930100	-2.28995100
C	-3.95495800	-1.40470000	-0.43467200
H	-4.95123400	-1.45044200	0.02977300
C	-2.88812300	-0.83296400	0.26388300
H	-3.02653700	-0.42936500	1.27954100
C	0.01394800	-1.08286600	-2.01313700
H	0.03325800	-0.58748800	-3.01300500
C	2.10002300	-0.09250100	-0.81288600
C	2.64704400	1.23323100	-0.97034600
C	3.96883400	1.46357300	-0.53424400
H	4.39981400	2.47247500	-0.63413600
C	4.75159900	0.42051400	-0.02230600
H	5.78322700	0.62005500	0.30759400
C	4.24121000	-0.89176800	0.04014500
H	4.88613500	-1.70697000	0.40512500
C	2.92624400	-1.18461100	-0.35254600
C	1.91702900	2.33658500	-1.70238900
H	0.87783900	2.06412200	-1.96593500
C	2.44288500	-2.61503200	-0.32251800
H	1.35487700	-2.71495000	-0.13722200
H	1.91951400	3.29214600	-1.13776500
H	2.44605000	2.54885300	-2.65657700
H	2.97845300	-3.20217700	0.44872800
H	2.65085800	-3.11348600	-1.29566300
C	-0.18622500	-1.43769500	2.26636500
H	0.49782200	-2.07648500	-2.15878100
H	0.59805300	-1.93920900	1.65452400
C	0.18926100	-0.24295900	2.89377800
C	1.29859900	0.50939000	2.43083200
C	-1.61538700	2.70213000	-0.37553000
H	-1.12346400	2.84412100	-1.35596300
C	-0.79781600	2.42434800	0.70969800
H	-1.21194700	2.38839500	1.73756900
C	-3.06048100	2.83186400	-0.38328400
H	-3.55288900	2.76246900	-1.36840300
C	-3.81136800	3.15302100	0.70727000
H	-3.36804600	3.33804200	1.70073400
H	-4.90037400	3.29939000	0.61988100
H	0.28363200	2.68466000	0.62962500
H	-0.53659500	0.22991100	3.58521400
H	2.20274800	-0.02301900	2.08068200
C	-1.33078700	-2.31015900	2.68627300
H	-1.81160700	-2.82695300	1.83147000
H	-0.94706400	-3.11401600	3.35468800
H	-2.09859900	-1.75481200	3.26173400
H	1.48595000	1.51410000	2.84678400

TS_{1-2Ti} syn-P/cis-S

E: -1021.79016348 A.U.

Ti	-0.13914800	0.75991500	0.06967400
N	-1.87788200	-0.50304900	-0.37680400
N	0.53435500	-0.96084500	0.13761300
C	-1.60586800	-1.84288200	-0.41518500
C	-2.58799100	-2.78714600	-0.75520600

H	-2.33213400	-3.85772600	-0.77472400
C	-3.88246400	-2.34869900	-1.07100500
H	-4.66479700	-3.07205800	-1.34900300
C	-4.16511700	-0.97142500	-1.01668400
H	-5.16858700	-0.58226900	-1.24502200
C	-3.14513900	-0.08718700	-0.65508000
H	-3.34013000	0.99241200	-0.57420700
C	-0.18224000	-2.20699700	-0.07277800
H	0.28357600	-2.80619400	-0.88902000
C	1.95510100	-0.80757300	0.05559600
C	2.56169100	-0.66157500	-1.24635700
C	3.95090300	-0.45030500	-1.31141700
H	4.43308400	-0.32845800	-2.29461700
C	4.73443300	-0.43247100	-0.14490400
H	5.82078200	-0.26724100	-0.21875000
C	4.14855300	-0.66340500	1.11070200
H	4.78422200	-0.69690700	2.00993900
C	2.76414600	-0.87781200	1.24213200
C	1.78077500	-0.85611500	-2.52426300
H	0.69359400	-0.65419700	-2.42344300
C	2.19601600	-1.24635500	2.58925100
H	1.09323900	-1.32810800	2.58433300
H	2.18169000	-0.23441400	-3.34979400
H	1.87120600	-1.91137200	-2.86618300
H	2.49876000	-0.52565000	3.37812000
H	2.59966100	-2.23136300	2.90955500
C	-1.60164400	0.45947400	2.41889100
H	-0.14488700	-2.85515800	0.83647300
H	-0.99216400	-0.44166800	2.62549400
C	-0.93097600	1.63777000	2.13082100
C	0.49097000	1.70873700	1.87396400
C	0.24279500	2.18227100	-2.02320500
H	0.36178600	1.60500700	-2.95567200
C	1.37051100	2.51262300	-1.32323500
H	1.35163400	3.13771700	-0.41333000
C	-1.14999800	2.50119200	-1.65798200
H	-1.92041200	2.03511200	-2.29596900
C	-1.54974600	3.35108400	-0.66702000
H	-0.83837200	3.93499800	-0.05789300
H	-2.61933000	3.55243800	-0.49279700
H	2.36666400	2.21569800	-1.68527500
H	-1.54631400	2.54905200	2.00877500
H	1.14581900	1.01204000	2.42458600
C	-3.06471300	0.33823700	2.66076200
H	-3.50237200	-0.54866600	2.15561100
H	-3.22850300	0.16015800	3.74963200
H	-3.63072900	1.24810300	2.38123800
H	0.92895500	2.71920300	1.77665400

1Ti syn-S/cis-P

E: -1021.79203260 A.U.

Ti	0.25521800	0.84923700	0.16667800
N	2.02481800	-0.45039900	0.14198200
N	-0.45411600	-0.79774800	-0.32385800
C	1.76233900	-1.71963500	-0.28511400
C	2.76271700	-2.70562700	-0.32972500
H	2.51547800	-3.71826400	-0.68391400
C	4.06015900	-2.38659300	0.09444200
H	4.85654100	-3.14681300	0.07620600
C	4.32436500	-1.08153000	0.55078700
H	5.32516700	-0.78770000	0.90106100

C	3.28795200	-0.14484900	0.55003800
H	3.46489200	0.88709400	0.89263900
C	0.32752600	-1.98074800	-0.66559800
H	-0.06718800	-2.87659200	-0.13237400
C	-1.88478300	-0.79388500	-0.28787000
C	-2.55312000	-1.17881900	0.93307300
C	-3.95669200	-1.10648600	0.97549000
H	-4.48266000	-1.39296100	1.90038900
C	-4.69624100	-0.71174700	-0.15100500
H	-5.79479000	-0.65792100	-0.09456100
C	-4.04484100	-0.43706800	-1.36566000
H	-4.64160900	-0.19705300	-2.26024500
C	-2.64433800	-0.49604700	-1.47477400
C	-1.82009200	-1.76268400	2.11977200
H	-0.72029300	-1.77138000	1.99827100
C	-2.01149500	-0.33069000	-2.83455400
H	-0.91381400	-0.45468400	-2.82008400
H	-2.07153500	-1.24326100	3.07051400
H	-2.13634000	-2.81688900	2.27300800
H	-2.25018500	0.65475600	-3.28850800
H	-2.42346500	-1.09130100	-3.53110100
C	1.78263800	1.96140400	-1.46282300
H	0.23995500	-2.21592600	-1.75400400
H	1.95845600	2.65025700	-0.59905200
C	0.48103500	1.89066500	-1.95532000
C	-0.62022100	2.36725100	-1.19432100
C	-0.47227000	2.52216600	1.93906500
H	-0.44320300	3.56294200	1.57531000
C	-1.66690600	1.85128200	1.91532500
H	-1.80302700	0.87170300	2.39885400
C	0.79870600	1.97363800	2.43214900
H	1.64209500	2.68433200	2.49993700
C	1.01438300	0.66164500	2.75111800
H	0.20474800	-0.09047800	2.75970900
H	1.99787600	0.31504500	3.10276600
H	-2.56881300	2.32263500	1.49450500
H	0.30810300	1.28111200	-2.85953000
H	-0.47490600	3.30329400	-0.62599100
C	2.99335900	1.52060900	-2.22238800
H	3.41404600	2.39958900	-2.76289400
H	3.80861600	1.14410500	-1.57433500
H	2.74884800	0.75332600	-2.98355600
H	-1.64779500	2.21131800	-1.55944900

TS1-2Ti syn-S/cis-P

E: -1021.77861477 A.U.

Ti	-0.14599100	0.57993100	-0.37675900
N	-1.85430700	-0.76017400	-0.15351400
N	0.60806300	-1.05137700	0.08979900
C	-1.53741100	-2.05428300	0.15350300
C	-2.52403700	-3.04918800	0.25105600
H	-2.23590700	-4.08072500	0.50552800
C	-3.86346100	-2.71314300	0.00896500
H	-4.65143800	-3.47952800	0.07491700
C	-4.18290100	-1.38434900	-0.32953900
H	-5.21878900	-1.08034500	-0.54152700
C	-3.15474000	-0.44127300	-0.39565200
H	-3.36388200	0.60583800	-0.66153700
C	-0.06481400	-2.31168700	0.34159700
H	0.28844700	-3.10775200	-0.35659000
C	2.01128700	-0.80952900	0.19574200

C	2.82727900	-0.82162100	-0.99433400
C	4.18118700	-0.44594700	-0.87294500
H	4.81815100	-0.43967300	-1.77203000
C	4.73912100	-0.13396200	0.37458000
H	5.80067800	0.15082000	0.44440700
C	3.96214300	-0.22650900	1.54547200
H	4.42915800	-0.03385600	2.52448200
C	2.60420300	-0.57654100	1.49092600
C	2.33991900	-1.34618400	-2.32787800
H	1.28476400	-1.67599700	-2.31369200
C	1.83056000	-0.76923800	2.77370500
H	1.96889400	-1.80853800	3.14735300
H	2.47988400	-0.61090400	-3.14914600
H	2.95147200	-2.22798800	-2.61518600
H	0.73990800	-0.61345700	2.65985900
H	2.19999700	-0.10275100	3.57807200
C	-2.01795100	2.44126400	1.38229700
H	0.15055600	-2.69287100	1.36816300
H	-1.88414400	3.45143800	0.94975600
C	-0.87559700	1.68764000	1.60882500
C	0.45738300	2.15036800	1.29097700
C	-0.34636500	2.84342800	-1.60112300
H	-0.81216500	3.83317800	-1.46233300
C	0.89241500	2.59024000	-0.95845200
H	1.55152100	1.75135600	-1.30009900
C	-1.07787200	1.85909300	-2.31613100
H	-2.10249000	2.11864400	-2.63492800
C	-0.61415700	0.54165900	-2.50856400
H	0.48212200	0.35889300	-2.59464400
H	-1.22495400	-0.20357800	-3.03960500
H	1.49941700	3.43287000	-0.60010800
H	-0.99344100	0.70724300	2.11335400
H	0.59661300	3.23989300	1.27462900
C	-3.39110000	2.08668400	1.81210700
H	-3.65668700	2.74845400	2.67312700
H	-4.15181900	2.33090800	1.03998500
H	-3.49784400	1.03783800	2.14892100
H	1.31696400	1.61143400	1.72275900

1Ti syn-S/cis-S

E: -1021.78928041 A.U.

Ti	-0.14209600	0.74432600	0.00573200
N	-1.85987200	-0.59215700	-0.31307800
N	0.55530200	-0.94143000	0.25988500
C	-1.57106400	-1.91913000	-0.14954500
C	-2.53212300	-2.91947600	-0.36730300
H	-2.26160800	-3.97653600	-0.22109000
C	-3.82149300	-2.55554500	-0.78108500
H	-4.58718100	-3.32491200	-0.96641200
C	-4.11822700	-1.19122400	-0.95278900
H	-5.11608900	-0.85711800	-1.27413900
C	-3.12096200	-0.24657400	-0.69679300
H	-3.33104300	0.82820100	-0.79701500
C	-0.14695900	-2.21242500	0.25364800
H	0.32941700	-2.92828700	-0.45522600
C	1.97116000	-0.77437600	0.14406400
C	2.55846900	-0.77948100	-1.17621800
C	3.94136300	-0.55122800	-1.28729000
H	4.40949800	-0.54386800	-2.28469200
C	4.73802300	-0.37311200	-0.14284800
H	5.81972300	-0.19730300	-0.25258300

C	4.17314000	-0.45961800	1.14065200
H	4.82118900	-0.37110400	2.02724600
C	2.79563600	-0.68388100	1.31905200
C	1.76261100	-1.14496900	-2.40633600
H	0.67633300	-0.93036100	-2.32177900
C	2.25280000	-0.89546600	2.70939100
H	1.15645300	-1.03352100	2.72833700
H	2.15455700	-0.64210600	-3.31297000
H	1.84919100	-2.23727400	-2.60196900
H	2.52114200	-0.06205100	3.39221800
H	2.70951000	-1.80686600	3.15202800
C	-1.98798200	1.50103800	1.98949100
H	-0.10756800	-2.70262700	1.25637000
H	-2.18588700	2.43291400	1.42215000
C	-0.67234600	1.20674200	2.30349200
C	0.46105900	1.86766000	1.70818600
C	0.23478500	1.93499600	-2.25777300
H	0.36944100	1.29146200	-3.14378000
C	1.34747000	2.29422500	-1.54774700
H	1.31709700	2.98243500	-0.68311600
C	-1.16149600	2.28667000	-1.94794300
H	-1.92298600	1.75257900	-2.54181800
C	-1.57628100	3.24622900	-1.06906600
H	-0.87540900	3.90338100	-0.52618300
H	-2.64862500	3.46630400	-0.93969500
H	2.34967200	1.97193600	-1.86765600
H	-0.48753700	0.33494800	2.95679500
H	0.28730900	2.91544900	1.37731500
C	-3.17837700	0.78808500	2.53300300
H	-3.67604300	1.44361000	3.28512600
H	-3.95071500	0.59881500	1.75797900
H	-2.91800000	-0.16563500	3.03167700
H	1.46101100	1.70261900	2.13966700

2Ti syn-P/cis-P

E: -1021.81319132 A.U.

Ti	-0.05654200	-0.49263400	-0.16798800
N	1.58443300	0.93847400	-0.33377400
N	-0.60042500	1.03933100	0.80744200
C	1.44537200	2.10836300	0.36399000
C	2.46106200	3.07691700	0.40531200
H	2.30971500	4.00100600	0.98397700
C	3.64843500	2.85521600	-0.30529900
H	4.45450000	3.60547300	-0.29542000
C	3.78624100	1.66221700	-1.03998500
H	4.69439300	1.44936100	-1.62349100
C	2.74129400	0.73665700	-1.02885400
H	2.81789100	-0.19843100	-1.60053400
C	0.11486600	2.26901000	1.04776300
H	-0.41281500	3.16716900	0.66187700
C	-1.96151400	0.76207600	0.67097600
C	-2.97064500	1.61705500	0.09945100
C	-4.19483900	1.01792800	-0.23276600
H	-4.98443600	1.65230300	-0.66698900
C	-4.45075200	-0.36385000	-0.06005800
H	-5.42688500	-0.77751300	-0.35642200
C	-3.49078700	-1.18350100	0.53006400
H	-3.71569700	-2.24097200	0.74094100
C	-2.25129700	-0.63106800	0.94887700
C	-2.76111700	3.08870400	-0.16164000
H	-1.93500800	3.27523800	-0.88150600

C	-1.34843400	-1.41952400	1.86457700
H	-0.30133400	-1.67455700	1.49078400
H	-3.67432800	3.53791300	-0.59568600
H	-2.53775100	3.65044800	0.76991500
H	-1.77557100	-2.41750400	2.08357300
H	-1.15053900	-0.88251700	2.81426100
C	1.98331500	-2.16101300	1.77604800
H	0.24735500	2.43747500	2.14326500
H	1.33191100	-2.75977800	2.44454400
C	1.93014600	-2.41819700	0.43282700
C	1.11525600	-3.51810000	-0.22817700
C	0.76568300	-1.86666100	-2.11037600
H	1.78559800	-2.09470500	-2.46570200
C	0.12087900	-2.93585100	-1.25981800
H	-0.81642700	-2.55933500	-0.74738900
C	0.15178600	-0.70939600	-2.56203500
H	0.75950200	-0.01240300	-3.16555300
C	-1.11799400	-0.26560200	-2.05567900
H	-1.95504900	-0.98600900	-1.98790600
H	-1.44817300	0.74874100	-2.33550600
H	-0.31514000	-3.73201900	-1.90973800
H	2.69008200	-1.92248800	-0.19796600
H	0.57865700	-4.13327800	0.52317900
C	2.91692000	-1.21631400	2.45569300
H	2.38195600	-0.54252600	3.15866100
H	3.61834400	-1.80137800	3.09344200
H	3.51868200	-0.61678600	1.74583500
H	1.81315100	-4.20998900	-0.74973100

2Ti syn-P/cis-S

E: -1021.82702768 A.U.

Ti	-0.09642900	0.52172000	-0.43910700
N	-2.06142600	-0.42457400	-0.29865000
N	0.18745400	-0.95751800	0.62849600
C	-2.09759700	-1.54988800	0.47899100
C	-3.29781400	-2.23328400	0.73323800
H	-3.28851400	-3.13864600	1.35949700
C	-4.49159300	-1.75337400	0.17577100
H	-5.44218100	-2.27981300	0.35432400
C	-4.45295700	-0.59285300	-0.61984400
H	-5.36388300	-0.18247700	-1.08063600
C	-3.22463200	0.03589400	-0.83702600
H	-3.16203400	0.93265700	-1.47228800
C	-0.75639900	-1.98791900	1.01205500
H	-0.47183900	-2.98304700	0.59753900
C	1.61027700	-1.01611200	0.59134400
C	2.26696400	-1.78662000	-0.44116000
C	3.66408400	-1.69481000	-0.54183600
H	4.18542900	-2.26346300	-1.32820900
C	4.40907300	-0.89743900	0.34852900
H	5.50357000	-0.83700800	0.24045800
C	3.77438200	-0.21696200	1.39832900
H	4.37892300	0.34406000	2.12892800
C	2.37718400	-0.28716500	1.57075200
C	1.50614400	-2.71366000	-1.35761100
H	0.48264800	-2.36051600	-1.59653600
C	1.76239600	0.27294600	2.83132200
H	0.66752400	0.12609100	2.87563200
H	2.04906600	-2.87521100	-2.30951100
H	1.40289800	-3.71756300	-0.88787100
H	1.99854400	1.34814800	2.97836300

H	2.19704100	-0.25053900	3.70987800
C	-1.04916500	2.20470900	1.59065400
H	-0.78199500	-2.11656100	2.12038400
H	-0.25793300	2.00546900	2.33815100
C	-0.65383200	2.64898300	0.35023700
C	0.76296600	3.06541900	-0.02515200
C	1.54221100	1.34571500	-1.85946300
H	2.59412300	1.05834100	-1.68643900
C	1.17592400	2.78217000	-1.51222000
H	0.38201900	3.16809300	-2.18762200
C	0.75418900	0.46460600	-2.61555600
H	1.22962900	-0.46691800	-2.96771200
C	-0.65623700	0.52660400	-2.60792400
H	-1.15234400	1.51845900	-2.51446400
H	-1.25459900	-0.24387100	-3.11647000
H	2.07903900	3.39572400	-1.71288800
H	-1.44865300	2.94831300	-0.36701200
H	1.51101800	2.65212500	0.69012800
C	-2.45191000	2.06611600	2.06567500
H	-2.62799100	1.08509800	2.55509900
H	-2.61737700	2.82297500	2.86803600
H	-3.20576200	2.23912800	1.27425600
H	0.81093700	4.16929700	0.11379900

2Ti syn-S/cis-P

E: -1021.81128377 A.U.

Ti	-0.05249400	-0.49147600	-0.08982200
N	1.57813400	0.98385000	-0.27136300
N	-0.64106400	1.07668000	0.80623800
C	1.39393400	2.17215800	0.38369800
C	2.38134900	3.17036600	0.41765200
H	2.19020900	4.10649800	0.96435500
C	3.58955900	2.96279200	-0.26029000
H	4.37430700	3.73532400	-0.25630600
C	3.77382500	1.75304800	-0.95604400
H	4.69887700	1.54785200	-1.51526600
C	2.75549300	0.79863500	-0.93684300
H	2.87792300	-0.15099800	-1.47398300
C	0.04460600	2.32516300	1.02840700
H	-0.49012600	3.20261300	0.60653400
C	-1.99237700	0.77904800	0.64089200
C	-2.99954200	1.59913500	0.01597000
C	-4.20491300	0.96801800	-0.32493300
H	-4.99277200	1.57327600	-0.80185000
C	-4.44468500	-0.41135700	-0.10968100
H	-5.40715100	-0.84951600	-0.41548100
C	-3.48912000	-1.19555300	0.53322000
H	-3.70434200	-2.24780800	0.77767000
C	-2.27019900	-0.60694700	0.96301000
C	-2.80577800	3.06357800	-0.29214200
H	-1.95820300	3.23866200	-0.98941200
C	-1.36767500	-1.33754400	1.92191500
H	-0.34444000	-1.67675500	1.53091400
H	-3.71084600	3.48015500	-0.77325900
H	-2.62480300	3.66285000	0.62518700
H	-1.80846500	-2.30639700	2.22935500
H	-1.12536000	-0.73445300	2.81922700
C	2.48177300	-1.92724800	0.98503000
H	0.14611600	2.52359700	2.12235100
H	3.09442900	-1.80023600	0.07359800
C	1.48055400	-2.85937500	0.95874000

C	1.09976000	-3.72910800	-0.22700600
C	0.88911400	-1.84142100	-1.91699500
H	1.94525000	-2.02527500	-2.17755000
C	0.18485400	-2.98069000	-1.21837400
H	-0.76599900	-2.65184000	-0.70067500
C	0.26004100	-0.71739100	-2.44033200
H	0.88332800	0.01239400	-2.98613300
C	-1.05920300	-0.33347600	-2.03900300
H	-1.86056100	-1.09325800	-1.97901500
H	-1.42313100	0.65950900	-2.35007300
H	-0.22901900	-3.67131300	-1.99357200
H	0.98602200	-3.09387300	1.92059000
H	2.00983500	-4.06806600	-0.76640500
C	2.95118400	-1.20016700	2.20805100
H	3.93874100	-1.61378300	2.51445200
H	3.12832900	-0.12129900	2.01755900
H	2.26151800	-1.31374000	3.06813500
H	0.59036400	-4.64532500	0.13134400

2Ti syn-S/cis-S

E: -1021.82499783 A.U.

Ti	0.22405100	0.56374500	0.33528600
N	2.27034000	-0.10552400	0.14637900
N	0.06943500	-1.26222900	0.22491200
C	2.42266100	-1.46103300	0.03923700
C	3.68729200	-2.04363600	-0.13527100
H	3.78080900	-3.13800700	-0.20935000
C	4.81742700	-1.21582800	-0.21533700
H	5.81847200	-1.65347200	-0.35385600
C	4.65590700	0.17877600	-0.10649100
H	5.51689600	0.86189300	-0.15616100
C	3.37245900	0.69393500	0.08770400
H	3.21294400	1.77719000	0.21199600
C	1.13298400	-2.24623800	0.12376500
H	1.14488600	-2.93018100	1.00587900
C	-1.29378400	-1.36766000	-0.17000900
C	-2.29943500	-1.72856900	0.79749900
C	-3.64107200	-1.74067400	0.37577400
H	-4.42872400	-2.00851000	1.09810800
C	-3.99001500	-1.44554500	-0.95378800
H	-5.04892300	-1.46747600	-1.25650100
C	-2.99994500	-1.15881700	-1.90997400
H	-3.28814200	-0.98177700	-2.95845000
C	-1.63907200	-1.13859500	-1.55466900
C	-1.94557200	-2.17444700	2.19224700
H	-0.90084000	-1.94239200	2.47157600
C	-0.57971700	-1.01162000	-2.62289800
H	0.36299200	-0.54031000	-2.27051300
H	-2.62935500	-1.74057500	2.95027700
H	-2.06643400	-3.27763600	2.27021000
H	-0.94754800	-0.44427300	-3.49958700
H	-0.29874600	-2.02033200	-2.99996300
C	0.11688600	2.45610900	-1.25383600
H	0.99517100	-2.89533000	-0.77128800
H	0.58568900	2.98332000	-0.38937000
C	-1.24802600	2.31391200	-1.24183500
C	-2.18734600	2.76416100	-0.15498300
C	-1.39827800	1.43895900	1.88343100
H	-2.33464500	0.87341600	2.03053800
C	-1.59002200	2.81212500	1.26570200
H	-0.66844800	3.43041100	1.30520800

C	-0.27276700	0.97395700	2.57718800
H	-0.39999600	0.06617300	3.19200100
C	1.05148600	1.35311400	2.24968700
H	1.25637000	2.37981900	1.87786400
H	1.89713700	0.87569700	2.76650600
H	-2.31329900	3.34457700	1.92579100
H	-1.72333600	1.90968800	-2.15528900
H	-2.54777700	3.77824300	-0.45284900
C	1.00467400	2.26099300	-2.45678000
H	1.39723600	3.25459300	-2.76990600
H	1.90073400	1.63750600	-2.25156500
H	0.45746800	1.83073300	-3.31648900
H	-3.09849000	2.12860800	-0.16832000

Titanium – Path 3

1Ti anti-S/trans-P

E: -1021.79474475 A.U.

Ti	0.18117400	0.69825600	0.55189900
N	2.08660300	-0.35242200	0.16806300
N	-0.23354700	-0.44868000	-0.84161600
C	2.03458600	-1.21371900	-0.88980400
C	3.14780700	-1.98261200	-1.27293900
H	3.06963100	-2.66393300	-2.13423900
C	4.33839000	-1.87814200	-0.54177000
H	5.21920600	-2.47809900	-0.81873700
C	4.38776500	-0.99347700	0.55334800
H	5.30082600	-0.87642200	1.15597400
C	3.25116500	-0.24635400	0.86772400
H	3.27014200	0.47219800	1.70254400
C	0.69808400	-1.28221500	-1.58700100
H	0.33503200	-2.33307500	-1.64420700
C	-1.64061700	-0.66795300	-0.75050600
C	-2.13301200	-1.75854100	0.05986700
C	-3.52344600	-1.89130300	0.21483900
H	-3.92042100	-2.71154300	0.83426200
C	-4.41677200	-1.01424400	-0.43171800
H	-5.50204400	-1.13890200	-0.29064000
C	-3.93452700	-0.01932600	-1.29398600
H	-4.64545200	0.61185900	-1.85085000
C	-2.55089500	0.15624700	-1.50451300
C	-1.21936700	-2.80972700	0.64940100
H	-0.19506200	-2.44629900	0.86412000
C	-2.09217200	1.08622300	-2.59843300
H	-0.99179300	1.12186500	-2.69914600
H	-1.64197200	-3.24194600	1.57884300
H	-1.11930200	-3.66213400	-0.05907000
H	-2.47873900	2.11766600	-2.46173900
H	-2.50242500	0.73418900	-3.56940700
C	2.05766700	2.46420500	-0.50525800
H	0.78524200	-0.93387400	-2.64473300
H	3.03585600	2.51652100	0.00523500
C	0.95090000	2.86169200	0.23841500
C	-0.42076100	2.70280700	-0.15395700
C	-1.23174000	1.17521800	2.59064900
H	-0.66985300	2.03739400	3.00094000
C	-2.43541800	1.85338200	1.97403900
H	-3.04230800	0.54442900	1.59557900
C	-0.64361700	-0.15280800	2.73102100

H	-1.30422100	-1.02157900	2.56949500
C	0.69280300	-0.34655600	2.95082600
H	1.35581300	0.50766800	3.19095700
H	1.13363900	-1.35302700	3.01739900
H	-2.86008100	2.39725500	1.87820700
H	1.15784500	3.21740300	1.26927200
H	-1.17527500	3.25642300	0.42249200
C	2.11353400	2.18218100	-1.96790200
H	2.61523700	3.04876300	-2.46021400
H	2.75849700	1.30851600	-2.19837300
H	1.12482000	2.05664900	-2.44778700
H	-0.65219700	2.61624100	-1.22714200

TS_{1-2Ti} anti-S/trans-P

E: -1021.77748180 A.U.

Ti	0.30561100	0.65835300	0.69711600
N	2.10655500	-0.43427400	0.19680700
N	-0.33239000	-0.48934800	-0.63546700
C	1.94711800	-1.28079100	-0.86134900
C	3.01619600	-2.05355500	-1.34816700
H	2.85707100	-2.72955000	-2.20254500
C	4.26855900	-1.96215600	-0.72486200
H	5.11603700	-2.56605800	-1.08497600
C	4.42429500	-1.09225800	0.37252600
H	5.38804100	-0.99226300	0.89380500
C	3.32487600	-0.34548300	0.79928500
H	3.41406800	0.35309000	1.64776800
C	0.55067200	-1.34090500	-1.43062300
H	0.17832500	-2.39109500	-1.43319700
C	-1.75095500	-0.69780300	-0.61017300
C	-2.29230300	-1.76280700	0.19623200
C	-3.69058400	-1.86787600	0.30337800
H	-4.12197600	-2.66541900	0.92927700
C	-4.54280000	-0.99065300	-0.38915800
H	-5.63446800	-1.08720800	-0.28148800
C	-4.00720700	-0.02675400	-1.25816000
H	-4.68430200	0.60158300	-1.85886000
C	-2.61584000	0.12415400	-1.41209500
C	-1.42741700	-2.81467800	0.85257500
H	-0.37221500	-2.50724500	0.97489300
C	-2.10187100	1.04174100	-2.49611800
H	-0.99742700	1.06964300	-2.54479800
H	-1.82645400	-3.11331200	1.84350200
H	-1.43118700	-3.74079200	0.23594100
H	-2.48882000	2.07730700	-2.39294600
H	-2.45989700	0.68328700	-3.48492400
C	2.01260200	2.38648100	-0.74019000
H	0.54538500	-1.02152700	-2.50126700
H	3.05381000	2.41082200	-0.36900700
C	1.04563300	2.78867700	0.16429300
C	-0.40839600	2.80683100	-0.04269500
C	-0.77606000	1.41698000	2.51335900
H	-0.01504100	2.01556200	3.05644400
C	-1.61716100	2.12186000	1.60514700
H	-2.42870000	1.58397100	1.08146400
C	-0.68300500	-0.00607800	2.64731200
H	-1.56070300	-0.63036500	2.40421900
C	0.56960300	-0.59072200	2.78672000
H	1.42887700	0.02002700	3.12930700
H	0.70877600	-1.68123900	2.82276000
H	-1.85353800	3.16655500	1.84700300

H	1.41548100	3.18419100	1.13235900
H	-0.86304700	3.76473400	0.24858600
C	1.86435400	2.08213700	-2.18801600
H	2.39870300	2.88156500	-2.75370700
H	2.38968600	1.14327800	-2.46539600
H	0.81988500	2.05618300	-2.54867900
H	-0.78082300	2.47817700	-1.02680600

1Ti anti-P/trans-S

E: -1021.79381949 A.U.

Ti	0.21482800	0.55594300	0.69315500
N	2.06626400	-0.37886100	-0.04771200
N	-0.37327500	-0.46698400	-0.74127200
C	1.88550700	-1.16097700	-1.15057100
C	2.95482800	-1.85494600	-1.74580700
H	2.77429600	-2.47537900	-2.63715000
C	4.23507600	-1.75109300	-1.18668500
H	5.08527100	-2.28928400	-1.63402500
C	4.41626900	-0.94869900	-0.04250700
H	5.40362400	-0.83896900	0.43047400
C	3.31422500	-0.27791800	0.49025600
H	3.42399000	0.36878300	1.37572500
C	0.46579300	-1.23306900	-1.65245600
H	0.12014000	-2.29192300	-1.70943000
C	-1.80505000	-0.53927700	-0.73427700
C	-2.44872300	-1.58982900	0.01342200
C	-3.85238600	-1.59081700	0.08532900
H	-4.36144100	-2.38075900	0.66056700
C	-4.61498300	-0.62091600	-0.58866300
H	-5.71348400	-0.63797000	-0.51253200
C	-3.98521800	0.33775600	-1.39687900
H	-4.59573300	1.04943800	-1.97531800
C	-2.58311400	0.38744200	-1.51201200
C	-1.68345800	-2.73997000	0.62845500
H	-0.59323100	-2.55654200	0.69312500
C	-1.96738600	1.32584400	-2.51970700
H	-0.86203100	1.29992800	-2.51364500
H	-2.06278300	-3.00187100	1.63843600
H	-1.82015600	-3.65489700	0.01120500
H	-2.30383300	2.37425500	-2.37492600
H	-2.29648500	1.04170200	-3.54246700
C	1.93091200	2.54480000	-0.28158200
H	0.39003400	-0.83719000	-2.69425300
H	2.94670600	2.57502900	0.15236700
C	0.88460000	2.79036400	0.59958900
C	-0.51834800	2.62047800	0.32925300
C	-0.99062200	0.09856800	2.67876800
H	-1.57728000	-0.79454100	2.40135900
C	-1.58396600	1.33770100	2.63202000
H	-1.08349100	2.22896700	3.04512000
C	0.40807500	-0.08762900	3.06229500
H	0.93143200	0.78013300	3.51219300
C	1.10105600	-1.24613800	2.84501100
H	2.16442100	-1.33530700	3.11716900
H	0.60718600	-2.15219500	2.45580900
H	-2.63013200	1.45216000	2.30685800
H	1.17347900	3.03735600	1.64188900
H	-1.23240800	3.16203100	0.96597600
C	1.88073600	2.46265600	-1.76900300
H	2.36394800	3.38413000	-2.17114100
H	2.49265700	1.62299300	-2.16068400

H	0.86027300	2.41485000	-2.19144200
H	-0.84504300	2.55925700	-0.72327400

TS_{1-2Ti} anti-P/trans-S

E: -1021.78733368 A.U.

Ti	0.27542900	0.72155100	0.55339100
N	2.07978600	-0.43587200	0.11032000
N	-0.37342100	-0.59571600	-0.59580100
C	1.88395200	-1.41841400	-0.81556900
C	2.93872700	-2.24477400	-1.24328500
H	2.74867200	-3.03154400	-1.98959400
C	4.21770200	-2.05869400	-0.70158500
H	5.05578300	-2.69922000	-1.01780600
C	4.41358700	-1.04413900	0.25649100
H	5.40037600	-0.86541500	0.70907900
C	3.32469100	-0.25611600	0.63312200
H	3.44007900	0.54917900	1.37683900
C	0.46519100	-1.55486400	-1.30927000
H	0.09165800	-2.59282000	-1.14827500
C	-1.80180600	-0.74645200	-0.52596200
C	-2.36268800	-1.67353800	0.42185100
C	-3.76162100	-1.74968900	0.52835000
H	-4.20772000	-2.44629700	1.25619600
C	-4.59881300	-0.96877400	-0.28860600
H	-5.69230500	-1.04151100	-0.18112200
C	-4.04560900	-0.12927000	-1.26541100
H	-4.70926800	0.43108300	-1.94322400
C	-2.65019900	-0.01225500	-1.42259400
C	-1.51742200	-2.60545000	1.26083800
H	-0.43490100	-2.37959400	1.21253700
C	-2.11963100	0.78595700	-2.58862600
H	-1.01526200	0.79264300	-2.63707700
H	-1.83122700	-2.59855500	2.32596900
H	-1.64707500	-3.65406500	0.91570300
H	-2.48799200	1.83413400	-2.58145000
H	-2.48453200	0.34635300	-3.54136100
C	1.91935400	2.31399200	-1.00478900
H	0.40859600	-1.38645800	-2.41235400
H	2.97779000	2.35220800	-0.68835500
C	1.00723000	2.82458600	-0.09739800
C	-0.45156300	2.78977500	-0.18196000
C	-1.03347900	0.99091000	2.27603200
H	-1.71516900	0.12482900	2.20430300
C	-1.41417600	2.24279900	1.72668000
H	-0.97593700	3.15488400	2.16336400
C	0.25343000	0.83675400	2.93244700
H	0.78618600	1.76042200	3.23698500
C	0.91808100	-0.36167200	3.01126200
H	1.93624200	-0.42221000	3.42611500
H	0.41921000	-1.31468100	2.76899600
H	-2.43221200	2.35502300	1.32247800
H	1.43129600	3.28840800	0.81686800
H	-0.95544500	3.72509100	0.10416300
C	1.70224300	1.90765100	-2.42112800
H	2.23801400	2.64823100	-3.06040000
H	2.18251200	0.93336600	-2.65310200
H	0.64446500	1.89766500	-2.74045400
H	-0.89893100	2.37590900	-1.10660500

1Ti anti-S/trans-P

E: -1021.80202653 A.U.

Ti	0.26511200	0.88506700	0.09029400
N	2.12398800	-0.36922800	0.03588600
N	-0.27680100	-0.70851100	-0.69753400
C	1.98549200	-1.49058100	-0.72940000
C	3.05670800	-2.36951100	-0.96222300
H	2.90507600	-3.26044900	-1.59096600
C	4.30285400	-2.10145400	-0.37926000
H	5.15555200	-2.77819700	-0.54465500
C	4.43894700	-0.95821900	0.42971100
H	5.39245600	-0.71285500	0.92082100
C	3.33416900	-0.12128300	0.60766000
H	3.41821200	0.77954200	1.23285300
C	0.59816300	-1.71796100	-1.27554300
H	0.23609200	-2.74188000	-1.03194700
C	-1.65491200	-0.93145900	-0.38985100
C	-1.98518600	-1.68926100	0.79455900
C	-3.33929500	-1.80591600	1.14839300
H	-3.61268700	-2.36962400	2.05474500
C	-4.35337500	-1.23976400	0.35010700
H	-5.40739900	-1.33987000	0.65351100
C	-4.03008800	-0.59859800	-0.85375300
H	-4.83541400	-0.22841400	-1.50828000
C	-2.68985800	-0.45697300	-1.27058500
C	-0.94171800	-2.43331200	1.59822800
H	0.07238300	-1.99277100	1.52922700
C	-2.41382600	0.05347500	-2.66171400
H	-1.33654300	0.12769800	-2.88981800
H	-1.22500100	-2.50535300	2.66778700
H	-0.86518500	-3.48270200	1.23605400
H	-2.89533700	1.03458100	-2.85527300
H	-2.85823200	-0.64931100	-3.39925000
C	1.61709200	1.95742900	-1.39955800
H	0.59669300	-1.65405500	-2.39105300
H	2.37811000	1.41278300	-1.97796000
C	0.32384000	2.08831800	-1.94377500
C	-0.71735000	2.64591900	-1.19061700
C	-0.96382400	2.00765400	1.97792500
H	-0.45883400	2.98634800	2.08820500
C	-2.18719000	1.95072800	1.36219000
H	-2.75854900	1.00906200	1.29834000
C	-0.28337700	0.82693500	2.49341000
H	-0.86718600	-0.10769700	2.54589800
C	1.03449300	0.81769700	2.86560500
H	1.61947600	1.75132600	2.94038000
H	1.52335100	-0.10751100	3.20871800
H	-2.67272000	2.86232900	0.98052900
H	0.09760000	1.53086400	-2.86714700
H	-0.49788400	3.45202300	-0.46934400
C	2.07859200	2.79466900	-0.23482400
H	1.71599600	2.44165200	0.78567200
H	3.18020100	2.78589800	-0.13891300
H	1.72777400	3.84696600	-0.29377700
H	-1.75287800	2.61111800	-1.55942000

TS_{1-2Ti} anti-S/trans-P

E: -1021.78063807 A.U.

Ti	0.34120300	0.81981300	0.22737800
N	2.17773800	-0.40207400	0.04499200
N	-0.27334000	-0.77413200	-0.53442700
C	2.00056100	-1.53396200	-0.69680900

C	3.06802400	-2.38988500	-1.01685100
H	2.88165500	-3.29082500	-1.62155700
C	4.35320000	-2.08957400	-0.54681000
H	5.20364900	-2.74868800	-0.78063700
C	4.53043900	-0.94043000	0.24592900
H	5.51505300	-0.67359300	0.65799500
C	3.42595500	-0.13027500	0.51884200
H	3.54094200	0.76413800	1.14836200
C	0.57736900	-1.81412300	-1.09760500
H	0.25996800	-2.81770300	-0.73082700
C	-1.67557800	-0.98195200	-0.32653800
C	-2.10155600	-1.69471800	0.85237100
C	-3.47995200	-1.77390300	1.11653000
H	-3.82491500	-2.29790800	2.02222200
C	-4.42296600	-1.21993500	0.23202500
H	-5.49741800	-1.28699000	0.46406700
C	-4.00216500	-0.63461000	-0.97271000
H	-4.75326600	-0.28520700	-1.69943900
C	-2.63497400	-0.52706600	-1.29507100
C	-1.13255900	-2.42476700	1.75494600
H	-0.09294700	-2.05159000	1.68141600
C	-2.25174200	-0.04782400	-2.67596000
H	-2.81770500	-0.62666600	-3.43530700
H	-1.45133400	-2.38670600	2.81655400
H	-1.11189900	-3.50423800	1.48560900
H	-1.17792700	-0.18426100	-2.89952700
H	-2.52489000	1.01511100	-2.84958100
C	1.47136000	2.09145400	-1.33553900
H	0.47276200	-1.85686300	-2.20891500
H	2.15247900	1.55406100	-2.01366600
C	0.12032600	2.15319700	-1.68096100
C	-0.89847100	2.85477400	-0.92767300
C	-0.78926100	2.08522100	1.82389000
H	-0.14935600	2.95624100	2.06980900
C	-1.80564100	2.29978100	0.84623600
H	-2.49645200	1.47179100	0.60277900
C	-0.40879500	0.82836200	2.38480500
H	-1.14452200	0.00572900	2.37469700
C	0.91816000	0.55932000	2.70518100
H	1.63506600	1.38135900	2.87585600
H	1.23017000	-0.44020500	3.04292300
H	-2.27793900	3.29340900	0.81414200
H	-0.20100500	1.59048000	-2.57030400
H	-0.57187100	3.80909700	-0.47946500
C	2.05905000	2.81389100	-0.15728900
H	1.97394800	2.23869300	0.82273900
H	3.15186100	2.95327500	-0.26747200
H	1.58359700	3.79670800	0.04056700
H	-1.86965800	2.92103100	-1.44492900

1Ti anti-S/trans-S

E: -1021.79992304 A.U.

Ti	0.33744600	0.85568100	0.06368600
N	2.11988800	-0.44691300	-0.06415500
N	-0.38964800	-0.80865600	-0.37150000
C	1.83585700	-1.70830400	-0.50025300
C	2.84079600	-2.67673900	-0.66964600
H	2.57287300	-3.68318800	-1.02657700
C	4.16995000	-2.34622600	-0.37514100
H	4.97232100	-3.08995000	-0.50002400
C	4.45878000	-1.04894700	0.08961500

H	5.48558400	-0.74571700	0.34318600
C	3.41335900	-0.13379100	0.22829200
H	3.61152300	0.88608000	0.59045300
C	0.37910600	-1.98289700	-0.76236400
H	0.03472400	-2.87893600	-0.19492000
C	-1.81979900	-0.86855600	-0.21665900
C	-2.36293300	-1.30062800	1.04521400
C	-3.75607000	-1.24897800	1.22404800
H	-4.18582000	-1.56561500	2.18804100
C	-4.60814600	-0.83582300	0.18514600
H	-5.69616700	-0.79588400	0.34986800
C	-4.07873800	-0.53615000	-1.07802500
H	-4.75902300	-0.30022300	-1.91214600
C	-2.69089700	-0.57194200	-1.32021900
C	-1.51246800	-1.90793200	2.13998700
H	-0.42583100	-1.77517900	1.97683400
C	-2.21095100	-0.41753600	-2.74484600
H	-1.13746500	-0.64776800	-2.87061000
H	-1.77443500	-1.51231300	3.14393700
H	-1.69923500	-3.00272700	2.19292800
H	-2.41019900	0.59641000	-3.15307900
H	-2.77214900	-1.11816200	-3.39764800
C	1.52024000	1.79183700	-1.69763600
H	0.21029300	-2.23112900	-1.83839900
H	2.21645900	1.17566600	-2.28671200
C	0.16614500	1.81836000	-2.06148500
C	-0.78043300	2.52949400	-1.29534200
C	-0.73000100	1.52044900	2.04620500
H	-1.29310700	0.59524300	2.25448300
C	-1.35974500	2.55487700	1.38973600
H	-0.89850700	3.55330900	1.32004500
C	0.65939800	1.59338600	2.48904400
H	1.13984400	2.58949600	2.51887000
C	1.38636800	0.49193300	2.84633000
H	2.44213400	0.57821300	3.14890200
H	0.92838300	-0.50882300	2.90527800
H	-2.40951400	2.46430900	1.07209200
H	-0.17322000	1.10757600	-2.82907200
H	-0.48759500	3.49730400	-0.85892500
C	2.09631300	2.79786500	-0.73315200
H	1.70525000	2.71644100	0.32660200
H	3.19642800	2.72545100	-0.65898000
H	1.82796000	3.83910400	-1.01974100
H	-1.85377900	2.41251800	-1.50930000

TS1-2Ti anti-S/trans-S

E: -1021.79118023 A.U.

Ti	0.31611000	0.82042800	0.01146100
N	2.17751900	-0.39782900	-0.00725800
N	-0.29018600	-0.94378200	-0.03943700
C	1.96213100	-1.74043100	-0.12721100
C	3.02112800	-2.66261600	-0.18916100
H	2.80232600	-3.73695300	-0.28809700
C	4.34058000	-2.19806400	-0.11965900
H	5.18582300	-2.90216500	-0.16747000
C	4.56368800	-0.81566100	0.02462700
H	5.58095700	-0.40319600	0.09930500
C	3.46486200	0.04372000	0.07997900
H	3.61642500	1.12461400	0.21231300
C	0.51634000	-2.14678400	-0.16564100
H	0.28452400	-2.86533500	0.65675400

C	-1.72260300	-0.99648800	-0.02076400
C	-2.41565200	-1.11599100	1.23564200
C	-3.82125400	-1.06844600	1.22596300
H	-4.36820600	-1.14303400	2.17956900
C	-4.53692800	-0.96702100	0.02070300
H	-5.63730900	-0.92648200	0.03851400
C	-3.85721900	-0.97718100	-1.20810300
H	-4.43159800	-0.98411000	-2.14836000
C	-2.45182900	-1.02303400	-1.26335200
C	-1.70161700	-1.39962400	2.53801700
H	-0.60119100	-1.30626800	2.46404100
C	-1.78174300	-1.25074800	-2.59927500
H	-0.69210400	-1.06117000	-2.59179500
H	-2.06292600	-0.75349800	3.36594700
H	-1.91779400	-2.44206700	2.85883000
H	-2.24725100	-0.64857500	-3.40689900
H	-1.92412600	-2.31209400	-2.90195500
C	0.84211600	1.45259800	-2.07998200
H	0.28005200	-2.69018900	-1.11150300
H	1.14995500	0.64746100	-2.76568100
C	-0.52116900	1.76088000	-1.96059100
C	-1.00911700	2.81150200	-1.12335700
C	-0.65752200	1.74249400	1.75802700
H	-1.08908500	0.84300600	2.22452800
C	-1.48530500	2.59016400	0.97624400
H	-1.30641300	3.67630500	1.01037400
C	0.71035000	2.10083800	2.09256800
H	1.05293100	3.13036700	1.87197100
C	1.61276800	1.19307800	2.58245200
H	2.66145500	1.47255600	2.77042100
H	1.30753600	0.17460900	2.87740000
H	-2.53634800	2.28915500	0.84958300
H	-1.25432600	1.10632400	-2.45603300
H	-0.34249800	3.67488700	-0.96169700
C	1.89926800	2.38636700	-1.54553800
H	1.90774600	2.48812700	-0.41604400
H	2.91585800	2.06321900	-1.83164000
H	1.74080600	3.43118700	-1.89305700
H	-2.06862600	3.07786900	-1.25415400

2Ti anti-P/trans-P

E: -1021.81173966 A.U.

Ti	0.09799600	-0.38192100	-0.14032900
N	1.38721100	1.33628700	-0.34278900
N	-0.74759500	0.99205300	0.87202700
C	1.06965300	2.43223100	0.41453900
C	1.86942200	3.58556300	0.40818200
H	1.59428100	4.44645700	1.03666900
C	2.99978200	3.63025000	-0.42169600
H	3.63262900	4.53111600	-0.45206900
C	3.30729000	2.51403500	-1.22316200
H	4.17576400	2.51342700	-1.89853100
C	2.48618600	1.38733200	-1.14830100
H	2.70156800	0.49636600	-1.75922700
C	-0.20532100	2.29058500	1.21127600
H	-0.90101900	3.12679100	0.99484800
C	-2.03946800	0.55997100	0.59425700
C	-3.10627500	1.32725200	-0.00366300
C	-4.22016100	0.61349800	-0.46465500
H	-5.05112100	1.17879800	-0.91679000
C	-4.31471600	-0.79987200	-0.39957300

H	-5.21427700	-1.30269400	-0.78656600
C	-3.29587900	-1.54156100	0.19017100
H	-3.39646300	-2.63265900	0.30174200
C	-2.16501200	-0.88013700	0.74322100
C	-3.05956300	2.82715100	-0.16423600
H	-2.19497600	3.15442700	-0.78049300
C	-1.22199600	-1.64789900	1.63488700
H	-0.17624500	-1.86855000	1.22169200
H	-3.97373700	3.18855100	-0.67187700
H	-3.00783200	3.35268200	0.81302000
H	-1.60100500	-2.67260900	1.81684400
H	-1.04456200	-1.14345600	2.60362700
C	2.24616400	-1.17624300	1.63749300
H	0.00957800	2.34564700	2.30535600
H	2.62500500	-0.13881500	1.69267100
C	2.37675500	-1.81314700	0.42327500
C	2.09688000	-3.27327200	0.11996600
C	1.04496700	-2.22302200	-1.88465100
H	1.73719300	-1.46636700	-2.30403200
C	1.68070800	-3.48597600	-1.36668000
H	0.99134000	-4.35012600	-1.45163200
C	-0.30059100	-1.90988500	-1.93302500
H	-1.04316000	-2.68015800	-1.64938300
C	-0.73990900	-0.54019600	-2.08819500
H	-0.06442200	0.13879200	-2.65491600
H	-1.81210400	-0.32178200	-2.22493800
H	2.57007600	-3.72525900	-1.98572100
H	2.94908600	-1.25937500	-0.34184900
H	2.99899600	-3.87586500	0.37246000
C	1.85410700	-1.78559300	2.94648900
H	2.79048900	-1.93568700	3.53359700
H	1.23055500	-1.10767000	3.56407500
H	1.36888500	-2.77712900	2.86399100
H	1.29412200	-3.65734000	0.78448500

2Ti anti-P/trans-S

E: -1021.81958009 A.U.

Ti	-0.07483800	0.38903600	-0.13025500
N	-1.55173800	-1.15750200	-0.31755800
N	0.61773300	-1.08261900	0.87963400
C	-1.36179100	-2.29170000	0.42489800
C	-2.30662900	-3.32958300	0.43248000
H	-2.13257800	-4.22383100	1.05040000
C	-3.45204900	-3.21879300	-0.36986000
H	-4.19924600	-4.02765500	-0.38782600
C	-3.62681000	-2.06661400	-1.16115500
H	-4.50186700	-1.94766700	-1.81723200
C	-2.66264500	-1.05871800	-1.10163500
H	-2.76694600	-0.14424400	-1.70670500
C	-0.05788800	-2.32639800	1.18209500
H	0.53221000	-3.22318500	0.90203000
C	1.94890800	-0.78388800	0.62531600
C	2.94346700	-1.64672300	0.03056100
C	4.11987900	-1.03864000	-0.42375000
H	4.89478300	-1.67756200	-0.87733100
C	4.35150200	0.35921900	-0.34649100
H	5.29652300	0.77504100	-0.72829200
C	3.41133100	1.19027800	0.25230300
H	3.62080100	2.26386900	0.38143300
C	2.21520500	0.63697300	0.79103500
C	2.76264500	-3.13715200	-0.12748000

H	1.89103300	-3.38923400	-0.76889500
C	1.34878800	1.47953100	1.69617700
H	0.35332400	1.83937400	1.26165100
H	3.65443300	-3.58339200	-0.60678000
H	2.63431400	-3.64922900	0.84960300
H	1.84532900	2.44365400	1.92198700
H	1.09059000	0.96686000	2.64208800
C	-2.20127500	1.49004600	1.47746100
H	-0.24048800	-2.41057100	2.28016500
H	-2.74318100	0.52653900	1.44567100
C	-2.03026000	2.14655800	0.28078300
C	-1.50565200	3.55051300	0.05649200
C	0.10977400	2.53102300	-1.54021200
H	1.11142100	2.61304300	-1.06375500
C	-0.85065900	3.67499600	-1.34244300
H	-1.63395700	3.64009700	-2.12927900
C	-0.15579500	1.41279100	-2.31366200
H	-1.10638000	1.39395800	-2.88106500
C	0.57432400	0.17991500	-2.15870700
H	0.28505900	-0.69312600	-2.76718900
H	1.66797100	0.25386200	-1.97554900
H	-0.34070000	4.65538800	-1.43983500
H	-2.52613500	1.69254700	-0.59976900
H	-2.35317100	4.26832200	0.14905400
C	-1.88104900	1.99993600	2.84566700
H	-2.84381200	2.26962000	3.33950800
H	-1.43346100	1.21659400	3.49142600
H	-1.24772300	2.90753500	2.85818300
H	-0.78359700	3.84402300	0.84814200

2Ti anti-S/trans-P

E: -1021.82165193

Ti	0.37540800	0.64229400	0.22011600
N	2.40955700	0.02674100	0.03780500
N	0.19746700	-1.18727800	0.10579000
C	2.57929300	-1.33252800	-0.00986400
C	3.85599100	-1.90064100	-0.12860000
H	3.96770100	-2.99530600	-0.16195900
C	4.97791900	-1.05952000	-0.20104600
H	5.98802800	-1.48856500	-0.29421800
C	4.79853600	0.33634900	-0.14541500
H	5.65302500	1.02770400	-0.19193500
C	3.50320100	0.84001100	-0.01662400
H	3.32525200	1.92618800	0.05415300
C	1.30337100	-2.13553900	0.08335900
H	1.30486500	-2.77196500	1.00107300
C	-1.18162200	-1.50713900	-0.07903700
C	-2.01904000	-1.73845500	1.07026300
C	-3.39524700	-1.94566200	0.85071300
H	-4.05700500	-2.11275800	1.71556600
C	-3.92514200	-1.98608600	-0.44792400
H	-5.00348000	-2.15634100	-0.59385400
C	-3.08217300	-1.85504800	-1.56762800
H	-3.50503100	-1.94817900	-2.58083800
C	-1.70261500	-1.63186100	-1.41739700
C	-1.46231800	-1.90759600	2.46318100
H	-0.42405900	-1.54424700	2.57447900
C	-0.81662400	-1.62563900	-2.64242100
H	0.19306600	-1.20640400	-2.46254700
H	-2.10107200	-1.41848600	3.22703300
H	-1.45922400	-2.98912000	2.72397100

H	-1.28317400	-1.07472200	-3.48411100
H	-0.67068900	-2.66698900	-3.00543900
C	-0.38888800	1.86397100	-1.76436600
H	1.20598400	-2.83827200	-0.77678100
H	-0.13133000	0.95642500	-2.34942300
C	-1.66552400	1.90894300	-1.24852700
C	-2.34181100	3.05428100	-0.54277800
C	-0.96328400	2.38362700	1.38189100
H	-0.18142200	3.09487100	1.02738900
C	-2.36509000	2.74801700	0.97612500
H	-3.07059200	1.92463400	1.21384200
C	-0.53577600	1.39411600	2.25576500
H	-1.28432000	0.72354700	2.71356300
C	0.85348400	1.05085000	2.29832300
H	1.58154600	1.88166900	2.17239500
H	1.21234700	0.23833200	2.94987400
H	-2.71498700	3.64134800	1.54192000
H	-2.27333100	0.98925000	-1.35138300
H	-1.81713400	4.01358100	-0.72866500
C	0.59956400	2.99935700	-1.85267900
H	1.61989700	2.71412200	-1.50320900
H	0.75088500	3.26884000	-2.92249800
H	0.28393500	3.91268400	-1.31442100
H	-3.37506800	3.16858400	-0.93357900

2Ti anti-S/trans-S

E: -1021.82535115 A.U.

Ti	-0.26903800	0.64759700	-0.08893200
N	-2.36022500	0.06636300	0.03039000
N	-0.21622300	-1.12805300	-0.57380400
C	-2.60027500	-1.21244800	-0.39736800
C	-3.89830800	-1.74385600	-0.43194100
H	-4.05925200	-2.77247800	-0.78976800
C	-4.97511700	-0.95444600	-0.00053900
H	-6.00077000	-1.35510700	-0.01638400
C	-4.72529800	0.35513900	0.45022000
H	-5.53955100	1.00833300	0.79754300
C	-3.41247000	0.83082100	0.43893500
H	-3.18990700	1.86052400	0.76051700
C	-1.36781800	-1.99090400	-0.80162100
H	-1.43114700	-2.30038300	-1.87233400
C	1.05966100	-1.51702300	-0.07230600
C	2.16106700	-1.69410200	-0.98408400
C	3.42255100	-2.00156600	-0.44037600
H	4.27993500	-2.14199000	-1.11791500
C	3.59583100	-2.17084700	0.94352700
H	4.59243800	-2.41788900	1.34240200
C	2.50247800	-2.06320600	1.82311900
H	2.64994100	-2.24030500	2.90046800
C	1.21631900	-1.76101400	1.34311100
C	1.96995900	-1.68320300	-2.47912100
H	0.99777400	-1.25677200	-2.79200200
C	0.03888200	-1.77541100	2.29219300
H	-0.79866200	-1.10512400	1.99635900
H	2.78966700	-1.14544100	-2.99788900
H	2.00174900	-2.72736600	-2.86220700
H	0.34352900	-1.50918700	3.32348900
H	-0.39805700	-2.79723900	2.35066700
C	0.60657700	1.80498600	1.82282200
H	-1.27954000	-2.93281200	-0.21370100
H	0.35291700	0.97646000	2.51655900

C	1.86973800	1.77685900	1.27860900
C	2.52076400	2.79991200	0.39621700
C	1.41903700	1.65309100	-1.58814000
H	1.49138000	0.75927700	-2.23394600
C	2.71559700	2.18767300	-1.01270800
H	3.15507600	2.94634000	-1.70023600
C	0.20881100	2.35149400	-1.60624000
H	0.16553700	3.34997600	-1.13060400
C	-1.02642600	1.71070300	-1.89194800
H	-1.96285300	2.28827200	-1.83187000
H	-1.04998300	0.85983100	-2.60006700
H	3.45566000	1.36287700	-0.96104300
H	2.48117600	0.87988300	1.49571600
H	1.93830600	3.74184000	0.35041700
C	-0.38539200	2.94060900	1.75028500
H	-1.27856900	2.71648400	1.10726500
H	-0.81436500	3.13549300	2.75557300
H	0.05098700	3.88046100	1.36298300
H	3.51354800	3.06117000	0.82452700

C	1.01758500	2.78765200	-0.40564000
C	-0.40508000	2.64937700	-0.52244200
C	-1.10922400	1.57526000	2.41010100
H	-0.49865100	2.46382500	2.66637000
C	-2.32696600	1.74553800	1.80795400
H	-2.97823800	0.88506900	1.57345000
C	-0.56328900	0.25938500	2.71941000
H	-1.25905900	-0.59627000	2.72199200
C	0.77662500	0.04395200	2.90222000
H	1.47865000	0.89624700	2.99335300
H	1.18543700	-0.95948600	3.09583600
H	-2.71660900	2.75023900	1.57919000
H	1.42796600	3.39719100	0.42656400
H	-1.02482000	3.36375000	0.03700100
C	3.40143400	2.26290700	-1.15925100
H	3.93591700	1.30157000	-1.30572300
H	3.71209200	2.90067800	-2.02080300
H	3.75782000	2.75961300	-0.23568400
H	-0.81335900	2.37191400	-1.50798100

Titanium – Path 4

1_{Ti} syn-p/trans-P

E: -1021.79550893 A.U.

Ti	0.20036600	0.74345800	0.42715500
N	2.02964300	-0.44708300	0.13245200
N	-0.34080200	-0.58138600	-0.75200400
C	1.88673800	-1.46662700	-0.76518400
C	2.93905800	-2.35247400	-1.05017700
H	2.79000100	-3.15807300	-1.78571100
C	4.16137200	-2.20630100	-0.37844600
H	4.99420100	-2.89876400	-0.57669400
C	4.30360100	-1.16027400	0.55208100
H	5.24329700	-1.00553400	1.10307800
C	3.22502100	-0.29787800	0.76711700
H	3.31782200	0.54728900	1.46767000
C	0.51897800	-1.56831600	-1.39273100
H	0.10394500	-2.59419700	-1.26897600
C	-1.76142600	-0.69606600	-0.65122400
C	-2.32320300	-1.60291100	0.32192200
C	-3.72064800	-1.62599000	0.47321600
H	-4.17118900	-2.30469700	1.21513500
C	-4.55380200	-0.82290900	-0.32946700
H	-5.64557300	-0.85661300	-0.18786100
C	-4.00563200	-0.02246900	-1.34233500
H	-4.67288300	0.54379800	-2.01167700
C	-2.61294100	0.03578000	-1.55232000
C	-1.48047800	-2.59673900	1.08986300
H	-0.42498900	-2.28625200	1.21811100
C	-2.08660300	0.74498300	-2.77460300
H	-0.98275600	0.74050800	-2.83910300
H	-1.91005600	-2.81121000	2.08944300
H	-1.46995900	-3.57175900	0.55353400
H	-2.44921800	1.79237800	-2.84017000
H	-2.47159600	0.23573600	-3.68461200
C	1.92307900	2.11026700	-1.21335700
H	0.57117500	-1.39571400	-2.49519300
H	1.51552400	1.55509200	-2.08131300

TS_{1-2Ti} syn-p/trans-P

E: -1021.78097993 A.U.

Ti	0.30550100	0.65889900	0.63326600
N	2.06986800	-0.48450300	0.13746900
N	-0.41206300	-0.61491100	-0.53512100
C	1.83686400	-1.48803800	-0.75750000
C	2.86452600	-2.35276300	-1.17067200
H	2.64643400	-3.15425900	-1.89328300
C	4.15295100	-2.19102400	-0.64063400
H	4.96849200	-2.86678300	-0.94198200
C	4.38572800	-1.15613700	0.28547500
H	5.37958900	-0.99516900	0.72911700
C	3.32330100	-0.32271700	0.64337300
H	3.47182000	0.50171900	1.36034700
C	0.40847900	-1.61025300	-1.22464300
H	0.02248500	-2.63673500	-1.02277400
C	-1.84431900	-0.68709100	-0.56470800
C	-2.53165200	-1.54524900	0.36415100
C	-3.93792800	-1.49350700	0.39676500
H	-4.48097700	-2.12997600	1.11368000
C	-4.65719000	-0.67083800	-0.48542100
H	-5.75679100	-0.64089900	-0.43489600
C	-3.98057400	0.07113000	-1.46807100
H	-4.55756100	0.64866200	-2.20807900
C	-2.57611300	0.06168500	-1.55000200
C	-1.82096100	-2.57396800	1.21527500
H	-0.73085200	-2.40763500	1.30072000
C	-1.91011800	0.72654700	-2.73313600
H	-0.80638000	0.74573200	-2.65881800
H	-2.25267100	-2.63676300	2.23576500
H	-1.96387600	-3.58318500	0.76964000
H	-2.27759800	1.76094800	-2.89774900
H	-2.16039100	0.16710600	-3.66074500
C	1.68912900	2.12371600	-1.23398800
H	0.33754200	-1.47921000	-2.33154100
H	1.16673900	1.58169700	-2.04643800
C	0.91374300	2.74241500	-0.27046600
C	-0.55136600	2.70729700	-0.24341700
C	-0.64213400	1.56555100	2.46676700
H	0.15927400	2.20752200	2.89023800
C	-1.56614400	2.19259300	1.58506000

H	-2.41873900	1.61318400	1.18564300
C	-0.52517200	0.15765800	2.68930100
H	-1.41148900	-0.48416200	2.54602700
C	0.73771100	-0.41687500	2.77598500
H	1.61420300	0.21087100	3.03137500
H	0.88084100	-1.50464900	2.86163800
H	-1.78113200	3.25585000	1.75495700
H	1.42800600	3.36529700	0.48937100
H	-0.98739400	3.68644400	-0.00115100
C	3.16040400	2.27919500	-1.38085800
H	3.66186600	1.31585300	-1.61003300
H	3.35053100	2.92286900	-2.27210900
H	3.64208200	2.76340500	-0.50920700
H	-1.04470600	2.25640600	-1.11981300

1Ti syn-p/trans-S

E: -1021.79599647 A.U.

Ti	0.27055200	0.63692100	0.64622500
N	2.03705900	-0.43172300	-0.06759300
N	-0.47972900	-0.59300100	-0.53554500
C	1.75097700	-1.41966600	-0.96304200
C	2.75562500	-2.26142600	-1.47131300
H	2.49450800	-3.04929600	-2.19459200
C	4.07849100	-2.08810800	-1.03980000
H	4.87917000	-2.74127800	-1.42043700
C	4.36678700	-1.06778100	-0.11262300
H	5.39043200	-0.89734500	0.25307200
C	3.32335000	-0.25788300	0.34202900
H	3.51169900	0.55710000	1.06034400
C	0.29562300	-1.53771300	-1.33717900
H	-0.07193400	-2.57789700	-1.17223100
C	-1.91676000	-0.56367000	-0.61228000
C	-2.68159500	-1.42349100	0.24980100
C	-4.08429200	-1.32606500	0.21088900
H	-4.68513000	-1.97237900	0.87068200
C	-4.72815500	-0.44510500	-0.67285600
H	-5.82735100	-0.38105800	-0.68094300
C	-3.97550100	0.32012000	-1.57669600
H	-4.49097500	0.96106700	-2.30981400
C	-2.56876600	0.26677600	-1.58564100
C	-2.05326600	-2.49743200	1.10946100
H	-0.94994900	-2.42805700	1.15886500
C	-1.82598200	1.01805600	-2.66685600
H	-0.72804800	0.89273400	-2.61458600
H	-2.45724600	-2.49534400	2.14413800
H	-2.29717000	-3.50029100	0.69652100
H	-2.05484200	2.10574300	-2.65585500
H	-2.14897600	0.65491400	-3.66564800
C	1.52796000	2.25817900	-1.06788600
H	0.14769200	-1.34111400	-2.42668300
H	0.93398900	1.78570000	-1.87377900
C	0.83183700	2.84270600	-0.01723500
C	-0.57876100	2.69400900	0.19557700
C	-0.82252900	0.40434900	2.65151100
H	-1.48927500	-0.45695700	2.47799200
C	-1.30796400	1.69228000	2.51727400
H	-0.73219800	2.55457400	2.89060600
C	0.57228600	0.15134900	3.00064600
H	1.16572800	1.00966500	3.37772100
C	1.19327700	-1.05336000	2.81171100
H	2.26289900	-1.18550400	3.03788800

H	0.63323300	-1.94948200	2.49592200
H	-2.35923600	1.87304100	2.24515400
H	1.41718700	3.39523900	0.74608500
H	-1.06825600	3.42784200	0.84939400
C	2.97919600	2.45187000	-1.34184600
H	3.46903800	1.53129300	-1.71949000
H	3.07536400	3.19487500	-2.16846600
H	3.53934200	2.85176400	-0.47388300
H	-1.20417600	2.39329600	-0.66483500

TS_{1-2Ti} syn-P/trans-S

E: -1021.79243370 A.U.

Ti	0.28529200	0.69912200	0.55623900
N	2.05561800	-0.46257500	0.04889500
N	-0.45420200	-0.73541900	-0.37772100
C	1.78481400	-1.60080400	-0.65164900
C	2.80764900	-2.48685500	-1.03198600
H	2.55968800	-3.39869900	-1.59687200
C	4.13283900	-2.19580000	-0.67816100
H	4.94806900	-2.87964700	-0.96165600
C	4.40523900	-1.01931800	0.04684800
H	5.43001600	-0.75509700	0.34777300
C	3.34283300	-0.17905100	0.38801400
H	3.51522700	0.74982600	0.95650700
C	0.32663800	-1.82572000	-0.95906300
H	-0.01684900	-2.80623300	-0.55139400
C	-1.88902200	-0.71515300	-0.48453400
C	-2.68038400	-1.38256300	0.51249300
C	-4.08108100	-1.28975100	0.42078900
H	-4.70214700	-1.78913100	1.18165400
C	-4.69745700	-0.59801700	-0.63437600
H	-5.79569800	-0.53484500	-0.68237800
C	-3.91812600	-0.02551300	-1.65133700
H	-4.41170200	0.45914500	-2.50894900
C	-2.51223400	-0.08336300	-1.61461700
C	-2.07964000	-2.24593000	1.59841800
H	-2.35766000	-3.30912100	1.43305400
C	-1.73668200	0.45345800	-2.79686000
H	-0.65876100	0.20669800	-2.75826200
H	-0.97473100	-2.19887000	1.63180800
H	-2.47487400	-1.98685100	2.60395200
H	-1.83864600	1.55580800	-2.90737200
H	-2.13714200	0.02249400	-3.73779900
C	1.39654100	2.06722700	-1.44184900
H	0.15575100	-1.88835300	-2.06062300
H	0.75973000	1.48246300	-2.13247600
C	0.76644200	2.78358000	-0.44002900
C	-0.65529600	2.72043600	-0.13639300
C	-0.84356800	0.95907200	2.40198500
H	-1.55171200	0.11444500	2.43027500
C	-1.25504400	2.22437400	1.90984900
H	-0.73393100	3.12240600	2.28106000
C	0.50769200	0.77623100	2.90409800
H	1.09324300	1.68859500	3.14202600
C	1.14700300	-0.43822100	2.93333800
H	2.20436300	-0.51822400	3.23008100
H	0.60337000	-1.38212400	2.75909000
H	-2.31787600	2.36845900	1.66171000
H	1.38726700	3.44844500	0.19475400
H	-1.09297500	3.67172700	0.19930500
C	2.83210400	2.20047300	-1.81711000

H	3.29822200	1.22278500	-2.05609900
H	2.88626000	2.78959000	-2.76254000
H	3.43654100	2.73488000	-1.05856700
H	-1.30692600	2.22194700	-0.88073500

1Ti syn-S/trans-P

E: -1021.79740144 A.U.

Ti	0.22943100	0.76115700	0.48121200
N	2.06376200	-0.39928600	0.10664500
N	-0.32256000	-0.47185900	-0.77821200
C	1.92469000	-1.30182700	-0.90810000
C	2.97260300	-2.15897300	-1.28439700
H	2.82459400	-2.86972400	-2.11206800
C	4.18746400	-2.10722300	-0.58653500
H	5.01666400	-2.77933000	-0.85695800
C	4.32506200	-1.18440900	0.46699200
H	5.25743400	-1.10859100	1.04626500
C	3.25138300	-0.34329700	0.77089700
H	3.34143400	0.40303500	1.57600700
C	0.56382200	-1.32450700	-1.56136600
H	0.16454000	-2.36219700	-1.61249700
C	-1.73877800	-0.65623400	-0.68548100
C	-2.24291200	-1.70295800	0.16979100
C	-3.63533500	-1.81330700	0.32670300
H	-4.04259300	-2.60279100	0.97856400
C	-4.51653800	-0.95292700	-0.35654800
H	-5.60338900	-1.05566600	-0.21090000
C	-4.01935400	-0.00140900	-1.25841400
H	-4.72075100	0.61822500	-1.83981900
C	-2.63337800	0.14975800	-1.47185600
C	-1.34245200	-2.74024500	0.80302400
H	-0.29922300	-2.39783500	0.94856400
C	-2.16037500	1.04482300	-2.58873600
H	-1.06016200	1.12143500	-2.64604000
H	-1.74108800	-3.08713700	1.77799600
H	-1.29969700	-3.64603800	0.15795800
H	-2.59280900	2.06501100	-2.52307700
H	-2.51279900	0.63178000	-3.55879300
C	1.90796000	2.41912300	-0.41429100
H	0.62446900	-0.96909300	-2.61864300
H	2.00712900	2.68506400	0.66788500
C	0.65145200	2.59009900	-0.98944000
C	-0.50928700	2.75442200	-0.18715700
C	-1.10862100	1.29643500	2.57057000
H	-0.55549400	2.18120200	2.94278300
C	-2.33365900	1.46656600	1.98381200
H	-2.93791700	0.60506700	1.65025200
C	-0.47803500	-0.00874100	2.73124700
H	-1.10963600	-0.90338500	2.59778700
C	0.86396900	-0.15398800	2.95435400
H	1.50208400	0.72435000	3.17231600
H	1.33312900	-1.14614300	3.03928600
H	-2.77291100	2.47019900	1.86785000
H	0.55178800	2.40360300	-2.07404000
H	-0.39308700	3.33967000	0.74541600
C	3.18283300	2.28499600	-1.18184600
H	3.67180000	3.28497500	-1.23667400
H	3.91908500	1.61553200	-0.69399900
H	3.01092100	1.94594400	-2.22252800
H	-1.49451000	2.84834100	-0.66794900

TS1-2Ti syn-S/trans-P

E: -1021.77793029 A.U.

Ti	-0.27685200	0.65246400	-0.58689600
N	-2.11967300	-0.39673800	-0.13603500
N	0.31099000	-0.63522300	0.61928300
C	-1.97626600	-1.36484900	0.81488900
C	-3.06359900	-2.14958700	1.23534500
H	-2.91308300	-2.92229600	2.00502800
C	-4.32314900	-1.94634800	0.65453000
H	-5.18526000	-2.55844400	0.96196400
C	-4.46506100	-0.95119300	-0.33130200
H	-5.43284700	-0.75873200	-0.81800400
C	-3.34672300	-0.19620200	-0.69196400
H	-3.42814700	0.59398300	-1.45626000
C	-0.57354100	-1.54563100	1.33969400
H	-0.23836200	-2.60046200	1.20904500
C	1.73620000	-0.76851700	0.61040200
C	2.34919100	-1.71622700	-0.28701100
C	3.75114000	-1.71246500	-0.39463700
H	4.23835600	-2.41632800	-1.08826800
C	4.53971900	-0.85075400	0.38878900
H	5.63559800	-0.86089600	0.28016200
C	3.93919800	-0.02407000	1.35161500
H	4.57179400	0.57895700	2.02275200
C	2.54031900	0.01662900	1.50775600
C	1.55886300	-2.77424100	-1.02334900
H	0.48811700	-2.52649400	-1.15066200
C	1.96144100	0.78445200	2.67316800
H	0.87001300	0.64785300	2.78310100
H	1.99436700	-2.99469400	-2.01928900
H	1.60571900	-3.73105000	-0.45686700
H	2.18642900	1.87129000	2.62332600
H	2.43018100	0.42758900	3.61438600
C	-1.66181600	2.51293900	0.46234800
H	-0.52993500	-1.35039800	2.43827100
H	-1.91768300	2.90278100	-0.55008100
C	-0.32457900	2.51961800	0.83575300
C	0.76924300	2.93290100	-0.02323000
C	0.81363500	1.40313900	-2.46369000
H	0.10013300	2.11463500	-2.93142800
C	1.79946800	1.95337400	-1.59912500
H	2.53656900	1.27658900	-1.12797800
C	0.54216500	0.00986400	-2.62728400
H	1.35336500	-0.71338700	-2.43976000
C	-0.77007100	-0.43361100	-2.73936300
H	-1.57131800	0.27384200	-3.03100500
H	-1.02185100	-1.50313800	-2.79757800
H	2.18805200	2.95883000	-1.81648400
H	-0.07487900	2.19579200	1.85993500
H	0.50011400	3.72590300	-0.74099700
C	-2.79842800	2.33000700	1.41426800
H	-3.64211700	1.75763500	0.97920100
H	-2.48370400	1.86009800	2.36681200
H	-3.21306500	3.33515600	1.65990500
H	1.72086400	3.10953300	0.50411600

1Ti syn-S/trans-S

E: -1021.79571382 A.U.

Ti	-0.25307500	0.64728500	0.27055700
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N	-2.21744900	0.03818200	-0.41134600
N	-0.10700200	-1.18415200	0.17971700
C	-2.38336700	-1.31721700	-0.50258800
C	-3.57172700	-1.87839400	-0.99510300
H	-3.67911500	-2.97277100	-1.04711200
C	-4.60178100	-1.03107900	-1.43092900
H	-5.53840200	-1.45232900	-1.82841900
C	-4.41879100	0.36261100	-1.35779000
H	-5.19668700	1.06268500	-1.69710700
C	-3.22385700	0.85633400	-0.82874300
H	-3.05875200	1.94221900	-0.73545700
C	-1.18391200	-2.13006800	-0.07211500
H	-0.89693000	-2.86351800	-0.85970600
C	1.29546600	-1.43563000	0.09117800
C	1.92675300	-1.45644000	-1.20682400
C	3.32201900	-1.62382900	-1.25701900
H	3.82656800	-1.64419900	-2.23649800
C	4.07470100	-1.80926300	-0.08350400
H	5.16566300	-1.94485800	-0.15085600
C	3.44234000	-1.86623000	1.16823200
H	4.03941600	-2.06680600	2.07213300
C	2.04908800	-1.70701300	1.28798300
C	1.14010900	-1.42700000	-2.49806800
H	0.10862100	-1.03670600	-2.39051000
C	1.39176000	-1.91860700	2.62839700
H	0.30865100	-1.69673300	2.62127600
H	1.65866500	-0.83904000	-3.28268000
H	1.04935900	-2.45823100	-2.90540100
H	1.87738000	-1.31973800	3.42695000
H	1.50903300	-2.98099100	2.93388400
C	-1.61131900	1.65245800	1.95036100
H	-1.41500100	-2.73178200	0.83978800
H	-1.48965800	2.55601700	1.29770000
C	-0.44593300	1.17421300	2.56051300
C	0.82939200	1.45578900	2.01584100
C	2.77409700	2.59777800	-1.34106700
H	3.09637900	1.61701000	-1.73228800
C	3.70033700	3.55526300	-1.04328100
H	3.40437000	4.54914300	-0.66497500
C	1.36404800	2.85124000	-1.20586900
H	1.08347900	3.84455500	-0.80376000
C	0.33934400	1.97425700	-1.54607800
H	-0.68426900	2.39030400	-1.64030900
H	0.56865900	1.09233800	-2.17627200
H	4.77837000	3.37776400	-1.18765700
H	-0.54778400	0.36670600	3.30836400
H	0.98936500	2.45450500	1.55762000
C	-2.99857200	1.38158900	2.45229700
H	-3.30826500	2.20164900	3.13849900
H	-3.75617200	1.35075000	1.64460400
H	-3.04994400	0.43489700	3.02621400
H	1.73463400	0.98410200	2.42618200

TS_{1-2Ti} syn-S/trans-S

E: -1021.79073217 A.U.

Ti	0.27759200	0.82778600	0.33554700
N	2.13514000	-0.29375300	0.13418700
N	-0.31407900	-0.83103000	-0.26502600
C	1.97337000	-1.55582300	-0.35790500
C	3.07301800	-2.40200500	-0.58421100
H	2.90941700	-3.41692000	-0.97806800

C	4.36527400	-1.93616200	-0.30549600
H	5.24019700	-2.58270900	-0.47614900
C	4.52748700	-0.62924200	0.19540900
H	5.52329200	-0.22294900	0.42735700
C	3.39242300	0.15696400	0.40199600
H	3.48442700	1.18055300	0.80159800
C	0.54530900	-1.95140800	-0.62866800
H	0.26819900	-2.86457900	-0.05013100
C	-1.74511900	-0.91129600	-0.31038800
C	-2.45711600	-1.45574600	0.81685200
C	-3.86130900	-1.43119400	0.78957300
H	-4.42280800	-1.83285000	1.64829500
C	-4.55962800	-0.92727600	-0.32312400
H	-5.66070800	-0.91043100	-0.31669800
C	-3.85995500	-0.49506400	-1.45870700
H	-4.41709200	-0.17474000	-2.35366800
C	-2.45117300	-0.50417600	-1.49622800
C	-1.75533500	-2.12442300	1.97751300
H	-0.66839300	-1.91689500	2.00828400
C	-1.76104100	-0.24009100	-2.81323400
H	-0.66279900	-0.15107100	-2.72476900
H	-2.20006700	-1.83858600	2.95345300
H	-1.87367700	-3.22784400	1.90426100
H	-2.15909500	0.66510000	-3.31774300
H	-1.96685400	-1.08369300	-3.50793700
C	1.24419000	1.98946300	-1.45824800
H	0.40649300	-2.22324500	-1.70238000
H	1.91743400	2.45967300	-0.69812200
C	-0.09774500	2.36409100	-1.39679500
C	-0.65093600	3.08851400	-0.28775200
C	-0.88620600	1.23929400	2.14717300
H	-1.39765000	0.27603300	2.29877800
C	-1.56907000	2.30892300	1.51072000
H	-1.39579000	3.33470900	1.87171000
C	0.44868400	1.42253100	2.69154000
H	0.84693100	2.45568200	2.75119100
C	1.27937200	0.37956300	3.01152900
H	2.31440500	0.55521200	3.34479200
H	0.92047600	-0.66369400	3.02493600
H	-2.58601700	2.11115400	1.13609200
H	-0.78310500	2.01401200	-2.18709400
H	0.05339700	3.74821700	0.25209900
C	1.92712800	1.39057600	-2.65071700
H	2.43012500	2.20264400	-3.22298100
H	2.71980000	0.66824600	-2.37184900
H	1.21312100	0.90261000	-3.34290600
H	-1.63784300	3.54249100	-0.46350600

2Ti syn-P/trans-P

E: -1021.81672453 A.U.

Ti	-0.40468400	0.78469700	-0.03891600
N	-2.43204000	0.08785700	-0.02144700
N	-0.15849400	-1.04358400	-0.18881200
C	-2.55465300	-1.26092900	-0.20274400
C	-3.81584300	-1.87568600	-0.24012100
H	-3.89123300	-2.96372700	-0.38980700
C	-4.96707600	-1.08806500	-0.08457600
H	-5.96525400	-1.55260800	-0.11135800
C	-4.83211200	0.30128500	0.10358900
H	-5.71020800	0.95223200	0.22800500
C	-3.54960400	0.85303200	0.12347400

H	-3.40300300	1.93837300	0.25731900
C	-1.24881400	-2.00187000	-0.35379500
H	-1.19021300	-2.49904200	-1.35180700
C	1.21524200	-1.43393800	-0.07620800
C	2.03051800	-1.52193300	-1.25826800
C	3.39881800	-1.81683100	-1.09521200
H	4.04258200	-1.88066400	-1.98710300
C	3.94161200	-2.07018100	0.17303600
H	5.01428700	-2.29756300	0.27524200
C	3.11286800	-2.08528700	1.30975500
H	3.53879200	-2.35165000	2.29034500
C	1.74086300	-1.79554100	1.21431200
C	1.45786700	-1.46080800	-2.65502200
H	0.41809000	-1.08750200	-2.69303500
C	0.86372100	-1.96872800	2.43393800
H	-0.11954400	-1.46561500	2.35279600
H	2.08615500	-0.85006000	-3.33615500
H	1.45288000	-2.48367400	-3.09181900
H	1.36696200	-1.61412900	3.35654400
H	0.66060100	-3.05015100	2.59797300
C	0.65351000	1.44533000	1.96884400
H	-1.16438400	-2.82040300	0.39891300
H	1.26586400	0.53498400	2.10703500
C	1.23225700	2.52368000	1.34226100
C	2.58494600	2.54750200	0.67524400
C	0.94976600	2.74135100	-1.18041500
H	0.21118000	3.50181500	-0.85556900
C	2.38976600	3.00456500	-0.80137400
H	3.09079500	2.46942000	-1.47205100
C	0.46710100	1.73860900	-2.01413000
H	1.19006000	1.05939000	-2.49931200
C	-0.92620900	1.42278200	-2.04898900
H	-1.63906400	2.24647400	-1.82284800
H	-1.31536900	0.67084500	-2.75371400
H	2.59796500	4.08975500	-0.91523000
H	0.68191900	3.48471800	1.36838600
H	3.26354800	3.22870100	1.23486600
C	-0.69356600	1.49788000	2.64570000
H	-1.42565100	0.74932800	2.23757600
H	-0.60894600	1.19982800	3.71400000
H	-1.15798100	2.50435000	2.60313600
H	3.04008700	1.53600800	0.70985500

2Ti syn-P/trans-S

E: -1021.81790690 A.U.

Ti	-0.37367400	0.69508500	-0.08139600
N	-2.39666400	-0.01973500	-0.04010900
N	-0.11373400	-1.13578200	-0.17982100
C	-2.50670400	-1.37657600	-0.16107000
C	-3.76086100	-2.00731200	-0.14220700
H	-3.82588200	-3.10115900	-0.24788500
C	-4.91713600	-1.22849600	0.01728000
H	-5.90961400	-1.70535400	0.03566100
C	-4.79432000	0.16827300	0.15108100
H	-5.67686000	0.81275800	0.27758300
C	-3.51964400	0.73656100	0.10661100
H	-3.38246700	1.82861300	0.18279300
C	-1.19444200	-2.11111900	-0.29932100
H	-1.14150600	-2.64696700	-1.27765800
C	1.25995200	-1.48834300	0.02240400
C	2.10763700	-1.71465600	-1.11756900

C	3.46645100	-1.99170000	-0.88496900
H	4.13338400	-2.16481900	-1.74469500
C	3.97964500	-2.07532500	0.42074600
H	5.04873300	-2.28927100	0.57591800
C	3.13014800	-1.92476600	1.52834000
H	3.53449700	-2.04431000	2.54624700
C	1.75831100	-1.65515000	1.36242100
C	1.57755900	-1.75373700	-2.53168700
H	0.55962900	-1.33226100	-2.63296200
C	0.86113000	-1.65009600	2.57870200
H	0.77604600	-2.68162600	2.98449000
H	2.25075600	-1.22660200	-3.23901200
H	1.53037600	-2.80651000	-2.88750600
H	-0.16845800	-1.30174900	2.36949100
H	1.28496600	-1.03721500	3.40051100
C	0.63290300	1.97206100	1.58478100
H	-1.09537900	-2.89867300	0.48417900
H	1.40576000	1.18570900	1.39517100
C	0.87400600	3.22648300	1.08525000
C	1.93217000	3.60531100	0.09632400
C	1.33275600	1.68321000	-1.46972600
H	1.62768100	0.72598800	-1.93748600
C	2.44203100	2.45178200	-0.78059800
H	3.13930000	2.85502500	-1.55098600
C	0.07217300	2.19735700	-1.80034200
H	-0.16987600	3.23685200	-1.50455000
C	-1.01736000	1.35186100	-2.12717000
H	-2.01480200	1.78796700	-2.29526700
H	-0.83423900	0.39693800	-2.65622500
H	3.06340100	1.74026800	-0.19505900
H	0.22072900	4.04906100	1.43863000
H	1.54859600	4.44590000	-0.52262300
C	-0.47275700	1.63809200	2.55845900
H	-0.07410400	1.22357400	3.50772200
H	-1.10436800	2.52023200	2.78413700
H	-1.17134400	0.83068900	2.19267300
H	2.77676000	4.07139300	0.66047200

2Ti syn-S/trans-P

E: -1021.82004193 A.U.

Ti	-0.43227100	0.79999400	-0.16400800
N	-2.45956700	0.08196900	-0.04168700
N	-0.15464000	-1.01602800	0.09378300
C	-2.55080600	-1.26982300	0.13184600
C	-3.79753500	-1.90374200	0.25182400
H	-3.84637100	-2.99527100	0.38659200
C	-4.96802300	-1.13150300	0.19587700
H	-5.95498800	-1.61151400	0.28686300
C	-4.86549900	0.26154900	0.01734000
H	-5.75879600	0.90151500	-0.03531300
C	-3.59585700	0.83032100	-0.10457900
H	-3.47524800	1.91579000	-0.26021100
C	-1.23067900	-2.00096200	0.17057400
H	-1.16274000	-2.73132300	-0.67064100
C	1.23248700	-1.36661900	0.15813400
C	1.91261700	-1.80043400	-1.03530100
C	3.29633000	-2.04310100	-0.95285500
H	3.83851500	-2.36221300	-1.85744000
C	3.98752800	-1.92149000	0.26454500
H	5.07069700	-2.11711200	0.30101800
C	3.29424800	-1.60368000	1.44354700

H	3.83265900	-1.58536700	2.40477500	H	-0.53400400	-1.65093900	2.05814100
C	1.91042900	-1.34629400	1.42729900	H	2.47950000	-0.74300000	-3.22250900
C	1.18711400	-2.12539900	-2.32051700	H	1.81037200	-2.37949300	-3.12039700
H	0.16467900	-1.70765200	-2.37497700	H	0.78772000	-1.83379100	3.26808700
C	1.17858500	-1.19212700	2.74026900	H	0.26724600	-3.22265800	2.30156600
H	0.12311100	-0.88417900	2.62068300	C	0.37135000	2.16939600	1.78873500
H	1.75706600	-1.79131500	-3.21186800	H	-1.21408900	-2.88148700	-0.13909200
H	1.09483700	-3.22958500	-2.42135400	H	-0.13816200	3.10896900	1.48810400
H	1.68639800	-0.47921700	3.42338600	C	1.67786000	2.00617400	1.40749200
H	1.17466600	-2.16623900	3.27623200	C	2.42447300	2.95072100	0.51140300
C	0.28386300	2.55541700	1.37148700	C	1.31331000	1.80822200	-1.47770700
H	-1.13406200	-2.60470800	1.10387500	H	1.37830100	0.93386500	-2.14946400
H	-0.06178300	3.48626500	0.87824500	C	2.61444100	2.29612100	-0.87957700
C	1.59312900	2.18137100	1.18346900	H	3.10506100	3.01879600	-1.57215600
C	2.54657900	2.88475600	0.24976000	C	0.10366100	2.50957200	-1.48732500
C	1.01687600	2.17768300	-1.57610000	H	0.04860400	3.49880000	-0.99448900
H	0.40494200	3.07977700	-1.35891500	C	-1.11687500	1.84921100	-1.78651300
C	2.46253900	2.27391500	-1.17845800	H	-2.06926700	2.40017300	-1.72655300
H	2.94664400	1.27551000	-1.21503100	H	-1.11623900	1.00735700	-2.50748500
C	0.38595500	1.17893400	-2.31147600	H	3.31392700	1.43820800	-0.79852700
H	0.98559600	0.33330100	-2.68842700	H	2.22425700	1.10481500	1.75222000
C	-1.03288200	1.06181800	-2.26751500	H	1.88904500	3.91958500	0.43145500
H	-1.62616700	1.99754800	-2.16780900	C	-0.39982600	1.24760900	2.69597300
H	-1.54928100	0.25204000	-2.80600500	H	-0.95053400	1.83041200	3.46531700
H	3.01984900	2.92630700	-1.88909000	H	-1.23084500	0.68136400	2.17949800
H	1.97920200	1.30741100	1.74172600	H	0.24486900	0.50030600	3.19379500
H	2.28846700	3.96392800	0.20166100	H	3.42091000	3.17148300	0.95118800
C	-0.68408600	1.91658800	2.33399200				
H	-1.27031600	2.69552900	2.86630200				
H	-1.49190000	1.29470400	1.84433700				
H	-0.18748300	1.26020600	3.07211500				
H	3.58374300	2.81133200	0.63379300				

2Ti syn-S/trans-S

E: -1021.82302366 A.U.

Ti	-0.33476300	0.74669800	-0.01222500
N	-2.40132900	0.09066300	-0.01240000
N	-0.18307900	-1.04976400	-0.44289100
C	-2.57445500	-1.20568600	-0.40740300
C	-3.85352300	-1.78007500	-0.48344000
H	-3.96655900	-2.82421000	-0.81343700
C	-4.97178300	-1.01126900	-0.12839200
H	-5.98280000	-1.44500300	-0.17732900
C	-4.78556100	0.32076300	0.28908200
H	-5.63606000	0.95718600	0.57534300
C	-3.48916400	0.83882900	0.32177900
H	-3.30625400	1.88572700	0.61728500
C	-1.29765600	-1.94399200	-0.73584200
H	-1.29026100	-2.26120600	-1.80659500
C	1.15286700	-1.44027700	-0.14312100
C	2.13824800	-1.48112700	-1.19562600
C	3.47187000	-1.75471900	-0.84199100
H	4.24199000	-1.78370700	-1.62947900
C	3.82807300	-2.03265800	0.48881600
H	4.87929500	-2.24456300	0.74034400
C	2.84508400	-2.09769900	1.49188300
H	3.12984700	-2.39139200	2.51495300
C	1.49283300	-1.83956800	1.20253700
C	1.76359200	-1.37084300	-2.65305300
H	0.73799100	-0.98900600	-2.81732200
C	0.44647500	-2.12541200	2.25454400