

# Supporting Information

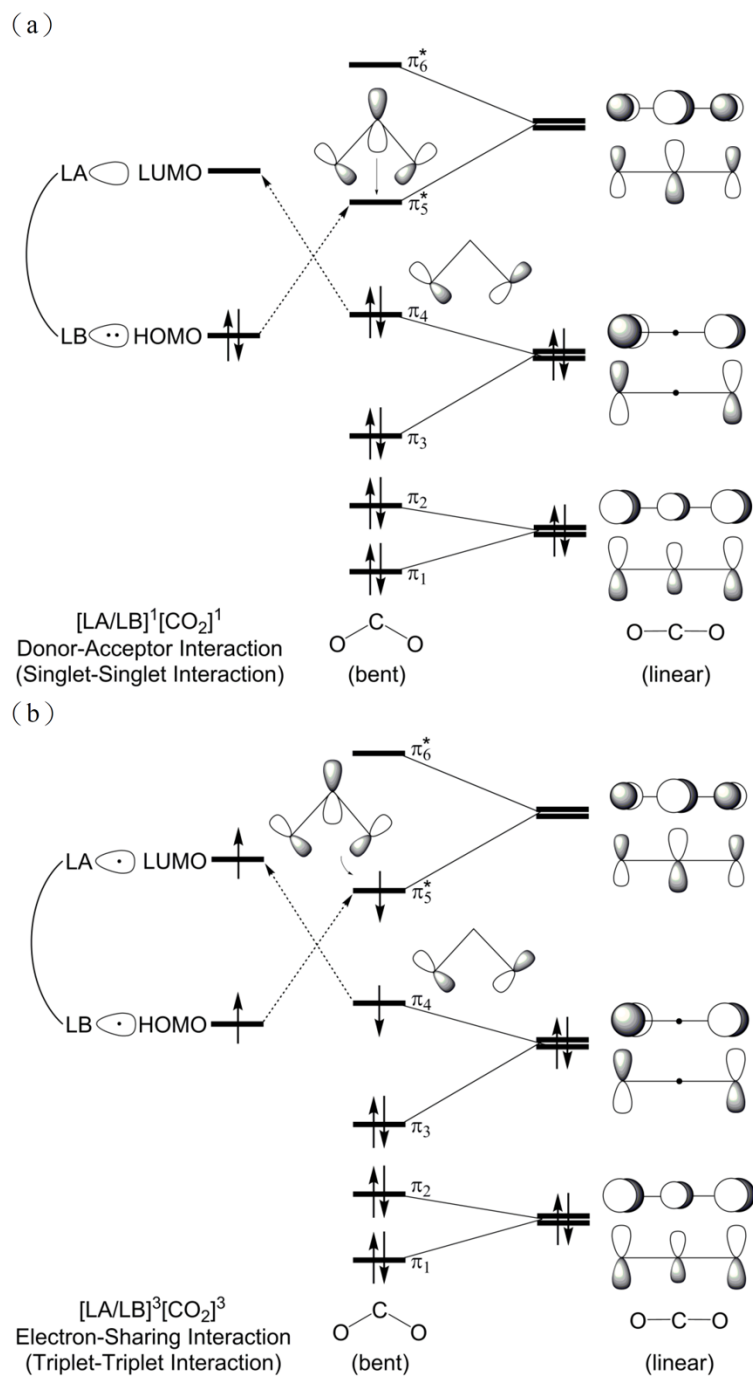
## Computational Insights into CO<sub>2</sub> Binding Reactions by Intramolecular Geminal Group-IV<sup>+</sup>/Phosphorus- and Zirconium<sup>+</sup>/Group-15-Based Frustrated Lewis Pairs

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**Figure S1.** Pictorial representation of the bonding situation in (a) donor-acceptor bonding or singlet-singlet interaction and (b) electron-sharing bonding or triplet-triplet interaction.

(All geometries were calculated at the M06-2X-D3/def2-TZVP level)

**Ti<sup>+</sup>/P-Rea**

Free energy (M06-2X-D3/def2-TZVP) = -2779.136479

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Ti	-0.07657300	0.14803700	1.05071200
C	2.07621600	0.40941900	0.09035600
C	1.23140600	1.24952600	-0.68175700
C	0.24746900	0.42745400	-1.30017000
C	0.56563900	-0.93604900	-1.02115800
C	1.70109000	-0.94768900	-0.16342000
C	-0.04591000	2.38305900	1.94083900
C	0.01169900	1.50836700	3.06068100
C	-1.22238100	0.80348900	3.13282800
C	-2.02440700	1.21231500	2.02745200
C	-1.29857000	2.18040100	1.28198400
C	2.60459900	-2.10039400	0.15937700
H	2.84488200	-2.16057800	1.23010300
H	3.55249100	-1.96202400	-0.38421600
H	2.18063000	-3.06358400	-0.14450000
C	-0.02117700	-2.09484000	-1.76751200
H	-1.08506700	-2.24535500	-1.54103900
H	0.50851000	-3.02632400	-1.53819500
H	0.06988200	-1.91445400	-2.84932400
C	-0.71959900	0.88183600	-2.35312400
H	-0.19351600	0.97422400	-3.31755300
H	-1.15641800	1.86238600	-2.12727600
H	-1.53530000	0.16197200	-2.49564600
C	1.52959700	2.65479100	-1.10387400
H	1.97147900	2.60543700	-2.11239000
H	2.25975800	3.14648500	-0.45385900
H	0.63839300	3.28752200	-1.18255600
C	3.30640500	0.79832400	0.85652400
H	3.31799800	1.86421700	1.11494600
H	4.20896500	0.59588100	0.25809200
H	3.40454600	0.21776600	1.78586900
C	-1.90567400	3.02719300	0.20258500

H	-2.53639000	3.80690800	0.65775700
H	-2.55047600	2.44001300	-0.46595200
H	-1.15242800	3.53652300	-0.40876700
C	-3.48663500	0.92082800	1.91566500
H	-3.71274100	-0.13895700	2.09538200
H	-3.89561900	1.20808600	0.94015100
H	-4.02205200	1.50469200	2.68212600
C	-1.80875700	0.06110800	4.29391800
H	-2.29187900	-0.87463900	3.98222000
H	-2.59028200	0.69506000	4.74248200
H	-1.07504200	-0.17640400	5.07080500
C	1.10687100	1.55115900	4.08662400
H	2.08600800	1.26442100	3.67290900
H	0.88685600	0.89889300	4.93959100
H	1.21192200	2.57789000	4.46980300
C	0.87982100	3.55133400	1.78234000
H	1.93927000	3.26513400	1.77288500
H	0.73799700	4.21990300	2.64671000
H	0.66489400	4.13633100	0.88316200
C	-1.43723100	-1.45789200	1.14875100
C	-2.60142900	-1.88480900	0.61768400
P	-0.10964800	-2.13736500	2.13621400
C	-0.10257500	-2.44125500	3.94101000
C	0.20678200	-2.96359200	6.67009900
C	0.90925200	-1.81038600	4.67143000
C	-0.91924500	-3.38823100	4.57035600
C	-0.77418300	-3.63221300	5.93386900
C	1.06255900	-2.06607100	6.03461900
H	1.58338900	-1.11528400	4.16745200
H	-1.65473300	-3.95006300	3.99336000
H	-1.42103700	-4.36110800	6.42391800
H	1.85369100	-1.56798500	6.59716500
H	0.31770600	-3.16235700	7.73684800
C	0.36583500	-3.80203400	1.53792500
C	1.17061700	-6.35707800	0.72148800
C	-0.29802200	-4.44941400	0.49434100
C	1.42284300	-4.45590600	2.19037700
C	1.82590100	-5.72176300	1.77843500

C	0.10492700	-5.72274100	0.08814600
H	-1.13452800	-3.96581900	-0.00363200
H	1.93507400	-3.97612500	3.02742000
H	2.65301500	-6.21733200	2.28807700
H	-0.42738000	-6.22132000	-0.72302900
H	1.48480600	-7.35144300	0.40196500
C	-3.33591300	-3.09988500	1.06167500
C	-4.72722800	-5.38754400	1.91105200
C	-3.85467700	-4.00984900	0.12692100
C	-3.55715900	-3.33856600	2.42255800
C	-4.24777600	-4.47311600	2.84667900
C	-4.53046800	-5.15100200	0.54949800
H	-3.70876600	-3.83885100	-0.94189200
H	-3.20271600	-2.60674300	3.15002800
H	-4.42165300	-4.63658800	3.91159000
H	-4.91118400	-5.85872800	-0.18796900
H	-5.26595700	-6.27697400	2.23964100
C	-3.26029300	-1.10797300	-0.49906800
H	-2.75010200	-0.14904700	-0.66296400
H	-4.32146800	-0.92556900	-0.27538200
H	-3.23465200	-1.67663100	-1.44293400

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### Ti<sup>+</sup>/P-TS

Free energy (M06-2X-D3/def2-TZVP) = -2967.490806

P	-0.09846200	-1.87142500	0.84367500
C	-1.85347900	-2.38088500	0.65565300
C	0.76139900	-3.43389600	0.38098000
C	-2.56658700	-2.27000400	-0.54031700
C	-2.47820000	-2.95994000	1.76884600
C	0.14758200	-0.49667800	-0.38977300
C	2.06172800	-3.63925200	0.86059100
C	0.13474600	-4.46076900	-0.33741800
C	-3.88731400	-2.71126000	-0.62368600
H	-2.07996700	-1.82766700	-1.40666900
C	-3.79944800	-3.39789200	1.68923600
H	-1.92760600	-3.07188000	2.70667300

C	0.44963500	-0.68749200	-1.69558700
Ti	0.12748200	1.43125100	0.67973800
C	2.74760600	-4.81946400	0.57672600
H	2.54523800	-2.87949200	1.47938300
C	0.81328500	-5.64704100	-0.60371600
H	-0.88457400	-4.33313700	-0.70469400
C	-4.50835000	-3.26926600	0.49396800
H	-4.43306500	-2.62076700	-1.56467000
H	-4.27660600	-3.84397700	2.56292100
C	0.69558500	0.45920400	-2.64688600
C	0.62365600	-1.99593100	-2.42111100
C	2.12396700	-5.82518100	-0.15976500
H	3.76181100	-4.96211900	0.95236000
H	0.31504500	-6.43522600	-1.17006300
H	-5.54220400	-3.61161500	0.43215400
H	1.71711200	0.40018200	-3.05443800
H	0.02906300	0.38236500	-3.52121600
H	0.55270500	1.43681000	-2.17295400
C	-0.39225100	-2.48185200	-3.25289300
C	1.85099100	-2.67236200	-2.40588500
H	2.65312600	-6.75503200	-0.37306200
C	-0.21211900	-3.64680800	-3.99911700
H	-1.33659900	-1.93779900	-3.33583400
C	2.03901800	-3.82641300	-3.16156800
H	2.66451700	-2.30820100	-1.77887700
C	1.00378100	-4.32490300	-3.95220500
H	-1.02178600	-4.01521800	-4.63058200
H	2.99887700	-4.34358900	-3.12376200
H	1.14891300	-5.23207700	-4.54019300
C	-1.20064400	2.89438200	-0.62593400
C	-0.85465300	3.63209400	-1.88658700
C	-1.95205200	1.67252800	-0.55507700
C	-1.19790100	3.48008000	0.67871100
H	0.07190800	4.21312800	-1.78413500
H	-1.65984600	4.34393300	-2.12917800
H	-0.74485700	2.95774500	-2.74475400
C	-2.50255400	0.93769300	-1.73779900
C	-2.30734000	1.46723500	0.80302200

C	-0.97373000	4.92158800	1.01492000
C	-1.82144000	2.57749100	1.56057300
H	-3.30408900	0.25709100	-1.42717200
H	-2.92902000	1.65925400	-2.45015200
H	-1.74798600	0.34342100	-2.26571500
C	-3.25099700	0.45429600	1.37508700
H	-0.45975300	5.06273100	1.97393900
H	-1.96566200	5.39156000	1.11379300
H	-0.43395200	5.46575200	0.23505400
C	-2.13528300	2.84886800	2.99957200
H	-2.80941900	-0.13389900	2.19219200
H	-4.12200500	0.98052400	1.79500400
H	-3.60800500	-0.25811300	0.62522500
H	-1.31281200	3.36234200	3.51501000
H	-3.02072900	3.50162500	3.06680700
H	-2.36770200	1.92735200	3.54769100
C	2.20174100	1.09395500	1.80651000
C	2.48571700	0.05728800	2.85083000
C	1.79769400	2.44381500	2.05297500
C	2.49641300	0.95982000	0.42641400
H	2.08617100	-0.93110400	2.58108600
H	3.57486500	-0.05134600	2.97177800
H	2.08480400	0.34555000	3.83222100
C	1.51390000	3.03368400	3.40202900
C	1.89504600	3.14895500	0.82643400
C	3.20317200	-0.20203500	-0.18734100
C	2.27032400	2.22729200	-0.19010300
H	0.87619900	2.37776900	4.01132200
H	2.45181600	3.18836800	3.95761000
H	1.01679000	4.00926700	3.32029500
C	2.01523100	4.62888100	0.63900600
H	2.82248000	-1.15886000	0.19032200
H	4.27670500	-0.14055400	0.05411200
H	3.09988000	-0.20776500	-1.27852200
C	2.74078200	2.66024500	-1.54847100
H	1.55723100	4.98013600	-0.29366000
H	3.09112400	4.85961300	0.56956800
H	1.61447300	5.20699300	1.47624400

H	1.96663300	3.17439600	-2.13399900
H	3.57712400	3.36603400	-1.42476900
H	3.10721000	1.81567500	-2.14086800
C	-0.40998200	-0.45658800	3.29805200
O	-0.50812300	-1.28110400	4.08775900
O	-0.36148700	0.52711200	2.65346700

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**Ti<sup>+</sup>/P-Prod**

Free energy (M06-2X-D3/def2-TZVP) = -2967.529194

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C	0.03882600	-0.40816300	-0.58479100
C	0.18803900	-0.56407600	-1.92266600
C	0.34228800	0.62340400	-2.83553200
H	1.30077700	0.56542400	-3.37508800
H	0.28465400	1.57392000	-2.29244000
H	-0.43922700	0.60400100	-3.61132600
C	0.26924300	-1.85362800	-2.68650400
C	0.49411800	-4.16981300	-4.26174600
C	1.40118600	-2.67192500	-2.59577900
C	-0.73276000	-2.19494500	-3.60852200
C	-0.63366500	-3.35440700	-4.37309300
C	1.51463200	-3.81861100	-3.38164600
H	2.19815500	-2.41800700	-1.89620600
H	-1.60121000	-1.54225200	-3.73375100
H	-1.43043700	-3.61329500	-5.07149200
H	2.40485600	-4.44320700	-3.29551300
H	0.58040000	-5.06965000	-4.87205100
P	-0.31416700	-1.82638300	0.47863600
C	0.64855700	-3.36658400	0.47543500
C	2.05614400	-5.77309700	0.47880600
C	1.73716000	-3.53863400	1.33836400
C	0.24504000	-4.41535800	-0.36222400
C	0.95188600	-5.61323500	-0.35981100
C	2.44393500	-4.73997000	1.33050600
H	2.00462200	-2.76255800	2.05396600
H	-0.61423600	-4.29448200	-1.02669400
H	0.63703700	-6.42566600	-1.01571500



H	3.28685100	-4.87392000	2.00901300
H	2.60621400	-6.71509500	0.48107700
C	-2.03230300	-2.40698400	0.37152700
C	-4.64161700	-3.37437300	0.28783900
C	-2.77839800	-2.29250200	-0.80221000
C	-2.57831400	-3.03078500	1.50184200
C	-3.88713100	-3.50330900	1.45582800
C	-4.08503500	-2.77869900	-0.84279900
H	-2.34059000	-1.82967100	-1.68420100
H	-1.98705100	-3.13337300	2.41484200
H	-4.31948600	-3.97754800	2.33752800
H	-4.66769000	-2.69022500	-1.76046700
H	-5.66618800	-3.74743200	0.25832800
Ti	0.19887400	1.48102800	0.64907900
C	2.52153500	0.95699200	0.16916900
C	2.37778700	1.04116400	1.57340300
C	2.00561600	2.37485800	1.91125200
C	2.01420900	3.14022900	0.71259400
C	2.26113200	2.25836200	-0.37221800
C	-1.16766200	3.14353300	-0.39843200
C	-1.04571100	3.54179300	0.96902900
C	-1.63993000	2.53660500	1.77008000
C	-2.21118500	1.56109200	0.90792600
C	-1.93024700	1.93359900	-0.43152000
C	-2.56338600	1.33386000	-1.64895100
H	-2.21533500	1.82184200	-2.56679100
H	-3.65337000	1.47719000	-1.59243200
H	-2.37213000	0.25761300	-1.73049700
C	-3.11837200	0.47555700	1.38723600
H	-2.63720800	-0.16162800	2.14401800
H	-3.48037900	-0.15805100	0.56959700
H	-3.99470900	0.93262300	1.87353200
C	-1.79238500	2.54618200	3.25868400
H	-1.15843200	3.30866500	3.72854800
H	-1.53508000	1.56581700	3.68405000
H	-2.83698900	2.76716700	3.52935100
C	-0.73551100	4.91900200	1.47279600
H	-0.28639200	5.55730600	0.70652300

H	-0.08972800	4.92064700	2.35888000
H	-1.68777600	5.38560800	1.77013900
C	-0.86475500	4.01107200	-1.58554700
H	0.00079600	4.66174200	-1.41150800
H	-1.72523100	4.66412500	-1.80092800
H	-0.66855800	3.42673500	-2.49442600
C	2.58340600	2.73439800	-1.75931000
H	3.47511100	3.38012400	-1.72050700
H	1.77412600	3.32782300	-2.20705400
H	2.81084700	1.90237100	-2.43456200
C	2.16340200	4.62548500	0.59683300
H	3.22959700	4.82829100	0.40308000
H	1.89560000	5.15506500	1.51550400
H	1.60475800	5.05704400	-0.24188800
C	1.83017600	2.85233400	3.32102100
H	2.79718700	2.84778300	3.84774800
H	1.15093100	2.19080300	3.87887500
H	1.43587100	3.87502300	3.36720300
C	2.71495900	-0.00928400	2.57926000
H	2.82057400	-0.99311800	2.10773100
H	1.96590300	-0.07856600	3.37922200
H	3.68444200	0.23038100	3.04365500
C	3.11176100	-0.19878400	-0.57462700
H	4.21070700	-0.14411500	-0.52431300
H	2.82264700	-0.19482600	-1.63289200
H	2.80409700	-1.16276800	-0.14455000
C	-0.15202500	-1.06844400	2.20998900
O	-0.12101400	0.21049700	2.14529600
O	-0.12484900	-1.77941900	3.17838300

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**Zr<sup>+</sup>/P-Rea**

Free energy (M06-2X-D3/def2-TZVP) = -1976.818974

Zr	-0.02025300	0.19460200	1.04351000
C	2.19941100	0.39640300	-0.10468100
C	1.34548200	1.28472000	-0.81285200
C	0.32153800	0.50461200	-1.43070800

C	0.60821700	-0.87458200	-1.19348700
C	1.76813900	-0.94343000	-0.37020500
C	-0.03710800	2.51214300	2.03209300
C	-0.04623200	1.62682300	3.14910600
C	-1.29651200	0.94390000	3.16259100
C	-2.04855200	1.38725700	2.03488900
C	-1.27734300	2.35661100	1.33424600
C	2.61105800	-2.14700700	-0.06185600
H	2.88818300	-2.20603300	1.00007600
H	3.54395700	-2.08506500	-0.64391100
H	2.11125300	-3.08556500	-0.32703300
C	-0.06802900	-2.00419100	-1.91174400
H	-1.13315400	-2.08643600	-1.65436400
H	0.41097300	-2.96296500	-1.68245900
H	0.00318900	-1.84438800	-2.99839900
C	-0.69434400	1.01269600	-2.41323900
H	-0.27974100	0.97305000	-3.43369900
H	-0.97479900	2.05511000	-2.21569400
H	-1.60808600	0.40242000	-2.41420200
C	1.64180300	2.71660400	-1.14061500
H	2.10526300	2.74899400	-2.13970000
H	2.35033300	3.16911800	-0.43893600
H	0.74329500	3.34320300	-1.18706900
C	3.45040400	0.74464200	0.65152200
H	3.48754000	1.80857300	0.91908000
H	4.34202700	0.52780600	0.04214900
H	3.54867400	0.15499100	1.57596700
C	-1.81350600	3.22088300	0.22933600
H	-2.45705200	4.00755000	0.65312000
H	-2.42692600	2.64959800	-0.48148000
H	-1.01707600	3.72230400	-0.33268500
C	-3.49681200	1.07360300	1.82054100
H	-3.71911000	0.02135500	2.04510000
H	-3.82195900	1.28794900	0.79479700
H	-4.10875800	1.69333800	2.49597100
C	-1.90461700	0.13149200	4.26569100
H	-2.31219800	-0.82034000	3.89725400
H	-2.74116500	0.69932800	4.70192800

H	-1.19367600	-0.09645400	5.06702500
C	1.02587100	1.60387100	4.20250500
H	2.00258400	1.26998400	3.81591000
H	0.75011500	0.95253400	5.04032700
H	1.17560500	2.61817400	4.60299600
C	0.97415300	3.60827400	1.86287200
H	2.00909700	3.23778700	1.85159700
H	0.89205800	4.30434900	2.71265500
H	0.80439500	4.18834000	0.94998800
C	-1.45515600	-1.53644700	1.17582100
C	-2.62793900	-2.02707400	0.71948400
P	-0.10884700	-2.21390300	2.18237000
C	-0.18926400	-2.55300500	3.97784400
C	-0.08749700	-3.10171800	6.71712400
C	0.70839500	-1.86782000	4.80318200
C	-0.99536700	-3.56055100	4.52187700
C	-0.95356900	-3.82007300	5.88961400
C	0.75723700	-2.13681500	6.17136900
H	1.37780300	-1.12188500	4.36996300
H	-1.64275900	-4.15355200	3.87459100
H	-1.59057500	-4.59879000	6.31135900
H	1.46014500	-1.59795000	6.80849600
H	-0.05607900	-3.31235100	7.78693700
C	0.41120500	-3.83879800	1.52782500
C	1.34246100	-6.29735300	0.57127800
C	-0.19905500	-4.44007600	0.42581600
C	1.48024400	-4.48650200	2.16457200
C	1.94484800	-5.70694000	1.68425800
C	0.26728700	-5.66636300	-0.05061800
H	-1.03753100	-3.94992900	-0.06457000
H	1.95301300	-4.03561300	3.04061200
H	2.77993800	-6.20129200	2.18201900
H	-0.21949600	-6.13169800	-0.90895200
H	1.70650200	-7.25481800	0.19670600
C	-3.32247400	-3.23825300	1.24235300
C	-4.71177600	-5.47313600	2.22326100
C	-3.71791700	-4.27126500	0.37788800
C	-3.65949200	-3.33131700	2.59710500

C	-4.35332100	-4.43919800	3.08491200
C	-4.39052400	-5.38673900	0.86731500
H	-3.48115100	-4.21251600	-0.68715500
H	-3.38970600	-2.51584400	3.27070000
H	-4.61842700	-4.48930400	4.14228600
H	-4.67336600	-6.19068300	0.18668500
H	-5.25104100	-6.34155900	2.60328000
C	-3.36347300	-1.32967000	-0.40131800
H	-2.84359600	-0.41102200	-0.70735900
H	-4.39250100	-1.08424600	-0.09873600
H	-3.45001900	-1.99202600	-1.27771100

**Zr<sup>+</sup>/P-TS**

Free energy (M06-2X-D3/def2-TZVP) = -2165.186941

P	-0.12266700	-0.16227800	0.20243200
C	-0.42859200	1.61689800	-0.14714600
C	-1.50329100	-0.96607200	-0.70984600
C	0.02432200	2.25423800	-1.30705800
C	-1.18896000	2.34750100	0.77541700
C	1.54426800	-0.49917600	-0.53097400
C	-2.20930200	-0.33393200	-1.74131600
C	-1.90022400	-2.24541300	-0.29944500
C	-0.25527600	3.60127600	-1.53327300
H	0.59191900	1.68295700	-2.04063900
C	-1.46396300	3.69718100	0.55449800
H	-1.57555100	1.85926800	1.67370200
C	1.78882900	-0.85820900	-1.81354900
Zr	3.18537200	-0.56142300	1.10944200
C	-3.26545700	-0.98761300	-2.37113300
H	-1.93055600	0.66970300	-2.06571600
C	-2.94712000	-2.90547200	-0.94131500
H	-1.39895000	-2.73049000	0.54206300
C	-0.99147500	4.32774100	-0.59646100
H	0.10125000	4.08564600	-2.44378900
H	-2.05332900	4.25676600	1.28217100
C	3.19446700	-1.13756600	-2.29267600

C	0.80006300	-1.05527800	-2.92806700
C	-3.62996800	-2.27678900	-1.98141600
H	-3.80362700	-0.48679100	-3.17719500
H	-3.24326800	-3.90299900	-0.61373400
H	-1.20629300	5.38325800	-0.76862700
H	3.45410400	-0.47238400	-3.13133500
H	3.95357800	-1.00404500	-1.50389600
H	3.27377200	-2.16433900	-2.68311100
C	0.66901100	-0.08401000	-3.92822200
C	0.08351500	-2.25189400	-3.05984300
H	-4.45725400	-2.78554900	-2.47831300
C	-0.20056200	-0.27631100	-5.00183100
H	1.26207400	0.83308100	-3.87640100
C	-0.77302900	-2.45254900	-4.13921500
H	0.17855600	-3.02723400	-2.29966000
C	-0.92634800	-1.46095300	-5.10804500
H	-0.29948300	0.49779400	-5.76406800
H	-1.33069200	-3.38696900	-4.21740700
H	-1.60167300	-1.61609900	-5.95044500
C	5.21283300	0.71249100	0.34805700
C	6.30121800	0.18990200	-0.54760600
C	4.09283600	1.50893100	-0.06333500
C	5.27304500	0.75400400	1.77755400
H	6.81858800	-0.67062700	-0.10223000
H	7.05758900	0.97172300	-0.71860900
H	5.92307500	-0.11633300	-1.53237000
C	3.78302300	1.94790800	-1.46328900
C	3.43306600	1.96844400	1.10719800
C	6.44690600	0.41231600	2.64431900
C	4.15546800	1.48686500	2.24159200
H	2.75645500	1.69130600	-1.75710800
H	3.89339100	3.04028700	-1.53705600
H	4.47549500	1.49729900	-2.18460100
C	2.31473900	2.96300500	1.17886400
H	6.15359700	-0.07293100	3.58480100
H	6.95471100	1.35180700	2.91536500
H	7.18142700	-0.21908100	2.13542800
C	3.89249600	1.85366300	3.67237400

H	1.48178400	2.62578300	1.81277700
H	2.69123800	3.90203600	1.61330000
H	1.90255900	3.18384000	0.18831600
H	4.03185700	1.00153000	4.35339900
H	4.59004800	2.64353100	3.99294500
H	2.87385100	2.23862800	3.80785300
C	3.57933200	-2.34821700	2.83680300
C	3.71545200	-2.01243900	4.29459800
C	2.35901000	-2.69313200	2.17286900
C	4.63830200	-2.52469400	1.90564000
H	2.92388800	-1.32989000	4.63698100
H	3.64969300	-2.92275000	4.91019200
H	4.68276800	-1.54003900	4.51106800
C	1.01384800	-2.83762600	2.82133500
C	2.66250500	-3.04812600	0.83160900
C	6.09899700	-2.66064700	2.20889200
C	4.07247400	-2.90945500	0.65443700
H	0.20413400	-2.41518200	2.20756800
H	0.78562700	-3.90436900	2.97088500
H	0.98600000	-2.36711000	3.81408700
C	1.70381300	-3.67001800	-0.13235600
H	6.73638500	-2.23224400	1.42480600
H	6.33502800	-3.73609800	2.25848800
H	6.37844200	-2.22187100	3.17165500
C	4.88970600	-3.38885000	-0.51181000
H	0.70711600	-3.21401900	-0.06652000
H	1.60339700	-4.74497200	0.08700800
H	2.04800500	-3.56716800	-1.16896800
H	5.61046100	-2.63742700	-0.86591500
H	5.46778300	-4.27682300	-0.21199400
H	4.25737300	-3.67778900	-1.35868000
C	0.48742400	0.13456500	2.95684700
O	-0.53663100	0.22763800	3.46154300
O	1.64080300	0.10272400	2.69244100

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**Zr<sup>+</sup>/P-Pro**

Free energy (M06-2X-D3/def2-TZVP) = -2165.225858

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C	0.02210600	-0.51261400	-0.59709100
C	0.20368500	-0.65488700	-1.93213700
C	0.34977700	0.55181700	-2.82283300
H	1.31608500	0.52404500	-3.35039900
H	0.26801000	1.49824000	-2.26715000
H	-0.42515500	0.53969200	-3.60570100
C	0.32530100	-1.94056600	-2.69324700
C	0.61492400	-4.28156000	-4.21417500
C	1.46991000	-2.73676400	-2.56456900
C	-0.65780800	-2.31629900	-3.62043800
C	-0.52436400	-3.48904800	-4.36062200
C	1.61547400	-3.89653000	-3.32402400
H	2.24886300	-2.45147300	-1.85615000
H	-1.53710100	-1.68337300	-3.76863000
H	-1.30491200	-3.77675200	-5.06605300
H	2.51390500	-4.50481000	-3.21079300
H	0.72630200	-5.19198900	-4.80439500
P	-0.32591200	-1.92003800	0.46903400
C	0.61406800	-3.46636000	0.40905300
C	2.06902900	-5.83613300	0.25707400
C	1.82305300	-3.58844000	1.10381500
C	0.12162200	-4.54018900	-0.34277600
C	0.85211600	-5.72248100	-0.41591800
C	2.55201800	-4.77229500	1.01956900
H	2.17924800	-2.77815200	1.74006100
H	-0.82321200	-4.45119300	-0.88414600
H	0.46934300	-6.55735800	-1.00389600
H	3.49018100	-4.86986400	1.56655200
H	2.63827600	-6.76489500	0.19927000
C	-2.06542900	-2.42725600	0.38840200
C	-4.71611100	-3.26993300	0.31080300
C	-2.80375300	-2.28824600	-0.78866500
C	-2.64049000	-3.01249000	1.52440900
C	-3.97039200	-3.42307400	1.48145400
C	-4.13148000	-2.71287700	-0.82593200
H	-2.34201400	-1.85225900	-1.67371500
H	-2.05474500	-3.13750400	2.43832800



H	-4.42607900	-3.86758500	2.36686000
H	-4.70966800	-2.60591200	-1.74444800
H	-5.75735700	-3.59378200	0.28374600
Zr	0.18091300	1.49633000	0.67282200
C	2.65010000	0.99039600	0.22359100
C	2.49045300	1.08699900	1.63095600
C	2.12954500	2.42965400	1.95151500
C	2.12409100	3.17868500	0.73959900
C	2.39503200	2.28455900	-0.33345000
C	-1.31802500	3.23234300	-0.38687100
C	-1.18467600	3.62073000	0.98308000
C	-1.78156500	2.60993000	1.78405900
C	-2.34813000	1.63309500	0.91753500
C	-2.06866600	2.01409300	-0.42298500
C	-2.65012200	1.37676600	-1.64999200
H	-2.24709500	1.82600700	-2.56598400
H	-3.74017100	1.52969200	-1.66181600
H	-2.46379800	0.29570300	-1.68184100
C	-3.22587600	0.51508900	1.38693500
H	-2.72168700	-0.11530800	2.13471000
H	-3.55861900	-0.12309600	0.55946400
H	-4.12122600	0.93341500	1.87256300
C	-1.91651400	2.61021200	3.27800800
H	-1.22844300	3.32537200	3.74791700
H	-1.71479400	1.61263000	3.69418900
H	-2.94002800	2.89401900	3.56939800
C	-0.80340900	4.97776400	1.49584200
H	-0.31825700	5.59132900	0.73026700
H	-0.14974300	4.93489800	2.37662100
H	-1.72212500	5.50160500	1.80276600
C	-0.97021400	4.08033100	-1.57848800
H	-0.10705700	4.72946800	-1.38232100
H	-1.81582300	4.73401600	-1.84376900
H	-0.73873600	3.47601100	-2.46696800
C	2.67225400	2.73698800	-1.73969800
H	3.56848900	3.37713300	-1.75121100
H	1.84837900	3.32865400	-2.16600000
H	2.86593300	1.89100200	-2.40919800

C	2.19295800	4.66916700	0.60001100
H	3.24302300	4.94385500	0.40887700
H	1.88007100	5.19362700	1.50822700
H	1.60749500	5.04887700	-0.24700400
C	1.94787100	2.94117800	3.35181100
H	2.91740100	2.98969300	3.87157900
H	1.29688000	2.27932300	3.94280600
H	1.51690800	3.95031000	3.36674300
C	2.78290200	0.03085100	2.65079400
H	2.87413900	-0.95956400	2.18828200
H	2.01044700	-0.02440500	3.43000500
H	3.74422200	0.24536600	3.14277400
C	3.20123400	-0.19015400	-0.51669500
H	4.30184300	-0.17012000	-0.48854400
H	2.89209800	-0.19007000	-1.57016800
H	2.87282300	-1.14185800	-0.07443200
C	-0.11423300	-1.19934800	2.21750100
O	-0.16338200	0.08879200	2.19741600
O	0.00040900	-1.93553400	3.15624700

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### Hf<sup>+</sup>/P-Rea

Free energy (M06-2X-D3/def2-TZVP) = -1977.779112

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Hf	-0.03287300	0.19407400	1.02827000
C	2.20335500	0.39918800	-0.10325700
C	1.35482900	1.29416300	-0.81109500
C	0.33009400	0.52074500	-1.43639000
C	0.61639400	-0.86170900	-1.20988600
C	1.77262300	-0.93838900	-0.38352000
C	-0.02809500	2.51383300	2.03084600
C	-0.04352100	1.62278100	3.14352000
C	-1.29981800	0.94918300	3.15352700
C	-2.04656200	1.40107200	2.02595200
C	-1.26793000	2.36837300	1.32947500
C	2.61066100	-2.14478100	-0.07359900
H	2.87078300	-2.21332400	0.99211000
H	3.55269900	-2.07801100	-0.64005300

H	2.11460700	-3.08066000	-0.35498000
C	-0.06752200	-1.98231600	-1.93450400
H	-1.13159800	-2.06278800	-1.67090400
H	0.41018700	-2.94450100	-1.71733100
H	-0.00303000	-1.81252600	-3.02001900
C	-0.68522400	1.03433100	-2.41699900
H	-0.29047200	0.95500100	-3.44288000
H	-0.92940600	2.08962100	-2.24151500
H	-1.61834500	0.45427700	-2.38711400
C	1.65697500	2.72679900	-1.12937200
H	2.11738700	2.76367100	-2.12965300
H	2.37017000	3.17005700	-0.42664300
H	0.76190600	3.35870100	-1.16813500
C	3.45290600	0.73938000	0.65933800
H	3.48914700	1.80049100	0.93793500
H	4.34652100	0.52863200	0.05082400
H	3.54757400	0.14127000	1.57865000
C	-1.79853300	3.23754500	0.22544300
H	-2.45543800	4.01399200	0.64731800
H	-2.39642500	2.66654100	-0.49878700
H	-0.99959500	3.75139900	-0.32143300
C	-3.49258500	1.08795600	1.79650400
H	-3.71938400	0.03973800	2.03470400
H	-3.80133400	1.28452400	0.76194100
H	-4.11436200	1.72014800	2.45098100
C	-1.91179600	0.13448300	4.25286500
H	-2.31687200	-0.81755200	3.88258100
H	-2.74940500	0.70088900	4.68869500
H	-1.20242300	-0.09422400	5.05541100
C	1.02601300	1.59151400	4.19946600
H	2.00266300	1.25760500	3.81295900
H	0.74658900	0.93567300	5.03251900
H	1.17655500	2.60278500	4.60720600
C	0.98949800	3.60531100	1.87096600
H	2.02232300	3.22917500	1.85842600
H	0.90989000	4.29506200	2.72610400
H	0.82424100	4.19346400	0.96255800
C	-1.46563200	-1.52932700	1.15400200

C	-2.63864500	-2.04473900	0.72565100
P	-0.11115700	-2.20649800	2.17606800
C	-0.20360300	-2.55997300	3.96725300
C	-0.12122800	-3.12935700	6.70224900
C	0.69037500	-1.88269400	4.80320100
C	-1.01548900	-3.56999800	4.49774300
C	-0.98363400	-3.83943400	5.86378200
C	0.72964200	-2.16250300	6.16950200
H	1.36451200	-1.13570600	4.37921500
H	-1.66002800	-4.15622600	3.84171300
H	-1.62544800	-4.61964300	6.27538900
H	1.42970300	-1.63047000	6.81541500
H	-0.09739100	-3.34802600	7.77065300
C	0.41311400	-3.82709200	1.51411900
C	1.35137300	-6.27773300	0.54425800
C	-0.18489900	-4.41647500	0.39925900
C	1.47367000	-4.48284600	2.15690800
C	1.94203700	-5.69905800	1.66969600
C	0.28441300	-5.63900500	-0.08376800
H	-1.01541600	-3.91839200	-0.09638400
H	1.93724400	-4.04130100	3.04250800
H	2.77073700	-6.19955800	2.17195100
H	-0.19276900	-6.09496500	-0.95251000
H	1.71832300	-7.23205900	0.16454300
C	-3.31539600	-3.25413400	1.27738900
C	-4.69265700	-5.47607600	2.30351000
C	-3.66551400	-4.32715400	0.44281300
C	-3.69250200	-3.30074000	2.62395600
C	-4.38077700	-4.40236200	3.13386100
C	-4.33130200	-5.43622000	0.95543100
H	-3.40058500	-4.30295200	-0.61702100
H	-3.45763200	-2.45605600	3.27424600
H	-4.67686100	-4.41652100	4.18403600
H	-4.57831300	-6.27129200	0.29876400
H	-5.22708100	-6.33961800	2.70110200
C	-3.40053000	-1.37755800	-0.39571200
H	-2.89557900	-0.46195200	-0.73388700
H	-4.42568000	-1.13380900	-0.07827400

H -3.49867000 -2.06269900 -1.25334100

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**Hf<sup>+</sup>/P-TS**

Free energy (M06-2X-D3/def2-TZVP) = -2166.148423

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Hf	3.17182700	-0.55605800	1.11005400
C	1.56148300	-0.50292600	-0.55042100
C	1.79814000	-0.85955400	-1.83568200
P	-0.10649600	-0.17422900	0.19147300
C	3.19845500	-1.13879300	-2.32941800
C	0.80002100	-1.05614000	-2.94201100
C	-0.41732700	1.60598600	-0.15012600
C	-1.49152800	-0.97422200	-0.71825000
H	3.44845300	-0.47303600	-3.17059000
H	3.96491600	-1.00861200	-1.54811200
H	3.27081100	-2.16497200	-2.72300400
C	0.65709200	-0.08216800	-3.93777100
C	0.08791900	-2.25559600	-3.07237000
C	0.03284100	2.24989600	-1.30749100
C	-1.18069000	2.33024800	0.77509600
C	-2.19888600	-0.33918000	-1.74706400
C	-1.89282800	-2.25164400	-0.30618600
C	-0.21991900	-0.27477500	-5.00531900
H	1.24705200	0.83697300	-3.88782900
C	-0.77603000	-2.45642500	-4.14576500
H	0.19265400	-3.03317900	-2.31571000
C	-0.25206700	3.59672100	-1.52845600
H	0.60241900	1.68361600	-2.04337600
C	-1.46099800	3.67968400	0.55970000
H	-1.56649100	1.83665800	1.67081900
C	-3.26010700	-0.98828900	-2.37296500
H	-1.91717700	0.66324500	-2.07259300
C	-2.94477000	-2.90737900	-0.94434600
H	-1.39110200	-2.73864200	0.53386200
C	-0.94115400	-1.46227600	-5.11006000
H	-0.32787900	0.50134200	-5.76428200
H	-1.33006600	-3.39308700	-4.22290600

C	-0.99092100	4.31667500	-0.58876000
H	0.10242700	4.08601200	-2.43713200
H	-2.05284000	4.23405400	1.28936700
C	-3.62862400	-2.27599300	-1.98205100
H	-3.79900600	-0.48511200	-3.17707800
H	-3.24391300	-3.90361200	-0.61555400
H	-1.62207500	-1.61771000	-5.94789300
H	-1.20990000	5.37200200	-0.75677800
H	-4.45977400	-2.78129100	-2.47602300
C	5.21014600	0.70970800	0.35423000
C	6.30066000	0.18693400	-0.53907300
C	4.09391400	1.51021200	-0.05923700
C	5.26968300	0.75633800	1.78441700
H	5.92488200	-0.11940500	-1.52466900
H	7.05768300	0.96844200	-0.70847900
H	6.81674800	-0.67396200	-0.09308900
C	3.78616900	1.94585200	-1.46048800
C	3.43513200	1.97692900	1.11037800
C	6.44094000	0.41239300	2.65391900
C	4.15643700	1.49760400	2.24566000
H	2.75628500	1.69937800	-1.75088400
H	3.90927300	3.03647500	-1.53995100
H	4.47169600	1.48366800	-2.18106500
C	2.31883300	2.97483000	1.17760400
H	6.14524300	-0.07573300	3.59222600
H	6.94842900	1.35084300	2.92901100
H	7.17661800	-0.21776900	2.14525200
C	3.89591600	1.86869500	3.67590500
H	1.48414000	2.64384100	1.81302100
H	2.69632900	3.91622700	1.60585900
H	1.90661800	3.19031000	0.18589700
H	4.02205400	1.01519400	4.35797900
H	4.60284200	2.64936300	3.99820200
H	2.88249100	2.26819400	3.80951700
C	3.57318600	-2.34922200	2.84270900
C	3.71292900	-2.01687300	4.30107800
C	2.35215400	-2.69509100	2.17974000
C	4.63120100	-2.52107500	1.90968800

H	2.91949900	-1.33975900	4.65005400
H	3.65545100	-2.92885500	4.91495300
H	4.67804400	-1.53861900	4.51446100
C	1.00721500	-2.83920300	2.82988900
C	2.65546400	-3.04732200	0.83759800
C	6.09208400	-2.65774400	2.21143100
C	4.06482600	-2.90264800	0.65713900
H	0.19738900	-2.40970500	2.22096100
H	0.77433700	-3.90542500	2.97541000
H	0.98388300	-2.37474400	3.82590500
C	1.69756100	-3.66523300	-0.12943500
H	6.72913700	-2.22571100	1.42917400
H	6.32832400	-3.73335300	2.25595600
H	6.37180700	-2.22321800	3.17602700
C	4.88133500	-3.38094200	-0.51028400
H	0.70242500	-3.20530000	-0.06867000
H	1.59167300	-4.73968500	0.08961500
H	2.04717600	-3.56395900	-1.16435200
H	5.61062400	-2.63388200	-0.85583900
H	5.44927800	-4.27754900	-0.21670600
H	4.24905100	-3.65578900	-1.36182100
C	0.51701500	0.14394700	2.99105200
O	-0.50996400	0.24377900	3.48414400
O	1.66441700	0.10217600	2.70698800

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### Hf<sup>+</sup>/P-Prod

Free energy (M06-2X-D3/def2-TZVP) = -2166.190301

C	0.02190000	-0.50620800	-0.60128900
C	0.20255500	-0.65311800	-1.93646700
C	0.35039900	0.54921700	-2.83230300
H	1.31622100	0.51573000	-3.36034200
H	0.27181800	1.49940300	-2.28275000
H	-0.42516200	0.53409300	-3.61446700
C	0.32238400	-1.94165800	-2.69286600
C	0.61100800	-4.28675400	-4.20734600
C	1.46788300	-2.73658400	-2.56376800

C	-0.66183200	-2.32034200	-3.61764900
C	-0.52891100	-3.49529400	-4.35443500
C	1.61286800	-3.89845300	-3.32007300
H	2.24799600	-2.44827000	-1.85790100
H	-1.54133900	-1.68803700	-3.76695500
H	-1.31028600	-3.78535400	-5.05797200
H	2.51201700	-4.50564900	-3.20677700
H	0.72201100	-5.19879700	-4.79514000
P	-0.32736200	-1.91600400	0.46485400
C	0.61483400	-3.46048300	0.40713300
C	2.07263500	-5.82838300	0.26011200
C	1.82641200	-3.57755800	1.09825500
C	0.12107600	-4.53805000	-0.33841300
C	0.85317900	-5.71951700	-0.40904800
C	2.55681700	-4.76060500	1.01645000
H	2.18356600	-2.76361000	1.72927400
H	-0.82581400	-4.45274800	-0.87674600
H	0.46962800	-6.55750200	-0.99207700
H	3.49707000	-4.85450400	1.56049000
H	2.64309300	-6.75652100	0.20424500
C	-2.06618800	-2.42439100	0.38431100
C	-4.71562500	-3.27027100	0.30657700
C	-2.80537600	-2.28358800	-0.79196800
C	-2.63969200	-3.01275400	1.51960200
C	-3.96905400	-3.42489000	1.47652700
C	-4.13251300	-2.70995600	-0.82932300
H	-2.34497100	-1.84461700	-1.67612100
H	-2.05342800	-3.13893500	2.43300100
H	-4.42369800	-3.87172800	2.36129300
H	-4.71148000	-2.60153600	-1.74716600
H	-5.75647900	-3.59537100	0.27950500
Hf	0.17918600	1.48687400	0.67222900
C	2.65676300	0.98795400	0.22544800
C	2.49842000	1.08384700	1.63303200
C	2.13223800	2.42537100	1.95392500
C	2.12438000	3.17455700	0.74182900
C	2.39631000	2.28118900	-0.33220200
C	-1.31958600	3.23349500	-0.38584700



C	-1.18611400	3.61945400	0.98522500
C	-1.78568500	2.60890100	1.78506700
C	-2.35449000	1.63467400	0.91698000
C	-2.07239700	2.01640600	-0.42321500
C	-2.65104400	1.37915000	-1.65149700
H	-2.24574400	1.82862000	-2.56645000
H	-3.74114900	1.53105100	-1.66687300
H	-2.46366200	0.29822100	-1.68325500
C	-3.23399700	0.51668000	1.38414400
H	-2.73290600	-0.11518300	2.13297600
H	-3.56477500	-0.12087900	0.55540700
H	-4.13076100	0.93432700	1.86769300
C	-1.92209400	2.61009300	3.27917400
H	-1.22759300	3.31896400	3.74928500
H	-1.72882000	1.61135000	3.69661200
H	-2.94296000	2.90305100	3.57072500
C	-0.80293900	4.97494000	1.50067600
H	-0.31955100	5.59007200	0.73525300
H	-0.14659500	4.92969900	2.37937800
H	-1.72035800	5.49862400	1.81159300
C	-0.97194600	4.08337400	-1.57636300
H	-0.10757700	4.73081600	-1.38004600
H	-1.81663800	4.73865200	-1.84055700
H	-0.74139000	3.48028900	-2.46596300
C	2.67370000	2.73481100	-1.73815700
H	3.57558800	3.36699900	-1.75185600
H	1.85353800	3.33447400	-2.16048900
H	2.85779400	1.88880100	-2.41043300
C	2.19147200	4.66509300	0.60225000
H	3.24055700	4.94084100	0.40742100
H	1.88126400	5.18885500	1.51177400
H	1.60245900	5.04472200	-0.24229600
C	1.95173000	2.93732000	3.35448600
H	2.92161400	2.98895500	3.87322200
H	1.30258800	2.27535300	3.94747400
H	1.51803400	3.94526400	3.36878500
C	2.79336800	0.02849500	2.65349700
H	2.90655200	-0.95867100	2.18847000

H	2.01276400	-0.04173100	3.42370500
H	3.74487000	0.25545700	3.15886900
C	3.20511800	-0.19189900	-0.51791900
H	4.30582700	-0.17183000	-0.49637100
H	2.89043000	-0.19090200	-1.56980900
H	2.87993200	-1.14452700	-0.07515900
C	-0.11606900	-1.19657200	2.21378200
O	-0.16090900	0.09380400	2.19824400
O	-0.00409400	-1.93283600	3.15186700

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**Zr<sup>+</sup>/N-Rea**

Free energy (M06-2X-D3/def2-TZVP) = -1690.24841

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Zr	-0.13429800	0.08785500	1.22439400
C	2.19827600	0.45426400	0.38079400
C	1.36457400	1.22530800	-0.48027300
C	0.51642900	0.32968000	-1.19230600
C	0.88476000	-1.00764400	-0.83914900
C	1.92458500	-0.93092200	0.12064700
C	-0.42283500	2.48039700	2.09796800
C	-0.24029000	1.64623600	3.23290400
C	-1.38754100	0.79108400	3.33986700
C	-2.25264600	1.08714400	2.26265900
C	-1.63576800	2.09804200	1.45100500
C	2.70951900	-2.11110100	0.62013800
H	3.36814000	-1.84443100	1.45702000
H	3.34843400	-2.48824600	-0.19269100
H	2.06271100	-2.94186200	0.94093900
C	0.43551700	-2.26406700	-1.51952400
H	-0.64603000	-2.28270700	-1.70327100
H	0.68492200	-3.15044700	-0.92346800
H	0.94058600	-2.35339000	-2.49441100
C	-0.40303700	0.73044100	-2.31102100
H	0.18723400	1.07362500	-3.17496900
H	-1.07546300	1.55417900	-2.03041300
H	-1.01714300	-0.11402000	-2.64773400
C	1.53179100	2.66683300	-0.85092000

H	2.07381600	2.71135200	-1.80930200
H	2.11914900	3.22887600	-0.11809900
H	0.57207900	3.17745700	-1.00333900
C	3.29667700	0.97751900	1.26405000
H	3.11477800	2.01859700	1.56330200
H	4.26490700	0.94825400	0.74101400
H	3.40958400	0.37836300	2.18041300
C	-2.28815100	2.80117400	0.29403300
H	-2.98986300	3.56813400	0.65683700
H	-2.86406600	2.10986300	-0.33872200
H	-1.55121800	3.30842600	-0.34305900
C	-3.65710100	0.57474900	2.16152500
H	-3.70875300	-0.52422500	2.17554900
H	-4.16472700	0.94403100	1.26243200
H	-4.22633400	0.93695600	3.03161500
C	-1.75297600	-0.11807800	4.47195000
H	-2.24057700	-1.03320100	4.10523300
H	-2.46598300	0.39312200	5.13843900
H	-0.88113600	-0.40966500	5.07006700
C	0.81065100	1.89287300	4.27780900
H	1.83485100	1.82586800	3.88013400
H	0.71772400	1.19154600	5.11435200
H	0.68965800	2.91084700	4.68011500
C	0.37479300	3.72769700	1.86850400
H	1.45713500	3.56165100	1.95316700
H	0.10301300	4.45583700	2.65008100
H	0.16380600	4.19583500	0.90200200
C	-1.08012600	-1.97238000	1.38252800
C	-2.27198000	-2.08887200	0.74204000
N	-0.49561300	-3.00290500	2.17000700
C	0.12091200	-2.57050200	3.36861700
C	1.40756100	-1.78391500	5.74624800
C	1.07553300	-1.54464900	3.36601700
C	-0.20215500	-3.17977200	4.58971200
C	0.43579900	-2.79136100	5.76194500
C	1.72519400	-1.16163900	4.54441400
H	1.47461300	-1.17911700	2.40925800
H	-0.94296200	-3.98125700	4.59635700

H	0.17689900	-3.28120700	6.70167400
H	2.50249700	-0.39760800	4.51247200
H	1.92036700	-1.49931400	6.66518700
C	-0.18629800	-4.31068400	1.70074300
C	0.53826200	-6.88523600	0.75940900
C	-0.74391600	-4.83769500	0.52336400
C	0.76870900	-5.09597400	2.37747900
C	1.11308300	-6.36309100	1.91503700
C	-0.38183200	-6.10321900	0.06702400
H	-1.45508700	-4.26295800	-0.05842700
H	1.26696400	-4.72127600	3.26934600
H	1.85302300	-6.94157100	2.47007200
H	-0.84097800	-6.47898600	-0.84858800
H	0.80795000	-7.87871500	0.40172600
C	-3.29306200	-3.15378600	0.91504300
C	-5.26809800	-5.12908100	1.26146400
C	-4.15039200	-3.50831800	-0.13762800
C	-3.45914000	-3.79706700	2.15282900
C	-4.43622300	-4.77153300	2.32385400
C	-5.12336900	-4.49234300	0.03118300
H	-4.05327900	-3.02529300	-1.11184100
H	-2.81455800	-3.51923800	2.98783300
H	-4.55253200	-5.25617600	3.29410300
H	-5.77215600	-4.76003700	-0.80376700
H	-6.03008000	-5.89764900	1.39561300
C	-2.62179200	-1.02057500	-0.27219100
H	-1.99392600	-0.10354300	-0.21391600
H	-3.66103500	-0.67883600	-0.18294000
H	-2.48617700	-1.38228600	-1.30327100

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**Zr<sup>+</sup>/N-TS**

Free energy (M06-2X-D3/def2-TZVP) = -1878.620466

C	-0.15486900	-0.80892600	-0.35938500
C	0.13766500	-0.87668300	-1.67815300
C	0.46557900	0.41107800	-2.40098200
H	1.50063300	0.41205600	-2.77187300

H	0.32824400	1.34371200	-1.80996400
H	-0.19141300	0.54505400	-3.27355400
C	0.18547900	-2.05429300	-2.60745800
C	0.29853000	-4.14394800	-4.48736600
C	1.18546800	-3.03207600	-2.53011200
C	-0.73487300	-2.12490500	-3.66579300
C	-0.69028300	-3.16533700	-4.58927200
C	1.23835600	-4.06807500	-3.46222700
H	1.92783100	-2.99565800	-1.73197300
H	-1.50622900	-1.35555100	-3.76697300
H	-1.42522400	-3.20861500	-5.39398900
H	2.02287200	-4.82157700	-3.37984400
H	0.33974600	-4.95855900	-5.21138800
N	-0.54858700	-1.99165100	0.42224600
C	0.38007500	-3.08895800	0.45956900
C	2.30516400	-5.12692900	0.52513100
C	1.69408500	-2.81655800	0.84787600
C	0.02374400	-4.39878100	0.13142400
C	0.98851900	-5.40617900	0.16516400
C	2.65446000	-3.82034000	0.87309500
H	1.95365300	-1.79240000	1.10893300
H	-0.99336500	-4.63243600	-0.18160800
H	0.70247700	-6.42306800	-0.10696100
H	3.67790000	-3.58673800	1.17376700
H	3.05142900	-5.92133700	0.54650200
C	-1.93938800	-2.38525000	0.34748100
C	-4.64176100	-3.16330500	0.27100900
C	-2.70238100	-2.19710700	-0.80505000
C	-2.53163900	-3.01948400	1.44959300
C	-3.87093800	-3.39529600	1.41175500
C	-4.04533300	-2.57720100	-0.84100400
H	-2.24291300	-1.76752800	-1.68816100
H	-1.93814800	-3.24601500	2.33408600
H	-4.31389600	-3.88077900	2.28233400
H	-4.62174500	-2.41812800	-1.75362400
H	-5.69129000	-3.45761500	0.24546500
Zr	0.17460500	1.32573700	0.51200800
C	2.71150000	0.84627000	0.19703500

C	2.49190300	0.90224200	1.59928600
C	2.06209700	2.22613800	1.93867200
C	2.10864100	3.01167600	0.75466000
C	2.43691400	2.15475800	-0.32920400
C	-1.27558300	3.13343900	-0.45502500
C	-1.14202600	3.49571300	0.91892500
C	-1.73640500	2.47252500	1.70004000
C	-2.34618300	1.52996300	0.81353000
C	-2.06540000	1.93506600	-0.51395400
C	-2.63755900	1.33177200	-1.76176400
H	-2.23729500	1.81620400	-2.66143000
H	-3.72909400	1.47217400	-1.77160800
H	-2.44153700	0.25435300	-1.82396800
C	-3.29159700	0.45934400	1.26179200
H	-2.84140900	-0.22822800	1.99166300
H	-3.65977800	-0.14171200	0.42343100
H	-4.15618000	0.93009300	1.75529900
C	-1.91155900	2.49585400	3.18944500
H	-1.07010300	2.98919200	3.69443600
H	-2.01171500	1.48204200	3.59892200
H	-2.82603500	3.05010300	3.45493100
C	-0.78095800	4.84292500	1.46684000
H	-0.28624600	5.48230500	0.72975500
H	-0.15428700	4.78718000	2.36579600
H	-1.71598000	5.34551200	1.76145900
C	-0.90401000	3.98293000	-1.63840200
H	-0.08561800	4.67546600	-1.40328600
H	-1.76440400	4.58969900	-1.96065100
H	-0.59420000	3.37915100	-2.50408000
C	2.76029500	2.65944600	-1.70807600
H	3.59320500	3.37740800	-1.65117500
H	1.91555400	3.18493800	-2.17863600
H	3.07072900	1.84998600	-2.37886500
C	2.18827300	4.50486700	0.65970800
H	3.24483600	4.77312800	0.49722900
H	1.86477500	5.00557700	1.57698100
H	1.62442800	4.91406800	-0.18813200
C	1.87243100	2.70851700	3.34803600

H	2.84717300	2.86244200	3.83789400
H	1.31452600	1.98038900	3.95494300
H	1.33512600	3.66476700	3.38574600
C	2.89616400	-0.10491700	2.63866200
H	3.48954900	-0.91843000	2.20495800
H	2.06127200	-0.55946500	3.19109500
H	3.52648500	0.39322800	3.38995300
C	3.34582100	-0.27095500	-0.58119300
H	4.07952000	0.13315800	-1.29243400
H	2.61976300	-0.87598700	-1.14381900
H	3.88455000	-0.95483100	0.08725100
C	-0.24350600	-1.15147800	2.60610300
O	-0.25121800	-0.00363300	2.29918000
O	-0.17176700	-2.10588300	3.24320500

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**Zr<sup>+</sup>/N-Prod**

Free energy (M06-2X-D3/def2-TZVP) = -1878.628744

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C	-0.06974700	-0.74520200	-0.40390200
C	0.21268600	-0.93617400	-1.70809000
C	0.40125400	0.30855300	-2.54849500
H	1.36443500	0.29829100	-3.07946900
H	0.33487600	1.25318700	-1.97238700
H	-0.38274000	0.35782100	-3.32066300
C	0.37742800	-2.17942000	-2.53396100
C	0.77449800	-4.41712800	-4.18601900
C	1.60405300	-2.85661200	-2.53810800
C	-0.62677900	-2.60730000	-3.41173700
C	-0.43595100	-3.72779600	-4.21999700
C	1.79878500	-3.96873600	-3.35244500
H	2.40494000	-2.52193000	-1.87858000
H	-1.56976900	-2.06011400	-3.48222900
H	-1.23417300	-4.05464500	-4.88765000
H	2.75665200	-4.49055600	-3.33021200
H	0.92489500	-5.29169100	-4.82006300
N	-0.42531100	-1.89230400	0.53694700
C	0.37117500	-3.14121700	0.35503600
C	1.95121700	-5.40399600	-0.01720000

C	1.69225100	-3.14550900	0.79414200
C	-0.17717100	-4.27189900	-0.24442500
C	0.62278600	-5.39867500	-0.43299500
C	2.48329600	-4.27350600	0.60268800
H	2.09530400	-2.27939400	1.31370400
H	-1.20984000	-4.28897600	-0.58692200
H	0.19322900	-6.27819200	-0.91334900
H	3.51448200	-4.27276600	0.95784100
H	2.56810000	-6.29150900	-0.16160000
C	-1.88983000	-2.23095400	0.49381400
C	-4.57328300	-2.99521000	0.37370300
C	-2.60795400	-2.06893800	-0.68384100
C	-2.49512500	-2.81642800	1.60862100
C	-3.83892000	-3.17868700	1.54484500
C	-3.94741400	-2.45312300	-0.74510900
H	-2.12283000	-1.65813800	-1.55943900
H	-1.93219800	-3.01207000	2.51886400
H	-4.30809000	-3.62377800	2.42276400
H	-4.49865600	-2.32205700	-1.67720700
H	-5.62264000	-3.28824100	0.33098800
Zr	0.13146700	1.38167300	0.59082000
C	2.63700800	0.91672200	0.19670100
C	2.45033400	0.96410300	1.60313300
C	2.04466700	2.28801900	1.95592300
C	2.06315100	3.07868700	0.77100700
C	2.36359700	2.22382900	-0.32253100
C	-1.31692300	3.17539200	-0.41506100
C	-1.18152700	3.55670800	0.95407700
C	-1.78382000	2.54650800	1.74919100
C	-2.39773400	1.60003300	0.87706400
C	-2.10641900	1.97723700	-0.45848000
C	-2.69084200	1.37537400	-1.70281100
H	-2.27662200	1.84332500	-2.60488700
H	-3.77901400	1.54002200	-1.71824200
H	-2.51899000	0.29449700	-1.76453500
C	-3.34350300	0.54958900	1.36540000
H	-2.88323700	-0.08430100	2.13628700
H	-3.71007600	-0.09157900	0.55654900



H	-4.21266200	1.04262500	1.82871500
C	-1.92498900	2.54197400	3.24257600
H	-1.22881800	3.24422100	3.71919500
H	-1.74019700	1.53967100	3.65579300
H	-2.94590800	2.83682400	3.53240600
C	-0.80969600	4.91066600	1.47962800
H	-0.32386100	5.53707900	0.72570000
H	-0.16782400	4.86644600	2.36827900
H	-1.73814900	5.42090600	1.78063100
C	-0.93974800	4.00640300	-1.60986200
H	-0.11469800	4.69406500	-1.38391900
H	-1.79434200	4.61720100	-1.94023100
H	-0.63416200	3.38899900	-2.46740400
C	2.65271500	2.71590500	-1.71308200
H	3.53670200	3.37275600	-1.69814600
H	1.82368300	3.30245600	-2.13622900
H	2.87113300	1.89015300	-2.40057200
C	2.15302300	4.57168200	0.67990400
H	3.21027800	4.83142700	0.50812400
H	1.84228700	5.07326400	1.60115800
H	1.58470600	4.98756700	-0.16149400
C	1.84673300	2.75714700	3.36875000
H	2.81779400	2.87571600	3.87522900
H	1.25933200	2.03494200	3.95481000
H	1.33575400	3.72768600	3.41023500
C	2.80456200	-0.08712700	2.61401800
H	3.36661400	-0.90861100	2.15178500
H	1.93780900	-0.50613000	3.14531100
H	3.46210900	0.35413600	3.37759000
C	3.27339800	-0.18881800	-0.58956300
H	4.35964900	-0.01774700	-0.65212700
H	2.88935100	-0.23708100	-1.61618400
H	3.11284600	-1.17104800	-0.13176700
C	-0.17118900	-1.32441100	2.04947400
O	-0.29849200	-0.07191900	2.09030000
O	0.06763900	-2.13453700	2.88150300

**Zr<sup>+</sup>/As-Rea**

Free energy (M06-2X-D3/def2-TZVP) = -3871.195241

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Zr	-0.01430500	0.27546800	1.01390300
C	2.19406600	0.45364100	-0.16750900
C	1.32988200	1.32878200	-0.87845800
C	0.29508100	0.53795700	-1.46598200
C	0.58625700	-0.83690700	-1.20860400
C	1.75741300	-0.89066400	-0.40139400
C	-0.01322900	2.60151000	1.96738000
C	-0.02564200	1.72154400	3.08797500
C	-1.28346500	1.05047900	3.10916900
C	-2.03483700	1.49260100	1.98253700
C	-1.25686600	2.45001100	1.27295300
C	2.60412300	-2.09068000	-0.08791600
H	2.90920500	-2.12784400	0.96732500
H	3.52125600	-2.04499600	-0.69606800
H	2.09440100	-3.03243200	-0.32076900
C	-0.09934000	-1.98234300	-1.89041100
H	-1.17369300	-2.01886600	-1.66481500
H	0.34169800	-2.94170300	-1.59631800
H	0.01237500	-1.88110100	-2.98090800
C	-0.73629500	1.02869000	-2.44103300
H	-0.34298700	0.95861400	-3.46817500
H	-1.00360200	2.07835900	-2.26500600
H	-1.65477100	0.42657100	-2.40726100
C	1.62245000	2.75445100	-1.23549300
H	2.07059100	2.76890200	-2.24192700
H	2.34238300	3.21764600	-0.55261400
H	0.72412900	3.38123600	-1.27896500
C	3.45995800	0.81299300	0.55761900
H	3.50446000	1.88117500	0.80603200
H	4.33810600	0.58427300	-0.06683000
H	3.57572500	0.23876200	1.48939800
C	-1.79398300	3.31451400	0.16890700
H	-2.43163300	4.10434500	0.59566700
H	-2.41443500	2.74437200	-0.53645800
H	-0.99919600	3.81215400	-0.39849500
C	-3.48358700	1.18099600	1.76883400

H	-3.70925000	0.13461200	2.01604900
H	-3.80288100	1.37201200	0.73664400
H	-4.09624400	1.81902100	2.42638200
C	-1.88794200	0.24088900	4.21604300
H	-2.23631700	-0.74340900	3.87222600
H	-2.76508200	0.77726800	4.60928600
H	-1.19244900	0.07945000	5.04613500
C	1.06978300	1.64749000	4.11596800
H	1.94709300	1.07089700	3.77797200
H	0.70734600	1.18889100	5.04454800
H	1.42744800	2.65760300	4.36223500
C	1.01136300	3.68156100	1.77395000
H	2.04072100	3.29676000	1.74782200
H	0.95207800	4.38682600	2.61784600
H	0.83373700	4.25521300	0.85851600
C	-1.44010900	-1.44720500	1.15816100
C	-2.60661900	-1.97714900	0.73675000
As	-0.00482300	-2.17276300	2.28803800
C	-0.23642700	-2.67488400	4.15190000
C	-0.32310200	-3.47745700	6.82508800
C	0.42548500	-1.92943400	5.13154200
C	-0.90024700	-3.85470800	4.50644500
C	-0.95156100	-4.24533800	5.84310500
C	0.37584800	-2.32536900	6.46835600
H	0.98843300	-1.03770700	4.84844900
H	-1.36487600	-4.47670500	3.73941200
H	-1.47484800	-5.16253700	6.11736300
H	0.89380500	-1.73987900	7.22924800
H	-0.36211500	-3.79003600	7.86940600
C	0.48828100	-3.90000400	1.56150800
C	1.32260000	-6.38202300	0.59140000
C	-0.17506000	-4.48573700	0.48352300
C	1.56088400	-4.56677400	2.16776200
C	1.97753900	-5.80241600	1.68010300
C	0.24471900	-5.72680900	-0.00040600
H	-1.01839100	-3.97683000	0.01927900
H	2.07390100	-4.12340500	3.02547100
H	2.81609800	-6.31601200	2.15204900

H	-0.28094300	-6.18426200	-0.83987400
H	1.64928000	-7.35059700	0.21090900
C	-3.26198300	-3.19888900	1.28631700
C	-4.56562700	-5.46440300	2.31775900
C	-3.71661100	-4.21609100	0.43129000
C	-3.49275900	-3.32730200	2.66013500
C	-4.14501000	-4.44892800	3.17298700
C	-4.34642600	-5.34588900	0.94384700
H	-3.55876600	-4.13443300	-0.64649900
H	-3.17019200	-2.53113000	3.33305200
H	-4.32531400	-4.52434700	4.24666600
H	-4.67624200	-6.13579500	0.26786500
H	-5.07273800	-6.34351300	2.71708600
C	-3.38001900	-1.30663700	-0.37828100
H	-2.88539900	-0.38034400	-0.70149700
H	-4.40715600	-1.07754600	-0.05666100
H	-3.46983500	-1.97586700	-1.24865900

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**Zr<sup>+</sup>/As-TS**

Free energy (M06-2X-D3/def2-TZVP) = -4059.564846

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As	-0.18129400	-0.16185600	0.26156800
C	-1.62057100	-1.01414300	-0.73693600
C	-0.49016100	1.71135300	-0.17581000
C	-2.31789300	-0.35558700	-1.75478900
C	-2.00140800	-2.30845600	-0.36475400
C	1.60337700	-0.52882500	-0.51138400
C	-0.03934800	2.29836800	-1.36147800
C	-1.20405200	2.48659500	0.74515300
C	-3.36414000	-1.00130700	-2.41101400
H	-2.04294700	0.65898200	-2.04859900
C	-3.03951200	-2.95704900	-1.03223200
H	-1.49682000	-2.81672200	0.46163500
C	1.82154900	-0.86458400	-1.80377700
Zr	3.21357200	-0.58040800	1.14385300
C	-0.28098700	3.64801900	-1.61698800
H	0.49822700	1.69188500	-2.08991200
C	-1.44219600	3.83820900	0.49233400

H	-1.57642800	2.03838800	1.67042300
C	-3.72075200	-2.30307400	-2.05842600
H	-3.90057500	-0.48363000	-3.20758200
H	-3.32866100	-3.96690800	-0.73773600
C	3.21849000	-1.14172300	-2.31213000
C	0.81483600	-1.04832500	-2.90419200
C	-0.97524300	4.42132200	-0.68543800
H	0.07271800	4.09761600	-2.54622600
H	-1.99606400	4.43646800	1.21715900
H	-4.54016400	-2.80445400	-2.57546700
H	3.28485400	-2.16515700	-2.71413800
H	3.98928800	-1.01797000	-1.53460600
H	3.46275000	-0.47047000	-3.15045200
C	0.68678400	-0.08200600	-3.90966300
C	0.08184300	-2.23633200	-3.02137500
H	-1.16025400	5.47825200	-0.88187000
C	-0.19603000	-0.26976200	-4.97314600
H	1.29408400	0.82641500	-3.86997200
C	-0.78646200	-2.43405100	-4.09206400
H	0.17770100	-3.00904400	-2.25859200
C	-0.93658600	-1.44656600	-5.06541200
H	-0.29264100	0.50058200	-5.73947100
H	-1.35504900	-3.36266900	-4.15994500
H	-1.62098800	-1.59891400	-5.90098600
C	3.62506200	-2.37754900	2.85330400
C	3.76723700	-2.04611400	4.31150200
C	2.40240700	-2.72423100	2.19550100
C	4.67870700	-2.53997300	1.91320000
H	2.97129400	-1.37186800	4.66025100
H	3.71271000	-2.95918000	4.92412300
H	4.73172900	-1.56630400	4.52434800
C	1.06344100	-2.87939300	2.85409900
C	2.69872100	-3.06828200	0.84933600
C	6.14281900	-2.66200600	2.20612400
C	4.10639900	-2.92074500	0.66330000
H	0.24083400	-2.49357800	2.23320600
H	0.85907700	-3.94605900	3.03539100
H	1.02779200	-2.37957800	3.83206700

C	1.73524700	-3.68556300	-0.11323000
H	6.77039100	-2.22505300	1.41874200
H	6.39110200	-3.73480700	2.25237800
H	6.42374400	-2.22141600	3.16775400
C	4.91766400	-3.38677400	-0.51243400
H	0.73403900	-3.24086600	-0.02931800
H	1.64668500	-4.76437300	0.09143900
H	2.06597100	-3.56339800	-1.15212600
H	5.64100300	-2.63340600	-0.85691600
H	5.49232700	-4.28200400	-0.22783300
H	4.28151800	-3.65913400	-1.36191600
C	5.22222800	0.71694900	0.36592600
C	6.31368600	0.20634600	-0.53280100
C	4.09128500	1.49818600	-0.04129400
C	5.28600100	0.75748500	1.79581600
H	6.83312100	-0.65710000	-0.09546300
H	7.06811300	0.99197400	-0.69469900
H	5.93760800	-0.09078500	-1.52105100
C	3.77053400	1.94152400	-1.43716200
C	3.42957300	1.94932800	1.13202300
C	6.46530300	0.42203100	2.65786700
C	4.16243000	1.47960300	2.26394700
H	2.73189700	1.71275100	-1.71183200
H	3.90942100	3.03057700	-1.51423100
H	4.43812800	1.47214500	-2.16960200
C	2.29133400	2.92141100	1.20065400
H	6.17850400	-0.06747400	3.59824300
H	6.96914600	1.36347500	2.92937600
H	7.20119300	-0.20430900	2.14452400
C	3.89635700	1.83834400	3.69621500
H	1.47162300	2.57499800	1.84712100
H	2.64949100	3.87434200	1.62010200
H	1.86621000	3.12138600	0.21054300
H	4.05460800	0.98750900	4.37474000
H	4.57884200	2.64126200	4.01672200
H	2.87044900	2.20215400	3.83566500
C	0.49796900	0.11592800	2.95981000
O	-0.49228100	0.24449700	3.52648500

O 1.65707900 0.05642300 2.70050400

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**Zr<sup>+</sup>/As-Pro**

Free energy (M06-2X-D3/def2-TZVP) = -4059.591832

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C	0.04427500	-0.42159000	-0.64677300
C	0.17234900	-0.56932900	-1.98538300
C	0.31139900	0.63700900	-2.88088800
H	1.27026100	0.59980500	-3.42186100
H	0.24983200	1.58357100	-2.32357300
H	-0.47420500	0.63409700	-3.65233800
C	0.25123400	-1.85677600	-2.74569800
C	0.46950500	-4.20234900	-4.27230100
C	1.35911900	-2.69966600	-2.60210200
C	-0.73487000	-2.19154300	-3.68750500
C	-0.63756000	-3.36523500	-4.42962300
C	1.47040100	-3.86198200	-3.36604700
H	2.14239900	-2.44364900	-1.88693200
H	-1.58882700	-1.52578000	-3.83995800
H	-1.41995900	-3.62118300	-5.14514300
H	2.34326600	-4.50489200	-3.24400500
H	0.55398000	-5.11288800	-4.86678600
As	-0.30311300	-1.94080800	0.48566200
C	0.72382000	-3.56634000	0.54419600
C	2.12163400	-5.96648100	0.66453000
C	1.74191900	-3.72739700	1.48893900
C	0.37889600	-4.61300000	-0.31860300
C	1.08479700	-5.81095700	-0.25776300
C	2.44516300	-4.93099000	1.53970700
H	1.96035400	-2.94331400	2.21479900
H	-0.43271900	-4.49435200	-1.04129000
H	0.82042600	-6.62804300	-0.93019500
H	3.23633700	-5.06271100	2.27839200
H	2.67002300	-6.90826800	0.71150700
C	-2.11868900	-2.55225100	0.34625300
C	-4.74266300	-3.45651100	0.24319800
C	-2.85494900	-2.39727900	-0.82894000

C	-2.67925500	-3.16925300	1.47054400
C	-3.99805100	-3.61502100	1.41365300
C	-4.17174100	-2.85512700	-0.87802500
H	-2.40499400	-1.92252400	-1.70114200
H	-2.09584800	-3.28815900	2.38759500
H	-4.44595500	-4.08836700	2.28810300
H	-4.75226600	-2.74007700	-1.79413800
H	-5.77451100	-3.80807800	0.20481400
Zr	0.21384800	1.54738800	0.65310400
C	2.66858300	1.04503000	0.10900600
C	2.53708300	1.08055300	1.52257000
C	2.19754900	2.41153300	1.90986000
C	2.16387300	3.20981800	0.73004600
C	2.40586100	2.36017400	-0.38687700
C	-1.29946300	3.28985500	-0.38088100
C	-1.16823900	3.65069900	0.99810200
C	-1.76390200	2.62316500	1.77818000
C	-2.31413800	1.65571200	0.89152900
C	-2.04034400	2.06795800	-0.44149900
C	-2.62752200	1.44751400	-1.67450500
H	-2.23924100	1.91678800	-2.58656600
H	-3.71883300	1.59148900	-1.67068300
H	-2.43312000	0.36760800	-1.72755500
C	-3.16944300	0.50504200	1.32237700
H	-2.67831600	-0.11129000	2.09086900
H	-3.44141600	-0.14159600	0.47925400
H	-4.10155900	0.88424300	1.76963200
C	-1.90312600	2.59990600	3.27130600
H	-1.18813400	3.27757700	3.75678800
H	-1.74114800	1.58825900	3.66900000
H	-2.91504200	2.92044100	3.56506500
C	-0.78412900	4.99497700	1.54199800
H	-0.29612900	5.62468000	0.79139200
H	-0.12980900	4.92805700	2.42125700
H	-1.70026400	5.51538700	1.86206000
C	-0.95758000	4.16622000	-1.55330700
H	-0.09748500	4.81517000	-1.34267100
H	-1.80670000	4.82162300	-1.80255000



H	-0.72368500	3.58328500	-2.45538500
C	2.64304700	2.86347900	-1.78299300
H	3.54513000	3.49517000	-1.80114000
H	1.81180200	3.47797100	-2.15945700
H	2.80455900	2.04075900	-2.48927900
C	2.22444800	4.70495600	0.65014800
H	3.27210700	4.99441600	0.46802000
H	1.90921300	5.19183300	1.57842000
H	1.63387900	5.11205000	-0.18056100
C	2.02594100	2.86962700	3.33017700
H	2.99844800	2.90856100	3.84467900
H	1.38247500	2.18247700	3.90031300
H	1.58586000	3.87400400	3.38295300
C	2.82160400	-0.04319600	2.46941100
H	2.70081000	-1.01819600	1.97778700
H	2.16322000	-0.01852200	3.34813700
H	3.86306900	0.01304100	2.82245100
C	3.20266800	-0.10810300	-0.68433500
H	4.30273600	-0.06443400	-0.70957600
H	2.84169500	-0.09861500	-1.72095100
H	2.91943800	-1.07309300	-0.23896400
C	-0.16605600	-1.10423800	2.31198600
O	-0.11195500	0.17614600	2.21879100
O	-0.17057000	-1.80035800	3.28619200

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### Zr<sup>+</sup>/Sb-Rea

Free energy (M06-2X-D3/def2-TZVP) = -1875.732149

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Zr	-0.00238500	0.38696400	0.95748800
C	2.18403100	0.54462200	-0.27921300
C	1.30019700	1.40406600	-0.98370600
C	0.25125400	0.60123700	-1.53332600
C	0.54580900	-0.76621900	-1.24800400
C	1.73706300	-0.80268000	-0.46988200
C	-0.00514500	2.72960300	1.87749400
C	0.01579500	1.85327400	2.99841200
C	-1.23610300	1.16988400	3.04804500

C	-2.01693100	1.60012700	1.93979400
C	-1.25884300	2.55767300	1.20584400
C	2.57980000	-2.00970100	-0.17144400
H	3.03017800	-1.97287000	0.83060200
H	3.40463800	-2.05386800	-0.90041200
H	2.01379300	-2.94490700	-0.25615800
C	-0.15681000	-1.94275500	-1.85046800
H	-1.24139500	-1.78480800	-1.89912600
H	0.02896500	-2.85925400	-1.27767100
H	0.20653100	-2.10631800	-2.87736500
C	-0.80234300	1.08260000	-2.48930500
H	-0.43618800	0.99507400	-3.52478700
H	-1.05771400	2.13654300	-2.32143200
H	-1.72412800	0.48862700	-2.42304500
C	1.57452000	2.82789900	-1.36235200
H	1.99657200	2.83760700	-2.38000700
H	2.30817000	3.30183300	-0.70154000
H	0.67090300	3.44815800	-1.38697800
C	3.46596300	0.92140500	0.40743400
H	3.50496400	1.99148600	0.64936000
H	4.32853900	0.70041800	-0.24097200
H	3.61216100	0.35334600	1.33846500
C	-1.82298200	3.40548100	0.10236500
H	-2.46684800	4.18898200	0.53142800
H	-2.44366900	2.82069500	-0.59058700
H	-1.04271700	3.91057300	-0.47862300
C	-3.46438500	1.26910500	1.74765600
H	-3.67253000	0.21974900	1.99727900
H	-3.79970200	1.45460400	0.71958300
H	-4.07616800	1.89945100	2.41304500
C	-1.78103100	0.33678500	4.16705500
H	-2.28667100	-0.56783500	3.80002900
H	-2.52969700	0.92208900	4.72336700
H	-1.00639200	0.03497100	4.87956500
C	1.12577800	1.79533100	4.00880800
H	2.11792100	1.77819000	3.53375400
H	1.04508200	0.90930400	4.65084700
H	1.09471000	2.68300000	4.66004700

C	1.01189900	3.80997100	1.65113000
H	2.04008800	3.42445300	1.59703100
H	0.97839700	4.51662700	2.49484300
H	0.80907200	4.37986300	0.73836900
C	-1.39155800	-1.33066300	1.11967500
C	-2.54890200	-1.89328100	0.72028000
Sb	0.21096500	-2.13416900	2.46171400
C	-0.25714200	-2.83806600	4.43525800
C	-0.61438500	-3.89263500	7.00190100
C	0.20679200	-2.14160800	5.55680900
C	-0.85806900	-4.09112600	4.60345800
C	-1.04448800	-4.60910300	5.88473000
C	0.02119400	-2.66295900	6.83742000
H	0.73535100	-1.19218600	5.44264700
H	-1.17670100	-4.67354800	3.73637900
H	-1.51901000	-5.58392600	6.00831300
H	0.38453600	-2.11181900	7.70577900
H	-0.75912300	-4.30227100	8.00245200
C	0.63617000	-4.06446800	1.65069600
C	1.26585200	-6.62338400	0.71709400
C	-0.14450200	-4.65964800	0.65707800
C	1.72827400	-4.76020900	2.18526400
C	2.04242500	-6.03453000	1.71633400
C	0.17181900	-5.93832100	0.19231500
H	-1.00864200	-4.13652500	0.24777300
H	2.34107100	-4.31742000	2.97571200
H	2.89572100	-6.57036800	2.13440100
H	-0.44705400	-6.40043700	-0.57830800
H	1.51202700	-7.62150400	0.35251200
C	-3.17861000	-3.12683100	1.27703000
C	-4.40835700	-5.43314200	2.31483400
C	-3.68312800	-4.11990300	0.42049300
C	-3.32414200	-3.30121600	2.65731000
C	-3.93941500	-4.44233200	3.17340600
C	-4.27545600	-5.26904200	0.93448600
H	-3.59045700	-4.00583700	-0.66145700
H	-2.96574700	-2.52677200	3.33762000
H	-4.05072700	-4.55149900	4.25356600

H	-4.64373800	-6.03865600	0.25485400
H	-4.88637200	-6.32731900	2.71657200
C	-3.35461900	-1.23786800	-0.38535800
H	-2.88744400	-0.29807000	-0.70894200
H	-4.38213800	-1.03423400	-0.04776500
H	-3.43952000	-1.90311200	-1.25875400

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**Zr<sup>+</sup>/Sb-TS**

Free energy (M06-2X-D3/def2-TZVP) = -2064.099866

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Sb	-0.29533800	-0.12397800	0.36099500
C	-1.84231500	-1.06889200	-0.77838900
C	-0.60714400	1.90872200	-0.24952400
C	-2.53212100	-0.37774800	-1.77915300
C	-2.20161300	-2.38647700	-0.47046100
C	1.69637400	-0.57878600	-0.46550800
C	-0.17154900	2.40802500	-1.48140500
C	-1.24147400	2.77068000	0.65300900
C	-3.55823500	-1.01169500	-2.47982800
H	-2.27014100	0.65386200	-2.02515300
C	-3.22038500	-3.02052900	-1.18021000
H	-1.69460300	-2.93094200	0.33225400
C	1.88324800	-0.88739000	-1.76938700
Zr	3.25965300	-0.62087400	1.20221200
C	-0.35470700	3.75380100	-1.80153100
H	0.30923300	1.74214200	-2.19888600
C	-1.42468300	4.11691300	0.33327900
H	-1.59089800	2.40122300	1.62170700
C	-3.89850600	-2.33198600	-2.18678700
H	-4.09199100	-0.46983100	-3.26215300
H	-3.49551400	-4.04809200	-0.93753300
C	3.26426800	-1.17084900	-2.32033900
C	0.84954000	-1.04445700	-2.84837700
C	-0.97565200	4.61019500	-0.89141300
H	-0.01307200	4.13474100	-2.76537200
H	-1.91865900	4.78181200	1.04333500
H	-4.70199400	-2.82382500	-2.73705100

H	3.48749900	-0.49703700	-3.16238300
H	3.30791200	-2.19167800	-2.73283600
H	4.05396600	-1.05902100	-1.56243900
C	0.07401000	-2.20721100	-2.93659800
C	0.73722500	-0.08675300	-3.86471200
H	-1.11556800	5.66308900	-1.14001600
C	-0.81671300	-2.39116100	-3.99180000
H	0.16105600	-2.97417000	-2.16661300
C	-0.16997100	-0.25782200	-4.90987100
H	1.37565800	0.80092000	-3.84438200
C	-0.94943300	-1.41177700	-4.97510900
H	-1.41652900	-3.30129000	-4.03847700
H	-0.25511500	0.50575100	-5.68431100
H	-1.65171700	-1.55206000	-5.79788300
C	3.71472900	-2.43954100	2.87569500
C	3.86439300	-2.12229800	4.33630600
C	2.49294200	-2.79581000	2.22241500
C	4.76279200	-2.56753400	1.92413500
H	3.04930900	-1.48194500	4.70390700
H	3.85121100	-3.04442700	4.93759400
H	4.81368400	-1.61047100	4.54345900
C	1.16133400	-2.97969400	2.88853600
C	2.78423800	-3.11624400	0.86864800
C	6.23166900	-2.65710000	2.20527100
C	4.18698900	-2.94348600	0.67376300
H	0.32587700	-2.60726600	2.27599700
H	0.97607500	-4.05065800	3.06464700
H	1.12052400	-2.48451300	3.86850700
C	1.82065800	-3.73330000	-0.09457200
H	6.84258400	-2.20232700	1.41477600
H	6.50685000	-3.72349800	2.24675200
H	6.50892400	-2.21178300	3.16601100
C	4.99619800	-3.38384300	-0.51307700
H	0.80737000	-3.32354400	0.02522000
H	1.76766100	-4.82004100	0.07747300
H	2.12304300	-3.56765200	-1.13608200
H	5.71180200	-2.61918600	-0.84838800
H	5.57943200	-4.27882500	-0.24541500

H	4.35824600	-3.64709900	-1.36404300
C	5.23263800	0.72208700	0.39773000
C	6.33108600	0.23512600	-0.50529300
C	5.30217600	0.76388100	1.82810800
C	4.08146500	1.47274400	-0.00424100
H	6.86148000	-0.62628100	-0.07716000
H	7.07562200	1.03191800	-0.65821500
H	5.95872700	-0.05566700	-1.49673300
C	6.49092100	0.44592600	2.68414900
C	4.16678100	1.46461200	2.30154600
C	3.74480900	1.91816700	-1.39522600
C	3.41423500	1.90832600	1.17318500
H	6.21621300	-0.05138200	3.62425600
H	6.98270700	1.39342600	2.95657600
H	7.23318700	-0.16831100	2.16514000
C	3.89822500	1.81285600	3.73602900
H	2.69075700	1.73070400	-1.64240200
H	3.92643800	3.00036800	-1.48295600
H	4.37391300	1.41820800	-2.14108300
C	2.23869000	2.83573300	1.23568900
H	4.05637200	0.95710000	4.40869700
H	4.57890800	2.61432300	4.06355900
H	2.87137300	2.17383900	3.87683700
H	1.43129800	2.46127200	1.88378400
H	2.55270600	3.80605400	1.65048000
H	1.80851300	3.01378300	0.24289900
C	0.56664200	0.04303400	3.08756000
O	-0.35263200	0.17720500	3.76742400
O	1.71484100	-0.04073900	2.76722600

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**Zr<sup>+</sup>/Sb-Pro**

Free energy (M06-2X-D3/def2-TZVP) = -2064.118059

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C	0.12281300	-0.25948800	-0.69644200
C	0.16402000	-0.40662900	-2.04071800
C	0.44595000	0.77174700	-2.94435600
H	1.40256500	0.61649200	-3.46919900

H	0.49538200	1.72070000	-2.38970600
H	-0.31901700	0.86237400	-3.72851400
C	-0.03721500	-1.69000700	-2.78083400
C	-0.45955800	-4.11747700	-4.12896000
C	0.79094400	-2.79439500	-2.54215100
C	-1.06072300	-1.80738800	-3.73377300
C	-1.27292600	-3.01368500	-4.39722900
C	0.57682400	-4.00441200	-3.20355000
H	1.62773300	-2.69902800	-1.84844100
H	-1.71081000	-0.95501700	-3.94333900
H	-2.08006700	-3.09451800	-5.12657200
H	1.23172200	-4.85328500	-3.00114200
H	-0.62680600	-5.06008000	-4.65149900
Sb	-0.35289200	-1.96888000	0.51728400
C	0.93039600	-3.66056100	0.72498300
C	2.46519100	-5.96959500	1.06414700
C	2.32237800	-3.60464800	0.59096300
C	0.30851000	-4.87629900	1.03117000
C	1.08017400	-6.02671600	1.20178300
C	3.08597800	-4.75792900	0.75812000
H	2.82979700	-2.66971800	0.34872100
H	-0.77672800	-4.94183200	1.13478500
H	0.59069800	-6.97131500	1.44185800
H	4.17008300	-4.70835000	0.64973700
H	3.06478100	-6.87111000	1.19577800
C	-2.22691300	-2.91236300	0.23218900
C	-4.66938900	-4.21561500	-0.04820000
C	-2.53313900	-3.55748300	-0.97117600
C	-3.12767000	-2.93520900	1.30458100
C	-4.35102100	-3.58931700	1.15686600
C	-3.76143700	-4.20376300	-1.10728900
H	-1.82268900	-3.57275900	-1.79957400
H	-2.87673300	-2.46068500	2.25715000
H	-5.05428500	-3.61245900	1.99024200
H	-4.00487600	-4.70426600	-2.04556100
H	-5.62805200	-4.72409700	-0.15950700
Zr	0.30640100	1.65389100	0.64732400
C	2.74796500	1.18038300	0.04233200

C	2.60787300	1.05860700	1.45172500
C	2.29903200	2.34687100	1.98355900
C	2.26875600	3.26816800	0.89759800
C	2.50477800	2.54198900	-0.30735700
C	-1.13420000	3.49601600	-0.36372900
C	-1.11524400	3.71152000	1.05314700
C	-1.78215200	2.61911100	1.67374300
C	-2.22765900	1.73842000	0.65114800
C	-1.85205900	2.28942300	-0.60642500
C	-2.36747100	1.80155900	-1.92625500
H	-1.90121300	2.32681400	-2.76809500
H	-3.45083900	1.99184400	-1.97897300
H	-2.21692100	0.72016000	-2.05518900
C	-3.07683000	0.52003300	0.83806300
H	-2.86163900	0.00667500	1.78645300
H	-2.95442900	-0.19340100	0.00989200
H	-4.14331400	0.79563300	0.86541900
C	-2.03649800	2.47300600	3.14475500
H	-1.23294800	2.92734000	3.74111400
H	-2.11216600	1.41853500	3.44097800
H	-2.97691600	2.97610300	3.41929600
C	-0.75691800	4.98096700	1.76952600
H	-0.21900000	5.68377600	1.12496300
H	-0.15485800	4.80544200	2.67185600
H	-1.68440600	5.47706100	2.09529900
C	-0.71741600	4.48207500	-1.41761400
H	0.09488900	5.13531200	-1.07384600
H	-1.56451100	5.13185800	-1.68763100
H	-0.38304000	3.98496800	-2.33961000
C	2.74452700	3.17705600	-1.64785500
H	3.69377300	3.73561700	-1.63273800
H	1.95488000	3.89018900	-1.92282800
H	2.81753600	2.42741600	-2.44533700
C	2.32583800	4.76289200	0.98867700
H	3.37844400	5.07472700	0.89306800
H	1.95980300	5.14234800	1.94838400
H	1.77232200	5.25771700	0.18057400
C	2.10822800	2.65973600	3.44049100



H	3.07369500	2.65730400	3.96896300
H	1.45991700	1.91691500	3.92828000
H	1.65824900	3.65107900	3.58390400
C	2.82973900	-0.18582400	2.25619200
H	2.38880200	-1.07450200	1.77869700
H	2.38676100	-0.10019700	3.25627200
H	3.90606000	-0.38524200	2.37416600
C	3.27174200	0.11650400	-0.87174900
H	4.37280900	0.13739200	-0.87612100
H	2.92862500	0.24933100	-1.90465000
H	2.95595100	-0.88258200	-0.54776700
C	-0.49533400	-0.85740400	2.43207600
O	-0.05332300	0.33558500	2.24236100
O	-0.95627400	-1.35183900	3.41885100

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**Zr<sup>+</sup>/Bi-Rea**

Free energy (M06-2X-D3/def2-TZVP) = -1850.038212

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Zr	-0.03463300	0.42497500	0.90897900
C	2.11934800	0.55186000	-0.38874000
C	1.22805200	1.43969700	-1.04821800
C	0.14892300	0.66291400	-1.58006500
C	0.42425300	-0.71291400	-1.32013000
C	1.63594600	-0.78256100	-0.57917000
C	0.08753000	2.71459200	1.95192200
C	-0.06643300	1.78404900	3.01914600
C	-1.36858500	1.20649500	2.92285800
C	-2.00504600	1.75721200	1.77605000
C	-1.11481500	2.69706500	1.17822400
C	2.45562800	-2.01304500	-0.31723100
H	2.94195300	-2.00001200	0.66958600
H	3.25859300	-2.07146200	-1.06938100
H	1.86361000	-2.93279200	-0.39432600
C	-0.32083400	-1.86667100	-1.91461200
H	-1.38512700	-1.63299200	-2.04034800
H	-0.23923900	-2.76602200	-1.29167100
H	0.09314600	-2.10351800	-2.90781600

C	-0.95199100	1.16402900	-2.47533400
H	-0.93450200	0.62243300	-3.43260000
H	-0.82439700	2.23035200	-2.70030100
H	-1.95772200	1.02688300	-2.04805500
C	1.50130600	2.87808100	-1.37074500
H	1.89596000	2.93894100	-2.39739900
H	2.25708700	3.31215100	-0.70676200
H	0.60184600	3.50217200	-1.33142200
C	3.43981700	0.88501100	0.24655300
H	3.56802100	1.96552200	0.38612100
H	4.26692500	0.53709900	-0.39192800
H	3.56562700	0.39584000	1.22488100
C	-1.53247400	3.66562200	0.10680500
H	-2.46230900	4.16596200	0.41505700
H	-1.73065800	3.18456200	-0.86112300
H	-0.77962300	4.44786900	-0.04547100
C	-3.43713300	1.55049400	1.38812400
H	-3.77473500	0.53391800	1.62803300
H	-3.60006500	1.72367300	0.31555400
H	-4.08068000	2.25697400	1.93685000
C	-2.05918500	0.34071200	3.93127900
H	-2.77695900	-0.33267100	3.44442800
H	-2.61980100	0.97176900	4.63851900
H	-1.36391300	-0.26749300	4.52355500
C	0.93304300	1.60297200	4.12567300
H	1.95908900	1.47753200	3.74858300
H	0.69185100	0.73307000	4.74818000
H	0.93458600	2.48758900	4.78170900
C	1.23915300	3.67217800	1.84495600
H	2.21030800	3.16179200	1.76243000
H	1.28174400	4.29867300	2.74907900
H	1.13284100	4.34140000	0.98418400
C	-1.40992300	-1.25647300	1.06998000
C	-2.53955300	-1.91259700	0.75679800
Bi	0.39354600	-2.06143600	2.53826100
C	-0.21893600	-2.86751100	4.53749300
C	-0.69766400	-3.98785400	7.05277400
C	0.01702200	-2.12205700	5.69620100

C	-0.66221500	-4.18883300	4.64066700
C	-0.90659800	-4.74222700	5.89823100
C	-0.23006800	-2.67872900	6.95211000
H	0.40938000	-1.10427200	5.64249300
H	-0.82363600	-4.79475200	3.74647900
H	-1.25751400	-5.77290000	5.97302000
H	-0.04647100	-2.08930100	7.85143000
H	-0.88801600	-4.42543000	8.03361200
C	0.73935100	-4.08783100	1.68419600
C	1.28957500	-6.65488700	0.73645600
C	-0.06963100	-4.65382400	0.69901700
C	1.82011600	-4.80759600	2.20318100
C	2.09519900	-6.08914500	1.72535700
C	0.20698300	-5.93964900	0.22760300
H	-0.92500500	-4.10752100	0.30231100
H	2.45462000	-4.38571900	2.98820700
H	2.94021400	-6.64788700	2.13026200
H	-0.43353100	-6.38285200	-0.53661700
H	1.50422200	-7.65827700	0.36654900
C	-3.06806800	-3.16183200	1.38276100
C	-4.12739000	-5.49557700	2.54119000
C	-3.55675100	-4.20635200	0.57923500
C	-3.13938500	-3.30186300	2.77227800
C	-3.67196700	-4.45643600	3.34779700
C	-4.06396800	-5.36797000	1.15198600
H	-3.51946500	-4.12166800	-0.50855700
H	-2.78932900	-2.49211100	3.41421300
H	-3.72717200	-4.53763100	4.43455800
H	-4.42157600	-6.17562800	0.51187400
H	-4.54126600	-6.39935300	2.98996600
C	-3.42983600	-1.35314900	-0.34017200
H	-3.03033000	-0.40997900	-0.73259900
H	-4.45019700	-1.18619500	0.03735300
H	-3.51531800	-2.06623000	-1.17410900

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**Zr<sup>+</sup>/Bi-TS**

Free energy (M06-2X-D3/def2-TZVP) = -2038.407152

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Bi	-0.23259500	-0.07937300	0.32213900
C	-1.91089900	-1.10302600	-0.72650400
C	-0.64091800	2.01193700	-0.33483600
C	-2.66467300	-0.40013200	-1.66628500
C	-2.20666100	-2.43495600	-0.42699900
C	1.85328400	-0.61580100	-0.52309700
C	-0.25881600	2.50927500	-1.58230300
C	-1.26560100	2.85105200	0.59239500
C	-3.71266100	-1.04659200	-2.32424500
H	-2.43989200	0.64316000	-1.90086400
C	-3.25155900	-3.07565500	-1.09291400
H	-1.63472300	-2.98739400	0.32429400
C	1.97604400	-0.90600500	-1.83398200
Zr	3.30975000	-0.64562900	1.22635100
C	-0.49394500	3.84909900	-1.89758300
H	0.21728300	1.85606300	-2.31453300
C	-1.49915200	4.19000100	0.27296000
H	-1.56871100	2.47734400	1.57515100
C	-4.00239300	-2.38107500	-2.04266500
H	-4.30310900	-0.50184500	-3.06261500
H	-3.48636200	-4.11587700	-0.86202900
C	3.33149800	-1.22066100	-2.43187600
C	0.88987800	-1.01131600	-2.86418700
C	-1.10918000	4.68941000	-0.96939600
H	-0.19614500	4.23676000	-2.87313900
H	-1.98631300	4.84359500	0.99806400
H	-4.82291600	-2.88145800	-2.55883100
H	3.54356300	-0.54460300	-3.27496700
H	3.33265400	-2.23926600	-2.85320500
H	4.14199500	-1.13606200	-1.69411500
C	0.06648700	-2.14228800	-2.92227600
C	0.76001700	-0.03387000	-3.85979700
H	-1.28957500	5.73633500	-1.21677500
C	-0.88925800	-2.27586000	-3.92768000
H	0.17190000	-2.92530700	-2.17044400
C	-0.21023400	-0.15487500	-4.85374200
H	1.43311200	0.82803400	-3.86069300

C	-1.03782200	-1.27707000	-4.88843400
H	-1.52613500	-3.16147300	-3.95238200
H	-0.30879200	0.62212000	-5.61313000
H	-1.79005400	-1.37755400	-5.67195100
C	3.71243700	-2.48107100	2.88123800
C	3.80630900	-2.15942800	4.34557600
C	2.51503900	-2.83419400	2.18428900
C	4.79260800	-2.59382500	1.96264800
H	2.98300900	-1.50786900	4.67318800
H	3.75904400	-3.07817500	4.95021400
H	4.75177000	-1.65609200	4.58836500
C	1.15900900	-3.00908900	2.80074100
C	2.85379800	-3.14235400	0.83847000
C	6.25217800	-2.67312300	2.29177600
C	4.26009300	-2.96014500	0.69029300
H	0.96977100	-4.07475900	3.00255600
H	0.34875800	-2.66312800	2.13966200
H	1.07052400	-2.47668800	3.75721700
C	1.92546500	-3.75659000	-0.16109200
H	6.88437700	-2.21275400	1.52154700
H	6.53464800	-3.73714800	2.34271400
H	6.49431100	-2.22519100	3.26087300
C	5.10462800	-3.37424500	-0.48126100
H	0.90075800	-3.37344100	-0.05111300
H	1.89291900	-4.84790900	-0.01524900
H	2.24369000	-3.56020300	-1.19244200
H	5.83374400	-2.60428600	-0.77220200
H	5.67575100	-4.27952500	-0.22186400
H	4.49254400	-3.60914500	-1.35944200
C	4.17756200	1.45459800	2.31334800
C	3.85734200	1.80376100	3.73673100
C	3.45435800	1.87912500	1.16088400
C	5.32843100	0.75079300	1.87851600
H	4.04452700	0.96323000	4.42073200
H	4.48593900	2.64399700	4.07133800
H	2.80849800	2.10617400	3.85014300
C	2.26514100	2.79034400	1.17701300
C	4.15533300	1.43154300	0.00606100

C	6.48957100	0.43774400	2.77404700
C	5.29906000	0.69509500	0.44688800
H	2.55872200	3.78371400	1.55026500
H	1.46317300	2.43222800	1.84164000
H	1.83836800	2.92109600	0.17522000
C	3.85782400	1.86209400	-1.39828200
H	6.18472800	-0.06184900	3.70373700
H	6.96943000	1.38603100	3.06380700
H	7.25025200	-0.17472100	2.28008400
C	6.41689300	0.19974100	-0.42703900
H	2.79520400	1.73798000	-1.64929500
H	4.11230600	2.92719600	-1.51251000
H	4.45494600	1.30206500	-2.12760000
H	6.05870300	-0.14736900	-1.40597400
H	7.13916400	1.00962100	-0.61422900
H	6.96929600	-0.62512000	0.04275000
C	0.50622400	0.04482000	2.83480800
O	-0.36091500	0.22455900	3.59057100
O	1.70499200	-0.08551000	2.65276400

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**Zr<sup>+</sup>/Bi-Prod**

Free energy (M06-2X-D3/def2-TZVP) = -2038.410247

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C	0.11176000	-0.17521800	-0.67884300
C	0.14331000	-0.39019200	-2.00840500
C	0.41774000	0.75845800	-2.95629000
H	1.37727600	0.59007100	-3.47207600
H	0.45989400	1.72547900	-2.43460700
H	-0.34853600	0.81350200	-3.74282600
C	-0.04564600	-1.70020400	-2.70426300
C	-0.41713600	-4.15683500	-4.01284600
C	0.81882100	-2.77527800	-2.46380700
C	-1.08232100	-1.86187600	-3.63616300
C	-1.26828000	-3.08201500	-4.28170600
C	0.62897900	-4.00057100	-3.10480800
H	1.66274500	-2.64748800	-1.78384600
H	-1.75947900	-1.03093600	-3.84649600

H	-2.08371600	-3.19634900	-4.99724500
H	1.31130500	-4.82704800	-2.89946300
H	-0.56330800	-5.11074700	-4.52105800
Bi	-0.34077600	-1.97971400	0.65679500
C	1.00007400	-3.76745500	0.68335700
C	2.55873200	-6.07559000	0.66714700
C	2.39202000	-3.66402800	0.73254600
C	0.38240700	-5.01797200	0.63409200
C	1.16910600	-6.17219300	0.62737300
C	3.16937100	-4.82241900	0.72165000
H	2.89257500	-2.69522600	0.77859200
H	-0.70542400	-5.10986200	0.59800200
H	0.68753000	-7.15036200	0.59129200
H	4.25664100	-4.74279400	0.75953200
H	3.16940100	-6.97923200	0.66036800
C	-2.29117300	-2.96436500	0.29454000
C	-4.75195800	-4.19842000	-0.06949500
C	-2.55913000	-3.61620600	-0.91070100
C	-3.23204900	-2.93922000	1.32738700
C	-4.46790800	-3.55998400	1.13779600
C	-3.79967700	-4.23088300	-1.08850400
H	-1.81305000	-3.66263400	-1.70642200
H	-3.00993400	-2.45237600	2.28127600
H	-5.20712800	-3.54810900	1.93987300
H	-4.01780500	-4.74012300	-2.02854100
H	-5.71933200	-4.68132200	-0.21381200
Zr	0.29572200	1.68782600	0.68096800
C	2.72897500	1.15961700	0.09178600
C	2.58880500	1.09122900	1.50496300
C	2.29743900	2.40169700	1.99175700
C	2.27604700	3.28282200	0.87316900
C	2.50244600	2.51082800	-0.30549900
C	-1.13859800	3.50380800	-0.37398000
C	-1.11045100	3.76128200	1.03597700
C	-1.77888000	2.69169900	1.69212700
C	-2.23079100	1.77971600	0.69872300
C	-1.86413700	2.29459800	-0.57754000
C	-2.39453300	1.77625700	-1.87938400

H	-1.92884400	2.27350300	-2.73828400
H	-3.47594900	1.97827500	-1.92896500
H	-2.25590600	0.69064800	-1.98052300
C	-3.07229000	0.56146100	0.92397200
H	-2.85656500	0.08084200	1.88966300
H	-2.94087400	-0.17821500	0.12033100
H	-4.14110500	0.82837700	0.93932800
C	-2.02868800	2.60062100	3.16830600
H	-1.19121100	3.01315500	3.74851000
H	-2.17872000	1.56314100	3.49365700
H	-2.92954900	3.17511500	3.43524600
C	-0.73774200	5.04792600	1.71270900
H	-0.19265200	5.72473100	1.04661100
H	-0.13666100	4.89241100	2.61947600
H	-1.65912800	5.56420000	2.02434900
C	-0.72266800	4.45827000	-1.45689700
H	0.10117000	5.11012200	-1.13875700
H	-1.56542600	5.11121200	-1.73275200
H	-0.40556400	3.93463200	-2.37005100
C	2.74559500	3.09653600	-1.66762000
H	3.69392000	3.65680400	-1.66869200
H	1.95612300	3.79828700	-1.97184400
H	2.82234600	2.31793300	-2.43609800
C	2.34542000	4.77933100	0.91050700
H	3.39998500	5.07984700	0.80148000
H	1.98432500	5.19528900	1.85692900
H	1.79341100	5.24895900	0.08643700
C	2.12253400	2.77297000	3.43694200
H	3.09448100	2.79800000	3.95287800
H	1.48453900	2.04854600	3.96397400
H	1.66868200	3.76701000	3.54530500
C	2.80572000	-0.12747100	2.34994300
H	2.30160500	-1.01582800	1.93840900
H	2.42595700	0.01742700	3.36902700
H	3.87819300	-0.36733600	2.41660300
C	3.23235300	0.05071500	-0.77980800
H	4.33372700	0.05042000	-0.78312300
H	2.89059600	0.15023600	-1.81733000



H	2.89763800	-0.93035600	-0.41736900
C	-0.49539100	-0.73189700	2.65203700
O	-0.07220800	0.42459300	2.35051300
O	-0.94632900	-1.20877500	3.64051300

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CO2

Free energy (M06-2X-D3/def2-TZVP) = -188.379677 Hartree

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O	-0.28202800	0.00000000	0.98993800
C	0.38551800	0.00000000	0.04590800
O	1.05306300	0.00000000	-0.89812100