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c1

C1

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Н

Н

Н

C

C

Н

Н

Н

Н

Н

Н

Н

Н

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C1

Dp3M

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Βi	-0.96369700	5.09499800	0.09632100
Βi	5.24011300	-1.77701300	-0.10615900

Dp2Ga SCF Energy = -5929.89202225 auC 1.71061800 2.87020000 0.75165100 C 0.49124500 3.21309700 1.32183100 C -0.64237400 3.48614200 0.56927700 C -0.56065800 3.38820200 -0.82202700 C 0.67032300 3.09264500 -1.39353200 C 1.81074200 2.84577200 -0.64195500 Н 0.41778200 3.25416500 2.40567200 Н 0.74067800 3.03696100 -2.47689800 C -1.32066500 3.10459800 2.50140500 C 3.27184400 0.99580800 -1.63718500 Н 3.93762100 2.84343700 -0.70465700 Н 2.93021800 0.80822300 -2.65753100 C 2.86398600 2.50029100 1.64191700 C 3.52213300 1.13361300 1.33193800 Н 3.27293300 3.64001200 1.60582100 Н 3.88529200 0.70494100 2.26908000 C 2.51071500 0.07340500 -0.72998300 C 1.65816700 -0.88092900 -1.27955800 C 2.60228200 0.15243800 0.66721500 C -0.51200800 0.84090000 -1.70405300 Н -0.96736500 -2.36172400 1.61012100 C 1.77344000 -0.66433100 1.43151600 C 0.86892700 -1.56383700 0.87685400 Н 1.82196400 -0.57723700 2.51362500 C -0.07843400 -2.68531300 -1.17676900 C -1.45592300 -2.09446200 -1.56167600 Н -0.21401900 -3.54946100 -0.52510400 Н 0.39662500 -3.06413000 -2.08462200 Н -2.20647600 -2.89117500 -1.53020400 Н -1.41517100 -1.74691200 -2.59624600 C -0.04745100 -2.34094800 1.77855200 C -1.54947900 -2.25943300 1.41501000 Н 0.09282500 -1.96473300 2.79422500 Н 0.24924800 -3.39542900 1.80250000 Н -1.84956000 -3.11871200 0.81575800 Н -2.32756100 -2.13082600 2.33745300 -1.90407400 C -0.93942800 -0.71362700 C -1.92566200 -1.00288800 0.68693300 C -2.28436300 0.25385800 -1.32310500 -2.24157400 C 0.15198900 1.39713300 C -2.60944500 1.40259100 -0.60970000 Н -2.29920400 0.29694700 -2.40876300 C -2.54711000 1.36263400 0.78467400 Н -2.22424400 0.10911800 2.48281700 C -2.97747000 2.66211400 -1.33612000 C -1.76456100 3.55154100 -1.70749400 Н 3.22938400 -0.72829400 -3.68424500

Dp2M Н -3.51004300 -2.25441500 2.40350000 Н -2.09267100 4.59692000 -1.72326600 Н -1.45679200 3.31728100 -2.72887200 C -2.78489400 2.57895000 1.63291100 C -1.93899600 3.81814800 1.24901600 Н -2.56411000 2.30704900 2.66734800 Н -3.84568400 2.85358000 1.61209100 Н -2.52228700 4.48130100 0.60782400 Н -1.73387600 4.38536200 2.16006200 Н 3.17772600 3.05535500 -2.25959100 Н 2.49629000 2.49065600 2.67041900 Н 4.33677700 0.74133400 -1.61446500 Н 4.40618200 1.26440700 0.70802900 C1-4.65088100 -3.27863600 -0.21721000 C15.92265000 -1.12946600 -0.26003100 Ga -4.85303200 -1.02133400 0.01059100 Ga 4.06803300 -2.40794900 0.07614700 Dp2In SCF Energy = -2460.99995119 au C -1.61531300 3.15163100 -0.75154800 C -0.38270500 -1.32385600 3.43919800 C 0.76295800 3.66229500 -0.57308700 C 0.67866300 3.56968400 0.81840600 C -0.56342900 3.32980000 1.39200200 C -1.71473300 3.13306900 0.64226900 Н -0.30913000 3.47607000 -2.40785000 2.47551700 Н -0.63472000 3.27846000 C -3.02180500 2.84612900 1.32222700 C -3.25377800 1.34968000 1.64081000 Н -3.83988600 3.22251700 0.70635900 Н -2.91971100 1.14878500 2.66120500 C -2.78571500 2.83283000 -1.63904500 C -3.50143300 1.49536600 -1.32830000 Н -3.52754700 3.63814300 -1.59965400 Н -3.88165600 1.08273500 -2.26590600 C -2.53458300 0.39374500 0.73394300 C -0.59851300 -1.72659600 1.28413900 C -2.62465600 0.47525900 -0.66337400 C -0.95354900 -1.46388100 0.51644700 Н -1.67668100 -0.68187800 2.36657100 C -1.83872900 -0.38252900 -1.42789800 C -0.97939800 -1.32628600 -0.87326300 Н -1.88271600 -0.29296800 -2.51013000 C -0.07486900 -2.48240500 1.18059600 C 1.32710300 -1.94851200 1.56009500 Н 0.02398300 -3.35275400 0.53053700 Н -0.56197500 -2.83954000 2.09095100 Н 2.04533600 -2.77442700 1.52294400

Dp2M 1.30479400 Н 2.59502400 -1.60019300 C -0.09947700 -2.14597500 -1.77353600 C 1.40671200 -2.11906600 -1.41693400 Н -0.23055400 -1.77270700 -2.79154500 Н -0.43537900 -3.18880300 -1.78750300 Н 1.68006300 -2.98884700 -0.81985700 Н 1.97994700 -2.20806400 -2.34269000 C -0.81255300 0.71033800 1.81883100 C 1.83448200 -0.87770700 -0.69040600 C 2.25312000 0.36271100 1.31890400 C 2.20314200 0.26064300 -1.40172400 C 1.49376900 0.60445300 2.63489100 Н 2.26732600 0.40704200 2.40462200 C 2.57015000 1.45546500 -0.79036200 Н 2.17836000 0.21950200 -2.48743300 C 1.32968100 3.06069400 2.73608200 C 1.88984200 3.67978000 1.70209200 Н 3.79142600 3.27073800 0.72049700 Н 3.58211700 2.45482100 2.24786200 Н 2.26496000 4.70925200 1.71646400 Н 1.57343600 3.46043100 2.72411900 C 2.86186000 2.65980000 -1.63938000 C 2.07222300 3.93559100 -1.25492500 Н 2.62807500 2.39767200 -2.67350000 Н 3.93375200 2.88787200 -1.62004400 Н -0.61502700 2.68555400 4.57239800 Н 1.89135900 4.51096300 -2.16600000 Н -3.07035300 3.40400400 2.26042000 Н -2.42158500 2.80871700 -2.66861300 Н -4.32869100 1.14082800 1.61708700 Н -4.38030100 1.66157000 -0.70543800 C14.42120500 -3.44220300 0.24645700 C1-6.12985100 -0.52935600 0.30379100 In -4.31483100 -2.16891700 -0.06846300 In 4.94940200 -1.03856200 -0.00879900 Dp2T1 SCF Energy = -2425.75827466 au -1.53729300 C 3.46920300 -0.75349800 C -0.29559300 3.71226200 -1.32682000 C 0.85770400 3.89543000 -0.57687700 C 0.77084100 3.80729500 0.81475600 C -0.47862500 3.61199600 1.38928500 C -1.63664200 3.45559600 0.64040000 Н -0.22152300 3.74539200 -2.41091700 Н -0.55118600 3.56398000 2.47286700 C -2.95268900 3.21465700 1.32063500 C -3.23442400 1.72745100 1.64139300 Н -3.75777400 3.61679200 0.70402200

Dp2M -2.90709100 2.66213200 Н 1.51704300 C -2.71911200 3.19069800 -1.63919400 C -3.47872900 1.87776900 -1.32749100 Н -3.43328100 4.02049900 -1.59774200 1.47751000 Н -3.87156400 -2.26526400 C -2.54805600 0.74666700 0.73573300 C -1.77636700 -0.27331300 1.28721700 C -2.63667700 0.82915500 -0.66178900 C -1.04119500 -1.17179900 0.52024500 Н -1.72547900 -0.35399000 2.36990400 C -1.88592900 -0.05973900 -1.42562000 C -1.06563000 -1.03742400 -0.87015900 Н -1.92634600 0.03051600 -2.50804300 C -0.19564900 -2.21815600 1.18447200 C 1.22339400 -1.72895400 1.56023100 Н 0.53579500 -0.12495400 -3.09232300 2.09689000 Н -0.69149400 -2.55786600 Н 1.91607300 -2.57659500 1.51902300 Н 1.21475800 -1.38026700 2.59529400 C -0.21455600 -1.88911400 -1.76874900 C 1.29313600 -1.90379900 -1.41687300 Н -0.33859200 -2.78859600 -1.51834200 Н -0.57911600 -2.92232200 -1.77531700 Н 1.54602200 -2.78080600 -0.82109300 Н 1.86032200 -2.00887300 -2.34467900 C -0.60919700 1.74861000 0.70917700 C 1.76001200 -0.67554400 -0.69174800 C 1.31705100 2.22511500 0.54984400 C 2.17049900 0.44769000 -1.40378900 C 2.65268500 1.66396700 0.60191600 Н 2.23855900 0.59506500 2.40283400 C 2.58728300 1.62676200 -0.79329300 Н 2.14099100 0.40799900 -2.48952700 C 3.12242100 2.89132000 1.32598400 C 1.98547400 3.87588000 1.69793700 Н 3.87084800 3.40018200 0.71602500 Н 2.59329100 2.24468000 3.63379000 Н 1.71138100 2.39653200 4.89157400 Н 1.66196300 3.66850700 2.72022200 C 2.92141300 2.82011800 -1.64284200 C -1.25964500 2.17535700 4.12249200 Н 2.67954800 2.56546000 -2.67698800 Н 4.00024600 3.01302000 -1.62328100 Н 2.81042300 4.73878700 -0.62077300 2.01400200 Н 4.70262300 -2.17137300 Н -2.98250200 3.77550300 2.25784300 Н -2.35770800 3.15519900 -2.66943700 Η -4.31580700 1.55369700 1.61606900 Н -4.35279700 -0.70565100 2.07146800

Dp2M Cl -3.43708300 4.20975400 0.25612100 C1-6.24275000 0.03617200 0.33692200 T1 4.89505100 -0.97277000 -0.00396900 T1 -4.45142900 -1.76689100 -0.04993600 Dp2Ge SCF Energy = -7154.36353623 au C -1.67853600 3.24609400 -0.50309800 C -0.45796000 3.65965000 -1.02118600 C 0.69053800 3.76723800 -0.24949200 C 0.62347300 3.42059200 1.10243000 C -0.60738300 3.05281500 1.63053600 C -1.76226900 2.97185900 0.86479100 Н -0.39619900 3.89564500 -2.08054600 Н -0.66679700 2.80448500 2.68710400 C 2.54336800 1.49323500 -3.05622100 C 1.01041500 1.53882100 -3.26172400 Н -3.88726700 3.01172200 0.96378000 Н 2.49923400 -2.91066200 0.62918300 C -2.85154900 3.07203000 -1.42779000 C -3.54660200 1.69039200 -1.35628000 Н -1.24323000 -3.60438300 3.84630700 Н -3.93894700 1.44538400 -2.34575500 C -2.53998700 0.24978000 0.46221500 C -1.67518000 -0.78989900 0.81962600 C -0.89900900 -2.64185400 0.58667100 -0.89243300 C -1.47631900 -0.09990200 Н -1.62030800 -1.07441500 1.86538500 C -1.83362500 -0.08375100 -1.80896700 C -0.94496000 -1.08725700 -1.44234800 -2.85577200 Н -1.89287800 0.20045400 C 0.00143200 -2.58943500 0.36077500 C 1.40368900 -2.12547900 0.82089700 Н 0.09737100 -3.32618100 -0.43783000 Н -0.47767200 -3.10799000 1.19418200 Н 2.12018900 -2.93275900 0.63756100 Н 1.39376500 1.90086000 -1.96988000 C -2.48861800 -0.06274800 -1.70803400 C 1.44490800 -1.74333000 -2.14178400 Н -0.20140900 -1.14396800 -3.41327800 Н -2.72944900 -2.70426500 -0.39490700 Н 1.71724700 -2.70570500 -1.71011300 Н 2.01520900 -1.66331600 -3.06967400 C 1.87834800 -0.84915900 0.18433400 C 1.86765300 -0.65049800 -1.20722900 C 2.27344900 0.21801800 0.99823100 C 2.18868800 0.60850400 -1.69931000 C 2.61677600 1.46682000 0.49734000 Н 2.31235400 0.05775100 2.07075000

Dp2M C 2.53713300 -0.88320800 1.67739300 Н 2.15015200 0.76639800 -2.77339900 C 3.02758600 2.56340900 1.43425300 C 1.84152000 3.39463300 1.98337400 Н 3.73897400 3.21698500 0.92698600 Н 3.56676900 2.12659100 2.27803900 Н 2.19410300 4.41234200 2.18419800 Н 1.54224200 2.98353100 2.94976200 C 2.79374000 3.02232800 -1.49996400 C 1.98623400 4.18900400 -0.87949800 Н 2.55230100 -2.56241100 2.94920500 Н -1.44811400 3.86150800 3.26277700 Н 2.59507400 4.70948700 -0.13846300 Н 1.78384900 4.91796100 -1.66770000 Н -3.10188900 2.91963300 2.51779200 Н -2.49491400 3.23542300 -2.44710600 0.79495100 1.50153300 Н -4.33470800 Н -4.41319000 1.73188100 -0.69711400 C14.51458100 -3.07114200 -0.92383000 C14.97611700 -1.60413200 2.04767000 C1-4.33221400 -2.64218200 1.92132000 C1-5.94910600 -0.30044300 -0.73270000 Ge 4.67452300 -1.01377500 -0.07662100 Ge -4.11318600 -1.99431500 -0.19655600 Dp2Sn SCF Energy = -3429.55809884 auC -0.49199600 -1.61183200 3.46260200 C -0.38218400 3.84110900 -1.01556600 C 0.77281200 3.91308400 -0.24941100 C 0.70248900 3.56504000 1.10205400 C -0.53602600 3.23250900 1.63570200 C -1.69679000 3.18816500 0.87581900 Н -0.31900900 4.07832200 -2.07458000 Н -0.59749700 2.98358900 2.69198200 C -2.99972500 2.79637200 1.50945900 C -3.24818600 1.26986100 1.55275400 Н 3.28908000 0.98474000 -3.81955700 Н -2.90542600 0.87574400 2.51090100 C -2.79435700 3.32523400 -1.41057100 C -3.52760100 1.96316200 -1.34090900 Н -3.52441600 4.11901300 -1.21806200 Н -3.92873900 1.73290300 -2.33045200 C -2.55177100 0.49253900 0.47138800 C -1.72520800 -0.57994400 0.82195000 C -2.65334300 0.83199400 -0.88936700 C -0.96905800 -1.29089800 -0.10435900 Н -1.67490900 -0.86936800 1.86666300 C -1.87122900 0.13646400 -1.80544500

Dp2M C -1.01271100 -0.89611600 -1.44577200 Н -1.92655100 0.42504900 -2.85134200 C -0.10404300 -2.42845300 0.35169600 C 1.30922300 -1.99760900 0.81009500 Н -0.02640100 -3.16553300 -0.44859300 Н -0.59333200 -2.93641700 1.18572700 Н 2.00664800 -2.82093000 0.62458500 Н 1.30470700 -1.84211200 1.89003800 C -0.15194500 -1.54026700 -2.49592000 C 1.35584200 -1.61433800 -2.15494700 Н -0.27993000 -0.97287800 -3.42011100 Н -0.50984800 -2.55319100 -2.71033700 Н 1.60753700 -2.58408900 -1.72721100 Н 1.92343800 -1.54625700 -3.08548500 C 1.81363300 -0.73306500 0.17244200 C -1.21926400 1.81055100 -0.53451600 C 0.98563300 2.25166600 0.31766700 C 2.17023900 0.71548100 -1.71158800 C 2.63493900 1.55686800 0.48370100 Н 2.29016000 0.15535100 2.05791300 C 2.55463200 1.77318900 -0.89624000 Н 2.13303900 0.87507600 -2.78554100 C 3.08300000 2.63839300 1.42121800 C 1.92338900 3.50193600 1.97733900 Н 3.81021000 3.27273900 0.91189200 Н 3.61263500 2.18387900 2.26177300 Н 2.30627500 4.50846100 2.17872200 2.94417100 Н 1.61716100 3.09726100 C 2.84775600 3.11136700 -1.51186400 C 2.07689200 4.29922500 -0.88496200 Н 2.59882100 3.04726600 -2.57318000 Н 3.92215400 3.32181100 -1.46525100 Н 2.70408000 4.80035800 -0.14591400 Н 5.03545300 -1.67058200 1.89169800 Н -3.03004600 3.17140900 2.53495000 Н -2.43925500 3.48344200 -2.43125800 Н -4.32679100 1.08429900 1.51699900 Н -0.68025900 -4.39185900 2.02538600 C14.36460800 -3.21245600 -0.90115000 C14.95589200 -1.55008500 2.21733300 C1-4.40220900 -2.45816100 2.09234200 C1-6.13745100 -0.29970000 -0.18137100 Sn -4.27968900 -1.83437700 -0.22549900 Sn 4.76897700 -0.97223500 -0.10775900 Dp2Pb SCF Energy = -3386.69685592 au3.71635500 C -1.51163200 -0.49831600 C -0.27124500 4.03713000 -1.03492100

Dp2M C 0.89164000 -0.27791800 4.06796600 C 0.81744700 3.73705700 1.07771800 C -0.42999800 3.46310600 1.62395500 C -1.59746200 3.46016400 0.87299700 Н 4.26121700 -0.20645200 -2.09671200 Н -0.49383000 3.22804400 2.68323000 C -2.91113700 3.12935600 1.51893800 C -3.22143700 1.61496000 1.57864300 Н -3.71363400 3.65005600 0.99453200 Н -2.89082500 1.21621600 2.53915100 C -2.70628000 -1.40610700 3.61951300 C -3.49206000 2.28774000 -1.32075700 Н -3.40301500 4.44242000 -1.21294900 Н -3.90595100 2.06495000 -2.30676800 C -2.56325700 0.79923400 0.50203800 C -1.78682700 -0.30746400 0.85961600 C -2.66177500 1.12630400 -0.86236300 C -1.07407700 -1.06636200 -0.06465500 Н -1.74341900 -0.58831300 1.90691700 C -1.92321800 0.38195300 -1.77671100 C -1.11194700 -0.68757400 -1.41112500 Н -1.97394100 -2.82573200 0.66014800 C -0.25212200 -2.23173300 0.40033500 C 1.17779100 -1.84488900 0.84553600 Н -0.20447200 -2.98066500 -0.39129300 Н -0.75563800 1.24315300 -2.71048000 Н 1.84660800 -2.69278500 0.66485100 Н 1.18441600 -1.67526900 1.92337700 C -0.28540200 -1.38170600 -2.45716000 C 1.22224200 -1.50055000 -2.12611400 Н -0.40229400 -0.82779000 -3.39094500 Н -0.67772700 -2.38622500 -2.64936500 Н 1.44762100 -2.47296500 -1.68929500

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Н

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Dp2M C 2.20546300 4.39257800 -0.92766300 Н 2.65905300 3.10259100 -2.60730200 Н 4.00259600 3.33386500 -1.51374100 Н 2.85969700 4.87366200 -0.19889200 -1.71924000 Н 2.04508600 5.12821100 Н -2.91916100 3.51496500 2.54083800 Н -2.35406100 3.75693400 -2.43080100 Н -4.30677800 1.47210400 1.54666700 Н -4.35106700 2.38809000 -0.65772500 C14.17186600 -3.26116800 -0.76279400 C15.02103800 2.32410700 -1.25825700 C1-4.42017100 -2.25341300 2.19118400 C1-6.23044300 0.17662400 -0.04795000 Pb -4.36806000 -1.49659600 -0.18939800 Pb 4.69939200 -0.89251000 -0.12650600 Dp2As SCF Energy = -8392.21753635 au C -0.92546100 3.75403100 -0.88840100 C 0.37685200 3.67444000 -1.36474800 C 1.48263300 3.61053200 -0.52854500 C 1.27621400 3.60012700 0.85340500 C -0.02226700 3.72946200 1.32932200 C -1.12593100 3.82027300 0.49277300 Н 0.53642600 3.64423000 -2.43959100 Н -0.18297100 3.74277900 2.40435100 C -2.50680000 3.92251200 1.07215800 C 2.55363200 1.38938500 -3.15800400 Н -3.14323000 4.48690700 0.38837900 Н -2.97404900 2.30795900 2.43730800 C -2.06999100 3.72569400 -1.86281800 C -3.14162700 2.64120200 -1.58588700 Н -2.56613300 4.70187900 -1.90293400 Н -3.55404000 2.31244900 -2.54279400 C -2.65307100 1.40584400 0.56128700 C -2.17564500 0.26602600 1.19672500 C -2.62134800 1.45020400 -0.83631300 C -1.63397000 -0.81442600 0.50856900 Н -2.22810400 0.21460300 2.28032700 C -2.04575900 0.38825700 -1.52275100 C -1.52690600 -0.73265500 -0.88561400 Н -1.98483600 0.44339800 -2.60630400 C -1.12267100 -2.00697700 1.26240300 C 0.34385200 -1.86228200 1.73824900 Н -1.23161200 -2.89599600 0.64016300 Н -1.75607100 -2.17553200 2.13653900 Н 0.80021900 -2.85764800 1.77424200 Н 0.34831900 -1.49137300 2.76530700 C -0.84074700 -1.79464100 -1.69637000

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Dp2M C 1.31955600 -3.16140700 2.75976100 Н -3.08839600 4.68576700 0.30732400 Н -3.00319600 2.51672800 2.37213400 C -1.98906400 -1.91959400 3.88856700 C -3.08726900 2.82749600 -1.65659300 Н -2.46520000 4.87380200 -1.97439700 Н -3.48770500 2.50062000 -2.61916500 C -2.66394000 1.59705000 0.50788800 C -2.22128500 0.45136600 1.15954300 C -2.60423300 1.63186100 -0.88972900 C -1.68495500 -0.64474000 0.48855900 Н -2.29772300 0.40645600 2.24169000 C -2.03690300 0.55390500 -1.55840300 C -1.54999000 -0.57334200 -0.90504400 Н -1.95419000 0.60084200 -2.64079700 C -1.20645600 -1.83934000 1.26099900 C 0.25085600 -1.71062400 1.76689600 Н -1.31608300 -2.73059300 0.64286600 Н -1.86058100 -1.99278100 2.12231100 Н 0.68904900 -2.71304600 1.82458000 Н 0.23921000 -1.32764400 2.78937000 C -0.86545500 -1.65068800 -1.69665000 C 0.54341200 -2.03362000 -1.18173500 Н -0.78267300 -1.30123100 -2.72778800 Н -1.48886800 -2.55014000 -1.72644900 Н -0.54095000 0.47808500 -2.91405200 Н 1.15472600 -2.32732800 -2.03826700 C 1.12383200 -0.80041300 0.94958500 C 1.23719900 -0.92946800 -0.43872900 C 1.81802300 0.22803100 1.57736900 C 1.97246500 0.02251300 -1.13621000 C 2.58249100 1.16037900 0.88560300 Н 1.74917000 0.31647500 2.65818100 C 2.63255200 1.07853300 -0.51327700 Н 2.03712200 -0.06168100 -2.21669000 C 3.28625000 2.26129300 1.62223400 C 2.41005300 3.51671900 1.85659500 Н 4.19238700 2.52753500 1.07762300 Н 3.62157600 1.88763700 2.59252700 Н 3.06481500 4.39463400 1.88609400 Н 1.95354000 3.44803300 2.84637300 C 3.33848600 2.10429600 -1.35364200 C 2.92324100 3.56879700 -1.07216400 -2.39961700 Н 3.13199200 1.86949300 Н 4.42274400 2.01135100 -1.23050200 Н 3.63517400 4.03021900 -0.38597300 Н 3.00030200 4.12899700 -2.00688200 Η -2.44350900 4.69875000 1.92716100 3.70805600 -2.90577800 Н -1.55612300

Dp2M Н -4.24431700 1.19763800 2.87560700 Н -3.92247300 3.28136000 -1.12062300 c14.85086000 -1.75486000 -2.16660200 C16.19733100 0.23347200 0.39249900 C15.92377500 -3.23382800 0.81830200 C1-4.13296300 -3.28352400 -0.62869200 C1-5.05704000 -1.42783900 2.20005600 C1-7.05479400 -1.35165500 -0.67185900 Sb -4.77656800 -1.07324200 -0.11230600 Sb 4.54718400 -1.43502300 0.14724700 Dp2Bi SCF Energy = -4350.38784625 au C -0.96268900 4.04855600 -0.88792300 C 0.33736700 3.98372000 -1.37263900 C 3.93623900 -0.54280800 1.44883500 C 3.92573200 1.25111200 0.84054500 C -0.04588900 4.03927200 1.32481600 C -1.15551700 4.11529000 0.49447200 Н 0.49098400 3.95596700 -2.44833200 Н -0.19982200 4.05591500 2.40072500 C -2.53400900 4.20584300 1.08164700 C -3.17081700 2.83157500 1.40447800 Н -3.17991600 4.76376500 0.40165100 Н -2.98368600 2.58849200 2.45206300 C 4.00804300 -2.11240200 -1.85590100 -1.57322800 C -3.17102300 2.91205200 Н -2.62055000 4.97780000 -1.89239400 Н -3.58374200 2.57727300 -2.52781900 C -2.65312700 1.68939100 0.57629000 C -2.15178400 0.55771500 1.21273700 C -2.63049400 1.72999100 -0.82377900 C -1.59508300 -0.51793800 0.52435100 Н -2.20449700 0.50492200 2.29584200 C -2.04257700 0.67242200 -1.51076700 C -1.49899800 -0.43977300 -0.87332000 Н -1.99006600 -2.59474600 0.72453800 C -1.07358800 -1.70514400 1.28047500 C 0.39300600 -1.54698500 1.75091600 Н -1.18102200 -2.59631500 0.66179200 Н -1.70383700 -1.87394200 2.15645300 Н 0.85565800 -2.53911400 1.78610100 Н 0.39962700 -1.17474200 2.77722900 C -0.80673200 -1.49618700 -1.68667100 C 0.62205900 -1.84685100 -1.20530500 Н -0.75642200 -1.14062300 -2.71770900 Н -1.40987000 -2.40967100 -1.70536000 Н 0.59245300 -2.73012800 -0.56614600 Н 1.22330400 -2.12222400 -2.07463900

Dp2M

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Dp1M Н 0.09174600 -2.74681000 3.15123800 Н 1.95354200 1.57238500 -3.80929500 Н 0.34485800 0.98717700 -3.46041000 C 3.09900900 2.73761200 -0.19676600 C 3.63278700 1.72834400 -1.24114100 Н 3.68413500 2.63802000 0.72013500 Н 3.28436700 3.75374400 -0.56379400 Н 3.60932100 2.17656100 -2.23623300 Н 4.68597700 1.53351700 -1.02382800 Н 0.41145900 -3.52108600 -2.31387200 Н 3.69315100 -2.38848700 1.30969400 Н -0.03365500 -0.68574300 -4.34763700 Н 1.38000200 -4.28365400 1.13739500 C1-4.43252700 -0.16784000 -1.18774400 Ga -2.32024700 -0.23956200 -1.96844100 Dp1In SCF Energy = -1810.69013583 au C 2.52852000 -2.01188100 0.54455100 C 3.24642000 -1.19159000 -0.31643000 C 2.78104300 -0.82185100 -1.57038300 C -1.98177000 1.52981100 -1.28514600 C 0.84705400 -2.16446800 -1.15040800 C 1.31017500 -2.53577200 0.10418000 Н 4.20603200 -0.80398100 0.01595500 Н -1.49349600 -0.10040000 -2.57020900 C 0.48370200 -3.43368900 0.98007200 C -0.53934400 -2.69083600 1.88055400 Н 1.14714600 -4.03770900 1.60166800 Н -1.51259000 -2.68543300 1.38110000 C 3.06396000 -2.28094800 1.92249500 C 2.07987400 -1.96784800 3.07536700 Н 3.38847000 -3.32414100 2.01112800 2.65917000 Н -1.63876400 3.94166000 C -0.18727700 -1.26722700 2.21200700 C -1.10660800 -0.25214700 1.96698700 C 1.05791200 -0.92107600 2.74046200 C 2.14713900 -0.81510700 1.09508900 Н -2.11519700 -0.51810200 1.65622900 C 1.35115400 0.42326900 2.91873300 C 0.45832600 1.44068700 2.60916800 Н 2.33127600 0.69283800 3.30395900 C -1.83812700 2.14613700 1.82182900 C -1.78237100 2.67768500 0.36316300 Н -1.72426900 2.97873100 2.51929200 Н -2.83726700 1.73753900 1.98536100 Н -2.06346300 3.73644800 0.36925000 Н -2.55661900 2.17036800 -0.21633100 C 0.89401200 2.87015500 2.76576700

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Dp1M C 3.51506500 -1.34249500 -2.35640800 Н 4.70889400 0.26792800 -1.54566100 Н 4.23225900 0.51171800 -3.20925600 Н 3.22197700 -1.57577100 -3.38149800 Н -1.92549200 4.41906100 -2.16339900 C 1.09057100 -1.78486400 -1.80631000 C 2.43195100 -1.79155000 -1.42005400 C 0.14300900 -2.27037900 -0.90906400 C 2.74877500 -2.19725700 -0.13142600 C 0.45749400 -2.67352000 0.38343700 Н -1.23795000 -0.88923700 -2.36440600 C 1.79423000 -2.60819600 0.78883800 Н 3.79108100 -2.17742300 0.17640700 C -0.62151700 -3.13428700 1.32399400 C -1.24127400 -2.01915200 2.21682400 1.96136200 Н -0.22077700 -3.92553300 -3.58418000 0.74518300 Н -1.43060100 Н -1.44767300 -2.44111900 3.20588300 Н -2.21340000 -1.74160900 1.80657800 C 2.22338100 -2.94634100 2.18747600 C 1.48667700 -2.15670900 3.29710900 Н 3.29460800 2.26221900 -2.74760000 Н 2.09973300 -4.01823800 2.37752500 Н 0.69058600 -2.77190800 3.72006300 Н 2.18861100 -1.96756200 4.11278800 Н 1.69094500 -1.78263300 2.93647500 Н 3.09439100 2.36312500 2.78198400 -0.04597900 Н -0.34163700 4.38432500 Н 1.61591300 4.35987800 1.12222700 C1-3.97981300 1.67089300 -0.00033200 C1-3.73973100 -1.86703100 -0.51170800 Sn -2.37146800 0.08330100 -0.82102500 Dp1Pb SCF Energy = -2273.53677927 au C -1.54614200 1.60772000 -2.35041200 C -2.06199900 -2.78070700 0.39175000 C -0.77210700 -2.84502800 -1.31140900 -0.72391700 C 0.03002000 -2.46284100 C 0.56944000 0.51228800 -2.10135000 C -2.00877900 -0.19230900 1.67944900 Н -3.10841800 0.34897900 -3.07133100 Н 1.65322400 0.59805600 -1.99734700 C 0.42506100 2.97818900 -1.56881500 C 0.29094400 3.30601700 -0.05189700 Н -0.01899400 3.78760200 -2.15244100 Н 1.23948400 3.06870800 0.43510000 C -2.45916300 2.79988100 -2.29304700 C -2.51137700 3.52660000 -0.92966100

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C1

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Dp1M Н 0.13245100 2.84422100 3.32600000 Н 1.24898800 2.32011400 1.96609500 C -3.07625300 3.20420200 0.61022700 C -2.74064700 2.83387500 2.07412700 Н 0.39714000 -4.10491600 2.90544900 Н -3.05113700 4.29514900 0.50863800 Н -2.12188800 3.61402400 2.52109600 Н -3.67016000 2.82002900 2.64851700 C -0.65463900 1.42955200 2.22121200 C -2.04798500 1.51184000 2.22180200 C 2.40769100 -0.06865900 0.18146100 C -2.78262800 0.33970400 2.32477200 C -0.80118500 -0.99697600 2.49634500 Н 1.01159300 0.12476100 2.52701200 C -2.19550300 -0.91426000 2.43272500 Н 0.40379800 2.30248500 -3.86744000 C -0.10426100 -2.32204100 2.63158900 C 0.20590000 -3.04567700 1.29042600 Н -0.70823700 -2.97574400 3.26435700 Н 0.84130400 -2.17653300 3.15886900 Н 0.13371700 -4.12583800 1.45834400 Н 1.24990200 -2.86212000 1.02625300 C -3.07558500 -2.13145100 2.46971200 C -2.73941800 -3.21396500 1.41714200 Н -4.10440000 -1.79801800 2.31751200 Н -3.05025600 -2.58889700 3.46531500 Н -2.12012400 -3.99067800 1.86933100 Н -3.66865100 -3.70511500 1.11811800 Н 0.84162000 -1.64726500 -3.46457100 Н -4.10415000 -1.10831700 -2.71548000 Н 0.13419700 0.80018800 -4.30206800 Н -2.12008300 0.37590400 -4.39080000 C13.54609500 -0.89484800 -1.81144800 C10.13126700 3.54597500 2.01672900 C13.54547900 -1.12156600 1.68108700 Sb 2.32841500 0.00028900 0.00007000 Dp1Bi SCF Energy = -2755.38952013 au C -2.35669800 2.35420200 1.09738700 C -2.94400000 2.34498900 -0.16110700 C -2.21068000 2.33387900 -1.33826800 C -0.81732900 2.33030000 -1.25813300 C -0.22956400 2.42186200 0.00156800 C -0.96227700 2.41164900 1.18552300 Н -4.02884100 2.32962500 -0.22600600 Н 0.84799900 2.56582100 0.06680500 C -0.26761200 2.44572800 2.51879200 C 0.02939200 1.05386600 3.14980900

Dp1M Н -0.86915700 3.21334300 3.03583200 Н 1.07788000 0.80537100 2.97015800 C -3.23825700 2.30280000 2.31282600 C -2.91058700 1.16770700 3.31060300 Н -3.20637900 3.26014900 2.84507000 Н -3.84289500 0.83232000 3.77126800 C -0.82429100 -0.07474100 2.64470900 C -0.23655000 -1.21203600 2.09531400 C -2.21761300 -0.00560700 2.68505700 C -0.96911100 -2.23194800 1.49379200 Н 2.18905200 0.84075600 -1.34122100 C -2.95082400 -1.03015900 2.10513700 C -2.36341100 -2.12551200 1.48540800 Н -4.03563700 -0.96502300 2.12202000 C -0.27458700 -3.40523800 0.85960000 -3.25731000 C 0.02646800 -0.66052100 Н -0.87784200 -4.30077200 1.02260900 Н 0.67512700 -3.57769200 1.37016700 Н -0.06789000 -4.24400600 -1.12633600 Н 1.07555400 -2.97843400 -0.78301000 C -3.24482200 -3.15162800 0.83190700 C -2.91442800 -3.44888400 -0.64939500 Н -4.27386000 -2.79225100 0.89958900 Н -3.21508700 -4.09111600 1.39518600 Н -2.30006900 -4.34817600 -0.71868900 Н -3.84596100 -3.67841300 -1.17231100 C -0.82408400 -2.25458000 -1.38751900 C -2.21766800 -2.32165700 -1.35105500 C -0.23294300 -1.21096100 -2.09602900 C -2.94765900 -1.30543100 -1.94938600 C -0.96227000 -0.17819100 -2.67933100 Н 0.84467200 -1.22964000 -2.25264400 C -2.35682600 -0.22176400 -2.58612400 Н -4.03268400 -1.35061000 -1.90415900 C -0.26443900 0.95696500 -3.37624900 C 0.03624400 2.19945800 -2.48769900 Н -0.86529500 1.26442800 -4.23471700 Н 0.59980600 -3.77866200 0.68576600 Н -0.05478000 3.09592000 -3.11021100 Н 1.08444600 2.16483400 -2.18207600 C -3.23493500 0.85861600 -3.15059600 C -2.90358200 2.28986100 -2.66730300 Н -4.26517000 0.62208800 -2.87614300 Н -3.20202900 0.84003200 -4.24576200 -2.28608700 Н 2.79793200 -3.40999900 Н -3.83439400 2.85901100 -2.60787800 Н 0.68366700 2.97144400 2.41340900 Η -4.26754200 2.18414400 1.96765600 Н -0.06481700 1.14354300 4.23726500

Dp1M

Н	-2.29480700	1.55554000	4.12386800
Βi	2.01252900	-0.00096800	0.00078700
Cl	3.28786400	1.65151000	1.30018000
Cl	3.28211900	-1.95511700	0.78527700
c1	3.28796400	0.29375200	-2.08054300

Dp-Ga+ SCF Energy = -3084.83025296 auC 1.27642400 2.47475900 0.61814100 C 1.18126400 2.42828700 -0.78157000 C -0.09297000 2.49841400 -1.35977600 C -1.27642400 2.47475900 -0.61814100 C -1.18126400 2.42828700 0.78157000 C 0.09297000 2.49841400 1.35977600 C 2.69359000 -0.19113900 0.78157000 C 2.78141600 -0.13196400 -0.61814100 C -1.35977600 2.21017500 -1.16869300 C 1.51232600 -2.23714800 -0.78157000 C 1.50499200 -2.34279600 0.61814100 C 2.11720500 -1.32972100 1.35977600 C -1.51232600 -2.23714800 0.78157000 -0.61814100 C -1.50499200 -2.34279600 C -2.11720500 -1.32972100 -1.35977600 C -2.69359000 -0.19113900 -0.78157000 C -2.78141600 -0.13196400 0.61814100 C -2.21017500 -1.16869300 1.35977600 C 0.75733500 -3.45455900 1.30281600 C -0.73045800 1.67024500 -3.17227800 C 0.73045800 -3.17227800 -1.67024500 C -0.75733500 -3.45455900 -1.30281600 C -3.11250200 0.95354400 -1.67024500 C -2.61306800 2.38315100 -1.30281600 C -3.37040300 1.07140800 1.30281600 C -2.38204400 2.21873400 1.67024500 C 3.37040300 1.07140800 -1.30281600 C 2.38204400 2.21873400 -1.67024500 C 3.11250200 0.95354400 1.67024500 C 2.61306800 2.38315100 1.30281600 Н -0.16622000 2.48711900 -2.44370800 Н 0.16622000 2.44370800 2.48711900 Н 2.23701800 -1.09960900 -2.44370800 Н 2.07079800 -1.38751000 2.44370800 Η -2.44370800 -2.07079800 -1.38751000 Н 2.44370800 -2.23701800 -1.09960900 0.81779400 Н -4.34846100 0.68173300 Н 1.27183000 -3.70491200 2.23307500 Н -2.75873300 -0.76150400 2.68018000 Н -1.24092800 -4.13933900 1.73000900 Н 1.24092800 -4.13933900 -1.73000900 Н 0.76150400 -2.75873300 -2.68018000 Н -0.81779400 -4.34846100 -0.68173300 Н -1.27183000 -3.70491200 -2.23307500 Н -4.20523700 0.99499400 -1.73000900 Η -2.76988500 0.71988500 -2.68018000 Н -2.57263400 2.95389300 -2.23307500

Dp-Mn+ -3.35698100 Н -0.68173300 2.88246100 Н -4.17477500 1.46600100 0.68173300 Н -3.84446300 0.75102000 2.23307500 Н -2.96430900 3.14434500 1.73000900 Н -2.00838100 2.03884800 2.68018000 Н 4.17477500 1.46600100 -0.68173300 Н 3.84446300 0.75102000 -2.23307500 Н 2.96430900 3.14434500 -1.73000900 Н 2.00838100 2.03884800 -2.68018000 Н 4.20523700 0.99499400 1.73000900 Н 2.76988500 0.71988500 2.68018000 Н 2.88246100 0.68173300 3.35698100 Н 2.57263400 2.95389300 2.23307500 Ga 0.00000000 0.00000000 0.00000000 Dp-In+ SCF Energy = -1350.35778049 auC 1.27842200 2.51527700 0.61887700 C 1.18242400 2.46535800 -0.78159300 C -0.09309800 2.55607300 -1.35951500 C -1.27842200 2.51527700 -0.61887700 C -1.18242400 0.78159300 2.46535800 C 0.09309800 2.55607300 1.35951500 C 2.72627500 -0.20867000 0.78159300 C 2.81750500 -0.15049200 -0.61887700 C 2.26017300 -1.19741100 -1.35951500 -0.78159300 C 1.54385100 -2.25668900 C 1.53908200 -2.36478400 0.61887700 C 2.16707500 -1.35866200 1.35951500 C -1.54385100 -2.25668900 0.78159300 C -1.53908200 -2.36478400 -0.61887700 C -2.16707500 -1.35866200 -1.35951500 C -2.72627500 -0.20867000 -0.78159300 C -2.81750500 -0.15049200 0.61887700 C -2.26017300 -1.19741100 1.35951500 C 0.75982800 -3.45942400 1.30151600 C -0.72915700 1.67293000 -3.16648800 C 0.72915700 -1.67293000 -3.16648800 C -3.45942400 -1.30151600 -0.75982800 C -3.10683700 0.95177600 -1.67293000 C 2.38774300 -1.30151600 -2.61603500 C -3.37586300 1.07168100 1.30151600 C -2.37768100 2.21471200 1.67293000 C -1.30151600 3.37586300 1.07168100 C 2.37768100 2.21471200 -1.67293000 C 3.10683700 0.95177600 1.67293000 C 2.61603500 2.38774300 1.30151600 Н -0.16634500 2.54466600 -2.44356100 Н 0.16634500 2.54466600 2.44356100

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C
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C
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C
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Dp-Mn+ C -2.27607900 -1.20864800 1.36042300 C 0.75978900 -3.45982600 1.30207800 C -0.73329900 -3.17116000 1.67035000 C 0.73329900 -3.17116000 -1.67035000 C -3.45982600 -1.30207800 -0.75978900 C -3.11295400 0.95052500 -1.67035000 C -2.61640300 2.38790900 -1.30207800 C -3.37619100 1.07191700 1.30207800 C -2.37965600 2.22063500 1.67035000 C 3.37619100 1.07191700 -1.30207800 C 2.37965600 2.22063500 -1.67035000 C 3.11295400 0.95052500 1.67035000 C 2.61640300 2.38790900 1.30207800 Н -0.16381500 2.56706500 -2.44467400 Н 0.16381500 2.56706500 2.44467400 Н -2.44467400 2.30505100 -1.14166400 2.44467400 Н 2.14123600 -1.42540100 Н -2.14123600 -1.42540100 -2.44467400 Н 2.44467400 -2.30505100 -1.14166400 Н 0.81090000 -4.35706100 0.68498000 Н 1.25921400 -3.71836700 2.23856400 Н -0.75553900 -2.73809200 2.67253300 Н -1.22575300 -4.14538800 1.76049300 Н 1.22575300 -4.14538800 -1.76049300 Н 0.75553900 -2.73809200 -2.67253300 Н -0.81090000 -4.35706100 -0.68498000 Н -1.25921400 -3.71836700 -2.23856400 Н -4.20288700 1.01116100 -1.76049300 Н -2.74902700 0.71473000 -2.67253300 Н -2.59059300 2.94969500 -2.23856400 Н -3.36787600 2.88079100 -0.68498000 Н -4.17877600 1.47627000 0.68498000 Н -3.84980700 0.76867200 2.23856400 Н -2.97713500 3.13422700 1.76049300 Н -1.99348800 2.02336200 2.67253300 Н 4.17877600 1.47627000 -0.68498000 Н -2.23856400 3.84980700 0.76867200 Н 2.97713500 3.13422700 -1.76049300 Н 1.99348800 2.02336200 -2.67253300 Н 4.20288700 1.01116100 1.76049300 Н 0.71473000 2.67253300 2.74902700 Н 3.36787600 2.88079100 0.68498000 Н 2.59059300 2.94969500 2.23856400 T1 0.00000000 0.00000000 0.00000000 Dp-Ge2+ SCF Energy = -3236.62933054 auC 1.27792000 2.40626900 0.62051600 C 1.18419000 2.36198000 -0.78311700

Dp-Mn+ C -0.09275700 2.39024600 -1.36430900 C -1.27792000 2.40626900 -0.62051600 C -1.18419000 2.36198000 0.78311700 C 0.09275700 2.39024600 1.36430900 C 0.78311700 2.63763000 -0.15545100 C 2.72285000 -0.09642300 -0.62051600 C 2.11639200 -1.11479300 -1.36430900 C 1.45344000 -2.20652800 -0.78311700 C 1.44493000 -2.30984600 0.62051600 C 2.02363500 -1.27545300 1.36430900 C -1.45344000 -2.20652800 0.78311700 C -1.44493000 -2.30984600 -0.62051600 C -2.02363500 -1.27545300 -1.36430900 C -2.63763000 -0.15545100 -0.78311700 C -2.72285000 -0.09642300 0.62051600 C -2.11639200 -1.11479300 1.36430900 C 0.75690200 -3.45009000 1.30795100 C -0.73493800 -3.18734100 1.66325500 C 0.73493800 -3.18734100 -1.66325500 C -0.75690200 -3.45009000 -1.30795100 C -3.12778700 0.95719600 -1.66325500 C -2.60941400 2.38054100 -1.30795100 C -3.36631600 1.06954900 1.30795100 C -2.39284900 2.23014500 1.66325500 C 3.36631600 1.06954900 -1.30795100 C 2.39284900 2.23014500 -1.66325500 C 3.12778700 0.95719600 1.66325500 C 2.60941400 2.38054100 1.30795100 Н -0.16425900 2.38201700 -2.44812100 Н 0.16425900 2.38201700 2.44812100 Н 2.14501600 -1.04875600 -2.44812100 Н 1.98075700 -1.33326100 2.44812100 Н -1.98075700 -1.33326100 -2.44812100 Н -2.14501600 -1.04875600 2.44812100 Н 0.84216800 -4.34101800 0.68681500 Н 1.28270900 -3.67844200 2.23637100 Η -0.79670000 -2.82668700 2.69100600 Н -1.26200900 -4.14616800 1.65076400 Н 1.26200900 -4.14616800 -1.65076400 Н 0.79670000 -2.82668700 -2.69100600 Н -0.84216800 -4.34101800 -0.68681500 Н -1.28270900 -3.67844200 -2.23637100 Н -4.22169100 0.98015300 -1.65076400 Н -2.84633200 0.72338100 -2.69100600 Н -2.54426900 2.95008000 -2.23637100 Н -3.33834800 2.89984700 -0.68681500 Н -4.18051500 1.44117000 0.68681500 Η -3.82697900 0.72836200 2.23637100 Н -2.95968300 3.16601600 1.65076400

Dp-Mn+ Н -2.04963300 2.69100600 2.10330600 Н 4.18051500 1.44117000 -0.68681500 Н 3.82697900 0.72836200 -2.23637100 Н 2.95968300 3.16601600 -1.65076400 2.10330600 Н 2.04963300 -2.69100600 Н 4.22169100 0.98015300 1.65076400 Н 2.84633200 0.72338100 2.69100600 Н 3.33834800 2.89984700 0.68681500 Н 2.54426900 2.95008000 2.23637100 Ge 0.00000000 0.00000000 0.00000000 Dp-Sn2+ -1374.22042148 au SCF Energy = C 1.28109900 2.45779100 0.62277000 C 1.18796300 2.41441900 -0.78257600 C -1.36425400 -0.09128600 2.47243800 -0.62277000 C 2.45779100 -1.28109900 C -1.18796300 2.41441900 0.78257600 C 0.09128600 2.47243800 1.36425400 C 2.68493000 -0.17840300 0.78257600 C 2.76905900 -0.11943100 -0.62277000 C -1.15716300 -1.36425400 2.18683700 C 1.49696600 -2.23601600 -0.78257600 C 1.48796000 -2.33836000 0.62277000 C 2.09555100 -1.31527500 1.36425400 C -1.49696600 -2.23601600 0.78257600 -1.48796000 C -2.33836000 -0.62277000 C -2.09555100 -1.31527500 -1.36425400 C -2.68493000 -0.17840300 -0.78257600 C -2.76905900 -0.11943100 0.62277000 C -2.18683700 -1.15716300 1.36425400 C 0.75825900 -3.45962700 1.30794800 C -0.73600800 -3.18926200 1.66597000 C 0.73600800 -3.18926200 -1.66597000 C -0.75825900 -3.45962700 -1.30794800 C -3.12998600 0.95722900 -1.66597000 C -2.61699500 2.38648500 -1.30794800 C -3.37525400 1.07314200 1.30794800 C -2.39397800 2.23203300 1.66597000 C 3.37525400 1.07314200 -1.30794800 C 2.23203300 2.39397800 -1.66597000 C 3.12998600 0.95722900 1.66597000 C 2.61699500 2.38648500 1.30794800 Н -0.16154700 2.47321900 -2.44841600 Н 0.16154700 2.47321900 2.44841600 Н 2.22264400 -1.09670600 -2.44841600 Н 2.06109700 -1.37651300 2.44841600 Η -2.06109700 -1.37651300 -2.44841600 -2.22264400 -1.09670600 2.44841600 Н

Dp-Mn+ Н 0.83356200 -4.35287100 0.68868300 Н 1.27225200 -3.69933200 2.24042300 Н -0.78650400 -2.80684100 2.68673900 Н -1.24975600 -4.15543800 1.68654900 Н 1.24975600 -4.15543800 -1.68654900 Н 0.78650400 -2.80684100 -2.68673900 Н -0.83356200 -4.35287100 -0.68868300 Н -1.27225200 -3.69933200 -2.24042300 Н -4.22359200 0.99539900 -1.68654900 Н -2.82404800 0.72228800 -2.68673900 2.95146900 -2.24042300 Н -2.56758900 Н -3.35291600 2.89832100 -0.68868300 Н -4.18647800 1.45455000 0.68868300 Н -3.83984100 0.74786300 2.24042300 Н -2.97383700 3.16003900 1.68654900 Н -2.03754400 2.08455300 2.68673900 Н 4.18647800 1.45455000 -0.68868300 Н 3.83984100 0.74786300 -2.24042300 Н 2.97383700 3.16003900 -1.68654900 Н 2.03754400 2.08455300 -2.68673900 Н 4.22359200 0.99539900 1.68654900 Н 2.82404800 0.72228800 2.68673900 Н 2.89832100 0.68868300 3.35291600 Н 2.56758900 2.95146900 2.24042300 Sn 0.00000000 0.00000000 0.00000000 Dp-Pb2+ -1352.79578915 au SCF Energy = C 1.28134700 2.47612200 0.62457900 C 1.18962900 2.43587700 -0.78190000 C -1.36501500 -0.08957800 2.50305800 C -1.28134700 2.47612200 -0.62457900 C -1.18962900 2.43587700 0.78190000 C 2.50305800 0.08957800 1.36501500 C 2.70434600 -0.18768900 0.78190000 C 2.78505800 -0.12838100 -0.62457900 C 2.21250100 -1.17395300 -1.36501500 -0.78190000 C 1.51471700 -2.24818800 C 1.50371000 -2.34774000 0.62457900 C 2.12292300 -1.32910500 1.36501500 C -1.51471700 -2.24818800 0.78190000 C -1.50371000 -2.34774000 -0.62457900 C -2.12292300 -1.32910500 -1.36501500 C -0.78190000 -2.70434600 -0.18768900 C -2.78505800 -0.12838100 0.62457900 C -2.21250100 -1.17395300 1.36501500 C 0.75897400 -3.46190600 1.30853400 C -0.73897800 -3.19322200 1.66404600 C 0.73897800 -3.19322200 -1.66404600

Dp-Mn+ C -3.46190600 -1.30853400 -0.75897400 C -3.13490000 0.95663800 -1.66404600 C -2.61861100 2.38824300 -1.30853400 C -3.37758500 1.07366200 1.30853400 C -2.39592300 2.23658400 1.66404600 C 3.37758500 1.07366200 -1.30853400 C 2.39592300 2.23658400 -1.66404600 C 0.95663800 3.13490000 1.66404600 C 2.61861100 2.38824300 1.30853400 Н -0.15880300 2.50969500 -2.44934100 Н 0.15880300 2.50969500 2.44934100 Н -2.44934100 2.25286100 -1.11732000 Н 2.09405800 -1.39237500 2.44934100 Н -2.09405800 -1.39237500 -2.44934100 Н -2.25286100 -1.11732000 2.44934100 Н 0.83359000 -4.35654200 0.69112000 Н 1.26655500 -3.70346800 2.24411100 Н -0.78964000 -2.80833800 2.68398500 Н -1.24470500 -4.16352200 1.69009000 Н 1.24470500 -4.16352200 -1.69009000 Н 0.78964000 -2.80833800 -2.68398500 Н -0.83359000 -4.35654200 -0.69112000 Н -1.26655500 -3.70346800 -2.24411100 Н -4.22806900 1.00381500 -1.69009000 Н -2.82691200 0.72032100 -2.68398500 Н -2.57402000 2.94860300 -2.24411100 Н -3.35608100 2.90018200 -0.69112000 0.69112000 Н -4.18967200 1.45636100 Н -3.84057500 0.75486500 2.24411100 Н -2.98336400 3.15970700 1.69009000 Н -2.03727300 2.08801700 2.68398500 Н 4.18967200 1.45636100 -0.69112000 Н 3.84057500 0.75486500 -2.24411100 Н 2.98336400 3.15970700 -1.69009000 Н 2.03727300 2.08801700 -2.68398500 Н 4.22806900 1.00381500 1.69009000 Н 2.82691200 0.72032100 2.68398500 Н 3.35608100 2.90018200 0.69112000 Н 2.57402000 2.94860300 2.24411100 Pb 0.00000000 0.00000000 0.00000000 Dp-As3+ SCF Energy = -3394.93945427 au C 1.28137100 2.37741100 0.62286700 C 1.18654700 2.32772300 -0.78667600 C -0.09484600 2.32501700 -1.36912800 C -1.28137100 2.37741100 -0.62286700 C -1.18654700 2.32772300 0.78667600 C 0.09484600 2.32501700 1.36912800

Dp-Mn+ C -0.13628200 2.60914100 0.78667600 C 2.69958400 -0.07900600 -0.62286700 C 2.06094700 -1.08036900 -1.36912800 C 1.42259400 -2.19144100 -0.78667600 C 0.62286700 1.41821300 -2.29840500 C 1.96610100 -1.24464800 1.36912800 C -1.42259400 -2.19144100 0.78667600 C -1.41821300 -2.29840500 -0.62286700 C -1.96610100 -1.24464800 -1.36912800 C -2.60914100 -0.13628200 -0.78667600 C 0.62286700 -2.69958400 -0.07900600 C -2.06094700 -1.08036900 1.36912800 C 0.76307100 -3.44768200 1.30890100 C -0.73658500 -3.18725300 1.66021900 C 0.73658500 -3.18725300 -1.66021900 C -1.30890100 -3.44768200 -0.76307100 C 0.95572500 -3.12853400 -1.66021900 C -2.60424500 2.38468000 -1.30890100 C -3.36731600 1.06300200 1.30890100 C -2.39194900 2.23152800 1.66021900 C 3.36731600 1.06300200 -1.30890100 C 2.39194900 2.23152800 -1.66021900 C 3.12853400 0.95572500 1.66021900 C 2.60424500 2.38468000 1.30890100 Н -0.16616000 2.30425100 -2.45313100 Н 0.16616000 2.30425100 2.45313100 2.07861900 -1.00822700 -2.45313100 Н 2.45313100 Н 1.91246000 -1.29602400 Н -1.91246000 -1.29602400 -2.45313100 Н -2.07861900 -1.00822700 2.45313100 Н 0.85565700 -4.33989100 0.69156900 Н 1.28645000 -3.66184300 2.24214100 Н -0.81383700 -2.85915300 2.69709200 Н -1.26567300 -4.14434100 1.60556400 Н 1.26567300 -4.14434100 -1.60556400 Н 0.81383700 -2.85915300 -2.69709200 Η -4.33989100 -0.69156900 -0.85565700 Н -2.24214100 -1.28645000 -3.66184300 Н -4.22194100 0.97606600 -1.60556400 Н -2.88301800 0.72477300 -2.69709200 Н -2.52802400 -2.24214100 2.94502000 Н -3.33062800 2.91096600 -0.69156900 Н -4.18628400 1.42892500 0.69156900 0.71682300 Н -3.81447400 2.24214100 Н -2.95626800 3.16827500 1.60556400 Н -2.06918000 2.13438000 2.69709200 Н 4.18628400 1.42892500 -0.69156900 Η 3.81447400 0.71682300 -2.24214100 Н 3.16827500 2.95626800 -1.60556400

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Dp-Mn+ C 1.66032400 -2.40243600 2.24329700 C 3.37801200 1.07155500 -1.31287000 C 2.40243600 2.24329700 -1.66032400 C 3.14397100 0.95892200 1.66032400 C 2.61700000 2.38966700 1.31287000 Н -0.15754100 2.44404900 -2.45391100 Н 0.15754100 2.44404900 2.45391100 Н 2.19537900 -2.45391100 -1.08559000 Н 2.03783800 -1.35845900 2.45391100 -2.03783800 Н -1.35845900 -2.45391100 Н -2.19537900 -1.08559000 2.45391100 Η -4.35535800 0.85125100 0.69732200 Н 1.27304000 -3.68718900 2.24977800 Н -0.81307700 -2.85476000 2.69183500 Н -1.25705300 -4.16781400 1.63683700 Н 1.25705300 -4.16781400 -1.63683700 Н 0.81307700 -2.85476000 -2.69183500 Н -0.85125100 -4.35535800 -0.69732200 Н -1.27304000 -3.68718900 -2.24977800 Н -4.23795900 0.99526700 -1.63683700 Н -2.87883300 0.72323500 -2.69183500 2.94607900 Н -2.24977800 -2.55667900 Η -3.34622500 2.91488400 -0.69732200 Н -4.19747600 1.44047400 0.69732200 Н -3.82971900 0.74111000 2.24977800 Н -2.98090600 3.17254700 1.63683700 Н -2.06575600 2.13152500 2.69183500 Н 4.19747600 1.44047400 -0.69732200 Н 3.82971900 0.74111000 -2.24977800 Н 2.98090600 3.17254700 -1.63683700 Н 2.13152500 -2.69183500 2.06575600 Н 4.23795900 0.99526700 1.63683700 Н 2.87883300 0.72323500 2.69183500 Н 3.34622500 2.91488400 0.69732200 Н 2.55667900 2.94607900 2.24977800 Βi 0.00000000 0.00000000 0.00000000