

Supplementary data for:

Rational Design of Co-based Redox Mediators
for Dye Sensitized Solar Cells by Density Functional Theory

Zhu-Zhu Sun^{a,c}, Kui-Ming Zheng^{a,c}, Quan-Song Li^{a,c,*}, Ze-Sheng Li^{a,b,c,d,*}

^a*Key Laboratory of Cluster Science of Ministry of Education, China*

^b*Beijing Key Laboratory for Chemical Power Source and Green Catalysis, China*

^c*School of Chemistry, Beijing Institute of Technology, Beijing 100081, China*

^d*The Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology,
Harbin 150080, China*

Fax: +86 10 68911354; Tel: +86 10 68918670;

E-mail: Q.-S. Li: liquansong@bit.edu.cn, Z.-S. Li: zeshengli@bit.edu.cn

Part 1

Cartesian coordinates of the optimized structures for classic and new designed redox mediators in acetonitrile at B3LYP/LANL2DZ level.

[C1]2+	N	-0.37338200	-0.25398300	-1.99298100			
Co	-0.07194700	-0.00009100	0.00002700	C	2.54267400	1.18311100	-0.14371800
C	-2.62088600	-0.15098400	-1.18228600	C	2.54353400	-1.18141500	0.14336400
C	-2.62071900	0.14950500	1.18294800	C	3.95051900	-1.20522000	0.14830600
C	-4.02591800	0.15224000	1.21222800	C	4.65302600	0.00162500	-0.00004900
C	-4.72542600	-0.00118400	0.00053600	C	3.94964500	1.20795000	-0.14847200
C	-4.02608900	-0.15432600	-1.21129200	C	1.68588400	2.38746600	-0.28879800
C	-1.70620300	-0.29822700	-2.33251500	C	-0.52547500	3.17731500	-0.38943200
C	0.56215000	-0.38009700	-2.96282800	C	-0.09160200	4.50592300	-0.54433100
C	0.21722500	-0.55440700	-4.31379200	C	1.29127500	4.76325100	-0.56910600
C	-1.14269600	-0.60050700	-4.66837700	C	2.19301100	3.69225700	-0.43976500
C	-2.11756800	-0.47107500	-3.66316300	H	4.49059600	-2.13607500	0.26511300
H	-4.56454000	0.27045600	2.14462700	H	5.73786400	0.00203000	0.00004500
H	-5.81025000	-0.00142200	0.00064600	H	4.48905300	2.13920600	-0.26516800
H	-4.56483800	-0.27275000	-2.14359000	H	-1.58255200	2.93488400	-0.36487300
H	1.59948800	-0.34148700	-2.65500800	H	-0.81756700	5.30561300	-0.64132000
H	0.99898600	-0.65086100	-5.05869500	H	1.66283800	5.77617400	-0.68634100
H	-1.44032300	-0.73442600	-5.70320100	H	3.25984300	3.88001900	-0.45691500
H	-3.17131700	-0.50526500	-3.91459000	C	-0.52321800	-3.17772000	0.38930700
C	0.56257200	0.38020300	2.96282800	C	-0.08842600	-4.50608400	0.54372800
C	0.21784500	0.55422100	4.31388000	C	1.29462700	-4.76251700	0.56798500
C	-1.14202700	0.59955900	4.66875700	C	2.19562300	-3.69088600	0.43875100
C	-2.11704400	0.46969500	3.66374200	C	1.68759400	-2.38638400	0.28833500
C	-1.70586800	0.29718100	2.33299000	H	-1.58045900	-2.93596900	0.36513200
H	1.59986600	0.34216800	2.65478600	H	-0.81383700	-5.30628200	0.64067400
H	0.99971200	0.65102100	5.05862600	H	1.66689500	-5.77523100	0.68478500
H	-1.43950600	0.73323400	5.70365500	H	3.26258400	-3.87794400	0.45550100
H	-3.17075600	0.50328900	3.91540400	N	0.34198000	-2.14646400	0.26492600
N	-0.37309900	0.25368600	1.99317100	N	1.87403300	0.00060300	-0.00020800
N	-1.96388700	-0.00061100	0.00027000	N	0.34043400	2.14666600	-0.26497600

[C1]3+

Co -0.00000200 -0.00000800 -0.00016500
 C 2.52554800 0.85322600 0.84176000
 C 2.52685500 -0.85006000 -0.84107000
 C 3.93044800 -0.86979500 -0.86097900
 C 4.62426400 0.00294800 0.00053900
 C 3.92911300 0.87475000 0.86196500
 C 1.58543300 1.66004600 1.63893700
 C -0.70981100 2.06733400 2.03974400
 C -0.39752000 3.04153500 3.00130300
 C 0.95026000 3.32182800 3.27956900
 C 1.95462000 2.62024800 2.58805200
 H 4.47123000 -1.53731200 -1.52015200
 H 5.70869100 0.00368000 0.00060500
 H 4.46885400 1.54307200 1.52117000
 H -1.73963600 1.83385400 1.80883400
 H -1.20111600 3.55920400 3.51138100
 H 1.21824000 4.06950400 4.01805800
 H 3.00096400 2.81959600 2.78652900
 C -0.70650100 -2.06786600 -2.04063600
 C -0.39257000 -3.04177400 -3.00193900
 C 0.95569100 -3.32091800 -3.27909800
 C 1.95886100 -2.61820500 -2.58703000
 C 1.58803000 -1.65803400 -1.63853600
 H -1.73672000 -1.83531200 -1.81053700
 H -1.19530200 -3.56025600 -3.51254500
 H 1.22493500 -4.06854400 -4.01718000
 H 3.00554200 -2.81681300 -2.78446300
 N 0.25888100 -1.39286200 -1.37532700
 N 1.88415000 0.00120300 0.00023000
 N 0.25671000 1.39341300 1.37502700
 C -2.52668900 0.83982300 -0.85175900
 C -2.52571500 -0.84301000 0.85152700

C -3.92926900 -0.86389700 0.87213500
 C -4.62426300 -0.00284200 -0.00015300
 C -3.93029500 0.85902700 -0.87243100
 C -1.58768200 1.63766400 -1.65918400
 C 0.70694800 2.04066000 -2.06763000
 C 0.39325300 3.00205900 -3.04151100
 C -0.95495300 3.27906700 -3.32110300
 C -1.95828600 2.58653400 -2.61908300
 H -4.46911500 -1.52343100 1.54004800
 H -5.70869000 -0.00351800 -0.00019600
 H -4.47098300 1.51780900 -1.54040700
 H 1.73710000 1.81072200 -1.83461200
 H 1.19610500 3.51289100 -3.55958100
 H -1.22402000 4.01728900 -4.06865500
 H -3.00491600 2.78409400 -2.81784000
 C 0.70936000 -2.03997300 2.06730900
 C 0.39684400 -3.00160000 3.04136900
 C -0.95099300 -3.28003100 3.32121400
 C -1.95519100 -2.58882900 2.61909700
 C -1.58577800 -1.63984200 1.65885900
 H 1.73923500 -1.80899300 1.83416200
 H 1.20032800 -3.51150800 3.55938200
 H -1.21913600 -4.01847600 4.06887600
 H -3.00158500 -2.78731000 2.81816900
 N -0.25700100 -1.37549400 1.39292600
 N -1.88415000 -0.00118600 -0.00008700
 N -0.25859400 1.37485900 -1.39334200

[C2]2+

Co 0.07635800 -0.10380700 -0.09150600
 N -0.47413200 2.00744100 -0.28141400
 N 0.50902400 0.12370600 1.86726100
 N -1.87352200 -0.22111800 0.00633000
 N 1.96914000 -0.03891200 -0.22475500

N	0.26301500	-0.31357500	-2.09089200	C	2.35134800	0.37511300	3.42454200
N	-0.23205400	-2.29983800	0.16906100	C	1.43981900	0.46131800	4.49206100
C	0.33734300	-3.51190100	0.28420200	C	0.06196400	0.37693000	4.22504500
C	-0.65283300	-4.53488300	0.42172300	C	-0.36509800	0.20892400	2.89689100
C	-1.87677900	-3.88002300	0.38477500	C	2.70415200	0.09892600	0.91432300
N	-1.60897000	-2.53048200	0.23193100	C	4.10530500	0.11964900	0.84357300
H	1.41235000	-3.61187900	0.26535700	C	4.71866800	-0.00411000	-0.41983000
H	-0.48859600	-5.59505200	0.53129400	C	3.94663300	-0.15072200	-1.58671700
H	-2.87940600	-4.26997500	0.45407700	C	2.55350700	-0.16543300	-1.43529500
C	-1.83056200	2.17484400	-0.24931100	H	3.41778100	0.44076900	3.60708100
C	-2.41239500	3.45291200	-0.34812500	H	1.79921200	0.59214300	5.50740200
C	-1.57488000	4.57416000	-0.48289000	H	-0.67252900	0.43933700	5.01991300
C	-0.18020300	4.39243100	-0.51460100	H	-1.41867200	0.14225600	2.65618900
C	0.33028500	3.08635000	-0.40981000	H	4.70825300	0.22606300	1.73659400
C	-2.61671400	0.92409600	-0.10400500	H	5.80055200	0.01073600	-0.49609000
C	-4.01925500	0.86354700	-0.07828700	H	4.41423300	-0.24904200	-2.55853900
C	-4.64669700	-0.38810900	0.06138600				
C	-3.87903900	-1.55615300	0.17062100	[C2]3+			
C	-2.48078700	-1.42488400	0.13627000	Co	0.00002800	-0.13332300	-0.00021300
H	-3.48755100	3.58229800	-0.32009000	N	-0.36898500	1.24791900	-1.34370100
H	-2.00460100	5.56765600	-0.56027100	N	0.36870500	1.24485500	1.34645200
H	0.49714900	5.23296700	-0.61691700	N	-1.88289900	-0.17009700	0.12396100
H	1.39888900	2.90110200	-0.42918700	N	1.88295200	-0.16941400	-0.12448400
H	-4.61716800	1.76118200	-0.16653000	N	0.16570100	-1.50202700	-1.39361300
H	-5.72923900	-0.45249000	0.08308900	N	-0.16532700	-1.50525900	1.39009600
H	-4.35358700	-2.52331000	0.27723600	C	0.57254900	-2.31462100	2.17199800
C	-0.43718600	-0.46042400	-3.22969600	C	-0.27842200	-3.11525500	2.98539400
C	0.44170300	-0.55498500	-4.35112200	C	-1.58297200	-2.75521700	2.66197800
C	1.73100800	-0.45776700	-3.83829500	N	-1.50715300	-1.77839700	1.69446300
N	1.61127900	-0.31147200	-2.47171400	H	1.65067600	-2.30443400	2.13377700
H	-1.51573000	-0.49358000	-3.21269200	H	0.02826100	-3.85373900	3.70789100
H	0.16493400	-0.67713900	-5.38590700	H	-2.52637100	-3.11578000	3.04127900
H	2.68873100	-0.48232500	-4.33384100	C	-1.71689000	1.48219600	-1.53605400
C	1.86017400	0.20533200	2.12121200	C	-2.15632700	2.43233800	-2.46457200

C	-1.20515300	3.15500600	-3.20775100	H	-0.92553700	3.43521900	3.55936600
C	0.16171300	2.90811000	-2.99948300	H	-1.59341200	1.73017700	1.87865600
C	0.54735000	1.94353900	-2.05494800	H	4.59203000	1.26911600	1.27479200
C	-2.59574200	0.65628800	-0.69011600	H	5.69692000	-0.29804300	-0.32050400
C	-3.99511300	0.62779500	-0.63823700	H	4.33663300	-1.79215300	-1.78636100
C	-4.61450900	-0.26438300	0.26348700				
C	-3.85733500	-1.11357500	1.09269100	[C3]2+			
C	-2.46387500	-1.03258800	0.98457100	Co	0.00002500	0.00037800	-0.00001500
H	-3.21600500	2.60763800	-2.60665600	C	0.40356200	2.75009800	0.61737600
H	-1.52857000	3.89479300	-3.93180300	C	0.83746700	3.91264600	1.27804600
H	0.92471400	3.44474000	-3.55056100	C	1.59850500	3.79380400	2.45222900
H	1.59301200	1.73513400	-1.87468900	C	1.90580200	2.51089800	2.93932400
H	-4.59230100	1.27152900	-1.27147100	C	1.44561000	1.38950200	2.23312500
H	-5.69684300	-0.29991300	0.31983100	C	-0.40345100	2.75005900	-0.61752800
H	-4.33618700	-1.79749200	1.78185900	C	-0.83733600	3.91256400	-1.27828700
C	-0.57205200	-2.30933500	-2.17778000	C	-1.59838700	3.79364700	-2.45245400
C	0.27907500	-3.10776600	-2.99318000	C	-1.90572000	2.51071000	-2.93944600
C	1.58355800	-2.74835700	-2.66881300	C	-1.44554600	1.38936000	-2.23316400
N	1.50758100	-1.77420900	-1.69862500	H	0.58878500	4.89278400	0.88997800
H	-1.65018400	-2.29921300	-2.13976500	H	1.94066400	4.68149000	2.97396700
H	-0.02745800	-3.84441000	-3.71761600	H	2.48783600	2.37227300	3.84329200
H	2.52700300	-3.10795000	-3.04891500	H	1.66113100	0.38977700	2.58286800
C	1.71656500	1.47881800	1.53952400	H	-0.58862800	4.89272700	-0.89029900
C	2.15577100	2.42640700	2.47075700	H	-1.94052900	4.68130000	-2.97425900
C	1.20440600	3.14682400	3.21588700	H	-2.48776700	2.37202800	-3.84339700
C	-0.16240200	2.90028800	3.00682400	H	-1.66108700	0.38961000	-2.58282300
C	-0.54780200	1.93827500	2.05956300	N	0.71285500	1.50142600	1.09621500
C	2.59560700	0.65513500	0.69162200	N	-0.71277600	1.50136000	-1.09627100
C	3.99498800	0.62695400	0.63982900	C	2.80720800	-0.95469700	-0.43901000
C	4.61457900	-0.26285700	-0.26409300	C	4.15797000	-1.04193600	-0.83096700
C	3.85759800	-1.11012800	-1.09544300	C	4.61388500	-0.24216200	-1.89294000
C	2.46412800	-1.02974400	-0.98712200	C	3.71349200	0.62651300	-2.53698400
H	3.21540900	2.60140100	2.61352600	C	2.38274500	0.66626900	-2.08726100
H	1.52765200	3.88460700	3.94205600	C	2.22061400	-1.75593100	0.66530600

C	2.91516600	-2.80107700	1.30441900	
C	2.29584100	-3.51610400	2.34131400	[C3]3+
C	0.98666400	-3.17134500	2.72171600	Co 0.00003000 0.00020300 0.00005000
C	0.34308400	-2.12606500	2.04514100	C -2.25604400 -1.58626000 -0.57014600
H	4.84668500	-1.70665100	-0.32378200	C -3.06921500 -2.56288800 -1.16420700
H	5.65112200	-0.29565000	-2.20792400	C -2.57429000 -3.30108600 -2.25200700
H	4.02704100	1.25716600	-3.36150800	C -1.27530100 -3.04234000 -2.72212000
H	1.65476200	1.31964700	-2.55506300	C -0.50578600 -2.05672500 -2.08885000
H	3.91993100	-3.06153600	0.99596100	C -2.65361600 -0.74916000 0.57198200
H	2.82316500	-4.32384300	2.83839400	C -3.92332800 -0.76486100 1.16796000
H	0.47039800	-3.69380100	3.51902400	C -4.18251300 0.08388100 2.25691000
H	-0.66172200	-1.82522000	2.30918200	C -3.16209400 0.92925000 2.72542400
N	1.94184000	-0.10388300	-1.06482100	C -1.91311600 0.90612000 2.08962900
N	0.94024100	-1.43349000	1.04087200	H -4.06745900 -2.74995100 -0.78899300
C	-2.80726500	-0.95460900	0.43902300	H -3.19079600 -4.06020900 -2.72095600
C	-4.15804400	-1.04176100	0.83094600	H -0.85585500 -3.58520200 -3.56070900
C	-4.61398100	-0.24181800	1.89278100	H 0.49139700 -1.83116300 -2.43547700
C	-3.71359400	0.62693800	2.53672500	H -4.69833900 -1.42155900 0.79347800
C	-2.38283000	0.66659600	2.08704300	H -5.15945600 0.08296000 2.72789100
C	-2.22065300	-1.75602000	-0.66515700	H -3.31794100 1.59677100 3.56446000
C	-2.91520800	-2.80125800	-1.30411800	H -1.10887800 1.53861800 2.43418400
C	-2.29587600	-3.51645400	-2.34089300	N -0.98673900 -1.34568600 -1.03760800
C	-0.98669000	-3.17176700	-2.72132900	N -1.66590900 0.08441500 1.03805100
C	-0.34311200	-2.12638700	-2.04490300	C 1.97782400 -1.92247000 0.57025300
H	-4.84675500	-1.70653900	0.32383700	C 2.62799600 -3.01402500 1.16506600
H	-5.65123000	-0.29523900	2.20773700	C 2.02262900 -3.66589200 2.25222800
H	-4.02715900	1.25772200	3.36114200	C 0.77897100 -3.20807600 2.72033000
H	-1.65485100	1.32002800	2.55477500	C 0.17332700 -2.11444400 2.08649600
H	-3.91998000	-3.06165900	-0.99563500	C 2.50246300 -1.15810800 -0.57166100
H	-2.82320100	-4.32426400	-2.83785600	C 3.75417000 -1.37298900 -1.16720500
H	-0.47041700	-3.69434900	-3.51855000	C 4.14392500 -0.57576300 -2.25612400
H	0.66169900	-1.82559400	-2.30898300	C 3.26870800 0.41855400 -2.72589300
N	-1.94190400	-0.10372100	1.06473600	C 2.03134600 0.59179500 -2.09069600
N	-0.94027200	-1.43365100	-1.04074900	H 3.58528800 -3.35461200 0.79092000

H	2.51286600	-4.51156700	2.72208500	C	-4.03932900	-0.07228700	-1.21020200
H	0.27876000	-3.67933000	3.55792100	C	-4.73172700	-0.09253100	0.01667800
H	-0.77746600	-1.73693700	2.43156000	C	-4.02469000	-0.08360300	1.23230000
H	4.41648700	-2.14278000	-0.79213800	C	-1.69766600	-0.04070000	2.35162800
H	5.10920800	-0.72966500	-2.72604900	C	0.57410300	-0.00273000	2.97449900
H	3.52746700	1.05282600	-3.56529100	C	0.23569500	-0.00708900	4.33850300
H	1.33638500	1.34271200	-2.43589900	C	-1.12165300	-0.02935100	4.70318700
N	0.76111700	-1.48644200	1.03650400	C	-2.10187500	-0.04620600	3.69464700
N	1.65804400	-0.18005300	-1.03843800	H	-4.58270200	-0.07931400	-2.14747600
C	-0.24714700	2.74594100	-0.57058300	H	-5.81605400	-0.11534900	0.02333800
C	-0.68908800	3.93815700	-1.16345800	H	-4.55821100	-0.09984200	2.17503000
C	-1.57691100	3.87801400	-2.25044700	H	1.60989400	0.01480400	2.66018200
C	-2.00196100	2.62338300	-2.72007000	H	1.02138500	0.00666400	5.08522900
C	-1.53097000	1.46457900	-2.08780500	H	-1.41363300	-0.03314100	5.74813100
C	0.67881500	2.67251600	0.57002300	H	-3.15398800	-0.06230000	3.95377800
C	1.30292600	3.78030900	1.16264600	C	0.51999600	0.02803300	-3.01068900
C	2.16861200	3.58153100	2.25091100	C	-1.10076800	0.01577100	-4.66121600
C	2.38885900	2.27589700	2.72226600	C	-2.11762800	-0.01241800	-3.69088400
C	1.74186000	1.20546100	2.08972900	C	-1.72690900	-0.01892200	-2.34461500
H	-0.35313100	4.89668000	-0.78873000	H	1.56736700	0.04471400	-2.73993200
H	-1.92757700	4.79135200	-2.71856200	H	-1.33653800	0.02231800	-5.71986700
H	-2.68271800	2.53101900	-3.55785000	H	-3.15842000	-0.02735100	-3.98727600
H	-1.83544400	0.48777700	-2.43245600	N	-0.39046400	0.00074500	-2.01002600
H	1.12263300	4.77957300	0.78715700	N	-1.96925900	-0.03518600	0.00291600
H	2.65843400	4.42842600	2.71902000	N	-0.36639500	-0.01948700	2.00149700
H	3.04514300	2.07787100	3.56128000	C	2.56682800	-1.15138200	-0.02427900
H	1.88777400	0.19317500	2.43566700	C	2.52076800	1.22598200	-0.01316000
N	-0.67333600	1.52624600	-1.03766900	C	3.92900500	1.27235500	-0.02531000
N	0.90626700	1.40093800	1.03811000	C	4.65397900	0.07144700	-0.03771600
				C	3.97114400	-1.15725700	-0.03688700
[Z1]2+				C	1.73487800	-2.37916600	-0.02073500
Co	-0.07627000	-0.00167600	-0.00358900	C	-0.43292900	-3.25117900	-0.01590000
C	-2.61819400	-0.05397500	1.19752400	C	1.32797700	-4.74737100	-0.01315600
C	-2.63672200	-0.04317200	-1.18388300	C	2.25082300	-3.68734600	-0.01700300

H	4.45168600	2.22030300	-0.02577200	H	5.71358200	-0.02615200	-0.03516700
H	5.73834800	0.09070500	-0.04790000	H	4.48765400	1.57803600	1.42588400
H	4.52439000	-2.08782500	-0.04671900	H	-1.71902000	1.90938500	1.74604000
H	-1.50184500	-3.07413500	-0.01519400	H	-1.15967600	3.69520100	3.37493600
H	1.66178400	-5.77951600	-0.01019600	H	1.26540000	4.21779400	3.84038800
H	3.31308900	-3.89337800	-0.01622100	H	3.03394900	2.91450300	2.64383800
C	-0.57565800	3.18945800	0.01566300	C	-0.70350700	-2.17071000	-1.96192300
C	-0.15982300	4.53288300	0.02914800	C	0.86074700	-3.43746800	-3.10615200
C	1.21893500	4.81119400	0.02825900	C	1.91576300	-2.74527100	-2.48338200
C	2.13592500	3.74521200	0.01415900	C	1.57807800	-1.73760600	-1.57429700
C	1.64677100	2.42568000	0.00110400	H	-1.74131400	-1.94771800	-1.75897900
H	-1.62942700	2.93237400	0.01602200	H	1.05471300	-4.22934700	-3.82084400
H	-0.89721300	5.32781000	0.03992600	H	2.94589700	-2.99118300	-2.70626800
H	1.57590800	5.83593200	0.03856000	N	0.24976300	-1.45532700	-1.31843300
H	3.20007000	3.94806000	0.01411500	N	1.88630400	-0.01204400	-0.01252900
N	0.30476700	2.16365500	0.00189200	N	0.27273600	1.44336600	1.31299400
N	1.87236000	0.02503700	-0.01469200	C	-2.52961800	0.81684500	-0.89220800
N	0.38206600	-2.17363100	-0.01996500	C	-2.53188700	-0.78988100	0.87938600
N	0.21733400	0.03645300	-4.32771700	C	-3.93798000	-0.80520500	0.89533100
N	-0.01671400	-4.53962300	-0.01259600	C	-4.62950200	0.01785200	-0.01269300
				C	-3.93029500	0.84166100	-0.92003100
[Z1]3+				C	-1.58590200	1.57717000	-1.72859100
Co	-0.00002700	0.00034300	-0.00108900	C	0.69371700	1.97305600	-2.16442100
C	2.53579300	0.87065300	0.78772400	C	-0.87617300	3.12056500	-3.42118300
C	2.52553400	-0.90081100	-0.81912400	C	-1.92808400	2.49072400	-2.73067100
C	3.92606800	-0.92977600	-0.84966800	H	-4.48054600	-1.43514900	1.58915400
C	4.62937600	-0.02283700	-0.02891100	H	-5.71372700	0.01941500	-0.01537500
C	3.94195600	0.88525900	0.79749100	H	-4.46633100	1.47431200	-1.61667600
C	1.60536400	1.71450600	1.55667200	H	1.73249400	1.77223200	-1.94416000
C	-0.68599200	2.14616400	1.95821000	H	-1.07368600	3.83917200	-4.20863000
C	-0.36168900	3.15579300	2.87887700	H	-2.95929700	2.71248000	-2.97301100
C	0.98877300	3.44253300	3.13436600	C	0.69574000	-1.94703000	2.15222900
C	1.98539100	2.71065400	2.46250300	C	0.37613300	-2.86304100	3.16756400
H	4.45890300	-1.62724600	-1.48410700	C	-0.97302600	-3.12187100	3.45745800

C	-1.97305000	-2.45693700	2.72388200	H	1.41376500	-0.07231500	-2.91084600
C	-1.59763600	-1.55454700	1.72286800	H	-1.81405000	-0.46410800	-5.52484800
H	1.72766000	-1.73251600	1.91268400	N	-0.47426200	-0.15548100	-1.99856400
H	1.17662800	-3.35314200	3.70870000	N	-1.96568200	-0.12626600	0.08698400
H	-1.24606600	-3.82496400	4.23664200	N	-0.29141700	0.08768000	2.00917300
H	-3.02067400	-2.64058400	2.93044900	C	2.62125900	-1.01371700	-0.05614100
N	-0.26627500	-1.30924900	1.44712200	C	2.45397000	1.34646000	-0.18852600
N	-1.88638600	0.01126100	-0.00543700	C	3.85983700	1.45276000	-0.25428900
N	-0.25631900	1.32223900	-1.45143900	C	4.64343300	0.28941200	-0.21819500
N	-0.44174400	-3.15262500	-2.84730000	C	4.02037700	-0.96867400	-0.11706200
N	0.42758100	2.86431300	-3.13982500	C	-0.19767400	-3.32306700	0.17929100
				C	1.73691300	-4.56285700	0.20096300
[Z2]2+				H	4.33520900	2.42234900	-0.33270800
Co	-0.07664700	0.00299500	-0.00251000	H	5.72444300	0.36059800	-0.26801000
C	-2.56773800	-0.10285700	1.30366900	H	4.58742000	-1.89063900	-0.08536800
C	-2.68051300	-0.24861100	-1.06303500	H	-1.27893000	-3.26984300	0.20874600
C	-4.07644300	-0.35127200	-1.04434700	H	2.23091000	-5.52622000	0.24832900
C	-4.72259800	-0.32529300	0.20901300	C	-0.73963000	3.14369900	-0.18004900
C	-3.97106100	-0.20196400	1.39142700	C	-0.39607100	4.50551000	-0.25737300
C	-1.60595500	0.02693700	2.41596500	C	0.96461700	4.85536400	-0.31449400
C	0.68440800	0.20917400	2.93883400	C	1.93751200	3.83991000	-0.29372600
C	0.39967100	0.27464000	4.31373800	C	1.52051300	2.49899800	-0.21587700
C	-0.93928800	0.21227000	4.73567400	H	-1.77778400	2.83337500	-0.13461500
C	-1.95652400	0.08653900	3.77206700	H	-1.17494900	5.25964500	-0.27191100
H	-4.62701900	-0.44816800	-1.97219000	H	1.26566500	5.89618000	-0.37413900
H	-5.80301600	-0.40217700	0.26262700	H	2.98878800	4.09786300	-0.33696300
H	-4.46856100	-0.18437000	2.35370400	N	0.19433100	2.16638200	-0.15933300
H	1.70543900	0.25370600	2.58189600	N	1.86487600	0.12092100	-0.09365200
H	1.21232900	0.37141000	5.02449500	N	0.49959000	-2.16638800	0.08451800
H	-1.18987000	0.25997500	5.79016700	N	-0.09023700	-0.26768900	-4.35131500
H	-2.99548100	0.03684000	4.07623900	N	0.37844900	-4.54828300	0.24079400
C	0.34788000	-0.15935500	-3.07540500	C	1.86069300	-2.27610500	0.04999700
C	-1.43388700	-0.37357200	-4.51435800	N	2.51805500	-3.45961600	0.10602600
C	-1.82282100	-0.26196100	-2.25751600	N	-2.33514900	-0.37257000	-3.50010200

[Z2]3+

Co 0.00000500 -0.00010000 0.00031600
C 2.53396100 0.85990100 0.81272200
C 2.53772400 -0.83133900 -0.86790000
C 3.93391400 -0.84926800 -0.92195000
C 4.63533700 0.02999300 -0.06628800
C 3.94293200 0.88944100 0.80623800
C 1.59889500 1.65381700 1.62739800
C -0.69751100 2.03010400 2.06391300
C -0.38082900 2.99825300 3.03108700
C 0.96669300 3.29286900 3.29116700
C 1.96993200 2.60989100 2.57794400
H 4.44548300 -1.52019800 -1.60130900
H 5.71927800 0.04257800 -0.08169800
H 4.48627600 1.56012000 1.46032100
H -1.72856000 1.78859000 1.84748000
H -1.18319600 3.50014900 3.55831000
H 1.23678100 4.03696700 4.03227100
H 3.01658000 2.82055500 2.76251800
C -0.64278200 -2.13434900 -2.07337700
C 1.03586400 -3.24908600 -3.18740300
C 1.59961600 -1.64786000 -1.64931800
H -1.69649000 -1.97266600 -1.89231500
H 1.34005700 -3.99266100 -3.91393800
N 0.26600000 -1.39901000 -1.38487800
N 1.88836600 0.00716400 -0.01889400
N 0.26741600 1.37565100 1.37869200
C -2.53767700 0.83116400 -0.86807600
C -2.53400400 -0.86002100 0.81260600
C -3.94297300 -0.88958200 0.80601400
C -4.63533100 -0.03022800 -0.06663900
C -3.93386200 0.84901900 -0.92227700
C 0.64292500 2.13400200 -2.07344100

C -1.03559800 3.24873800 -3.18766300
H -4.48638600 -1.56012500 1.46018200
H -5.71927000 -0.04288900 -0.08214400
H -4.44536600 1.51991200 -1.60172300
H 1.69662100 1.97214700 -1.89248300
H -1.33971300 3.99224800 -3.91429800
C 0.69735200 -2.02943500 2.06482500
C 0.38058000 -2.99715300 3.03239900
C -0.96695600 -3.29204100 3.29210400
C -1.97011100 -2.60965500 2.57819700
C -1.59898400 -1.65377700 1.62750000
H 1.72843200 -1.78799800 1.84844000
H 1.18289200 -3.49855600 3.56017300
H -1.23712800 -4.03587000 4.03344800
H -3.01676400 -2.82063400 2.76238000
N -0.26749500 -1.37545500 1.37903300
N -1.88835900 -0.00729400 -0.01897700
N -0.26595200 1.39889900 -1.38482200
N -0.29343100 -3.06826600 -2.98314800
N 0.29367600 3.06776400 -2.98342100
C -1.59953100 1.64772200 -1.64943600
N -2.01232000 2.56113200 -2.54166200
N 2.01251000 -2.56139600 -2.54138100

[Z3]2+

Co 0.00006000 -0.00004300 -0.09638300
C 2.73901300 0.24659800 0.74202700
C 2.00577200 1.80613900 -0.90761600
C 3.27409900 2.40024100 -0.95669600
C 4.29311200 1.89140200 -0.12864700
C 4.03028800 0.81503100 0.72896600
C 2.35130100 -0.87734000 1.61272300
C 0.41925900 -2.20591100 2.29351800
C 1.16563500 -2.93150500 3.13809600

C	2.65476400	-2.71312000	3.31776300	H	-0.67787400	3.71282800	3.71148200
C	3.14899400	-1.58185400	2.44353600	H	-2.88937500	2.49795300	4.36857700
H	3.47193600	3.23838100	-1.61277800	H	-4.20518900	1.33359000	2.49338500
H	5.28145600	2.33800600	-0.14963000	C	1.45409800	-1.82828500	-2.10768700
H	4.80795900	0.43042100	1.37655400	C	1.51179000	-2.87220100	-3.04574400
H	-0.64249100	-2.31464500	2.12168100	C	0.34474100	-3.61223700	-3.30795300
H	0.67490000	-3.70898400	3.71574400	C	-0.84142100	-3.28996500	-2.62549200
H	2.88734900	-2.49592700	4.37156400	C	-0.82993800	-2.23495200	-1.69751200
H	4.20363500	-1.33222300	2.49694200	H	2.33094200	-1.23432200	-1.88058400
C	-1.45287900	1.82720200	-2.10905500	H	2.44586500	-3.09156500	-3.55036300
C	-1.51022300	2.87095300	-3.04731500	H	0.35540600	-4.42410800	-4.02780900
C	-0.34316000	3.61115300	-3.30899600	H	-1.74829900	-3.85091700	-2.81739500
C	0.84268800	3.28918400	-2.62584500	N	0.31259700	-1.51697900	-1.45032400
C	0.83087800	2.23432400	-1.69770400	N	-1.76532000	-0.74667200	-0.07322200
H	-2.32974900	1.23314400	-1.88232300	O	0.95773400	-1.15884900	1.48968500
H	-2.44405900	3.09008500	-3.55247400	O	-0.95834300	1.15900300	1.48934300
H	-0.35357200	4.42292000	-4.02897200	H	-3.21243800	3.63594300	3.08060800
H	1.74957700	3.85025700	-2.81734200	H	3.20973600	-3.63465900	3.08407300
N	-0.31167700	1.51621400	-1.45101200				
N	1.76543700	0.74656900	-0.07257500	[Z3]3+			
C	-2.73919100	-0.24671500	0.74103400	Co	-0.00004700	-0.00001900	0.06839800
C	-2.00519400	-1.80655300	-0.90804300	C	-2.68590400	-0.13081800	-0.79413700
C	-3.27339700	-2.40089400	-0.95729900	C	-2.18010500	1.54702400	0.84428000
C	-4.29269000	-1.89213300	-0.12953600	C	-3.50560600	1.99079100	0.85338500
C	-4.03029800	-0.81554900	0.72792700	C	-4.43255900	1.34291100	0.00672000
C	-2.35206000	0.87771900	1.61135300	C	-4.03432600	0.28219600	-0.82138200
C	-0.42083500	2.20775400	2.29162800	C	-2.09081700	-1.21249100	-1.58004700
C	-1.16791200	2.93408400	3.13495000	C	0.09473500	-2.25337400	-2.08166500
C	-2.65690200	2.71485300	3.31468100	C	-0.49315900	-3.12918000	-2.90311100
C	-3.15043800	1.58295600	2.44087600	C	-1.98154400	-3.16929700	-3.16297800
H	-3.47092100	-3.23923300	-1.61322200	C	-2.70213000	-2.08588300	-2.40251300
H	-5.28091400	-2.33901200	-0.15058800	H	-3.81958800	2.80816300	1.49032000
H	-4.80814900	-0.43109600	1.37539100	H	-5.46609800	1.67104400	-0.00458600
H	0.64089000	2.31691400	2.11990000	H	-4.74895400	-0.20598800	-1.47219300

H	1.15001700	-2.17777700	-1.87315500	C	-0.06371500	-3.47755600	3.24572500
H	0.14662400	-3.84322700	-3.41252600	C	1.10225000	-3.10375400	2.55388200
H	-2.18577800	-3.06169900	-4.23848000	C	1.04491300	-2.05014700	1.63517200
H	-3.77772600	-2.00878700	-2.52857000	H	-2.17429400	-1.18550100	1.86575100
C	1.26620000	1.73671000	2.06987700	H	-2.17983600	-3.03931300	3.51506200
C	1.25886000	2.78559100	3.00082200	H	-0.03416400	-4.29267100	3.96044700
C	0.06156600	3.47887500	3.24429700	H	2.03628600	-3.62410200	2.72793200
C	-1.10399000	3.10464800	2.55199500	N	-0.14287500	-1.38366100	1.40274500
C	-1.04603900	2.05067300	1.63374300	N	1.81709700	-0.51321800	0.03012700
H	2.17314600	1.18645700	1.86645300	O	-0.65723400	-1.25207900	-1.36309200
H	2.17758700	3.04098300	3.51494900	O	0.65820500	1.25183600	-1.36281600
H	0.03154100	4.29428200	3.95866400	H	2.39734300	4.15032400	-2.88851700
H	-2.03817500	3.62496600	2.72533800	H	-2.39480700	-4.15139700	-2.88860000
N	0.14195900	1.38424800	1.40219900				
N	-1.81716500	0.51311500	0.02877700	[Z4]2+			
C	2.68635300	0.13028300	-0.79258400	Co	0.07938800	-0.10105800	-0.11006800
C	2.17946000	-1.54694000	0.84612200	N	0.55478400	-0.11902400	1.84841400
C	3.50487200	-1.99095400	0.85599700	N	-0.48668700	2.03363400	-0.00745700
C	4.43234400	-1.34354600	0.00954000	N	1.97455000	0.03501700	-0.27845000
C	4.03470000	-0.28302300	-0.81909400	N	-1.87385400	-0.23337700	0.04033200
C	2.09187000	1.21185700	-1.57908500	N	-0.14580700	-2.30869300	-0.12119100
C	-0.09315700	2.25336100	-2.08171100	N	0.15970100	-0.04595100	-2.09469200
C	0.49533500	3.12879700	-2.90312300	C	-0.64221500	-0.07778600	-3.12754900
C	1.98381000	3.16825700	-3.16258900	C	1.55433900	0.08800100	-3.94013900
C	2.70378900	2.08490200	-2.40146900	H	-1.71805400	-0.15242800	-3.03387200
H	3.81839700	-2.80818400	1.49334200	H	2.41831500	0.15931100	-4.58649700
H	5.46581900	-1.67189900	-0.00118800	C	1.90853400	-0.03779200	2.08378400
H	4.74971200	0.20478800	-1.46976200	C	2.42522700	-0.04193600	3.38910200
H	-1.14852600	2.17822800	-1.87344400	C	1.53731500	-0.12901300	4.47586300
H	-0.14399900	3.84306100	-3.41279900	C	0.15538000	-0.21000900	4.22684400
H	2.18830900	3.06012800	-4.23799100	C	-0.29721900	-0.20259300	2.89712100
H	3.77943600	2.00755400	-2.52693600	C	2.72567800	0.04896200	0.85651000
C	-1.26751800	-1.73573900	2.06994700	C	4.12536400	0.13706800	0.77468100
C	-1.26080000	-2.78423300	3.00133100	C	4.72418300	0.20614800	-0.49926100

C	3.93168100	0.18569500	-1.66120500	C	-1.56363100	-2.60778300	-0.03118200
C	2.53508500	0.09752300	-1.51908100	C	-0.43178200	-4.63081800	-0.13686100
H	3.49406800	0.02079500	3.55813400	H	-0.33379700	-5.26215000	-1.03269300
H	1.91732000	-0.13336900	5.49223000	H	-0.21813100	-5.28687500	0.72036900
H	-0.56179500	-0.27825200	5.03704500				
H	-1.35359600	-0.26408800	2.66798300	[Z4]3+			
H	4.73679700	0.15214100	1.66870500	Co	-0.00000700	-0.13225400	-0.00007500
H	5.80377600	0.27455100	-0.58318900	N	-0.45682900	1.24905200	-1.32705400
H	4.38236000	0.23634500	-2.64574800	N	0.45679400	1.24838000	1.32761400
C	0.50103800	-3.44364000	-0.18116700	N	-1.88082700	-0.16119100	0.25477100
C	-1.77870300	-3.95472800	-0.03759900	N	1.88081200	-0.16102600	-0.25496200
H	1.58097600	-3.49564100	-0.25406800	N	0.02779400	-1.49274200	-1.38363800
H	-2.72375300	-4.47776600	0.01778800	N	-0.02777400	-1.49334900	1.38288500
C	-1.84214700	2.18092400	0.08245300	C	0.82810700	-2.23220400	2.03884700
C	-2.43496900	3.45699800	0.14884700	C	-1.33316800	-2.75905900	2.80269900
C	-1.60994600	4.59492100	0.12296400	H	1.89796000	-2.19009600	1.88227600
C	-0.21508900	4.43308200	0.03180500	H	-2.16266800	-3.19924300	3.33818500
C	0.30609600	3.12868100	-0.03175000	C	-1.81189800	1.48950200	-1.42425200
C	-2.61671800	0.91296800	0.10346100	C	-2.31119200	2.44276600	-2.32023600
C	-4.01951200	0.84937500	0.18084700	C	-1.41189700	3.15903400	-3.13054900
C	-4.64900000	-0.40857500	0.19163000	C	-0.03472200	2.90306200	-3.02135500
C	-3.87593500	-1.57654400	0.12451600	C	0.41002200	1.93718700	-2.10518500
C	-2.47385100	-1.46154000	0.04763100	C	-2.63396700	0.66757800	-0.51767900
H	-3.50979600	3.57205700	0.21907000	C	-4.03005800	0.65735700	-0.38447100
H	-2.04888700	5.58624800	0.17323600	C	-4.60834500	-0.22058200	0.55635800
H	0.45292100	5.28703400	0.00969900	C	-3.80695600	-1.07045800	1.34058700
H	1.37489700	2.95643100	-0.10338700	C	-2.41285300	-1.02383100	1.16526400
H	-4.61522500	1.75192000	0.23107000	H	-3.37697400	2.62543400	-2.38680200
H	-5.73048800	-0.47321300	0.25073400	H	-1.78163800	3.90074600	-3.83020800
H	-4.34313400	-2.55438300	0.12988300	H	0.69004800	3.43361600	-3.62731800
C	1.53134600	0.05670500	-2.58083200	H	1.46389500	1.71932200	-1.99946000
C	0.12434000	0.00231700	-4.42345800	H	-4.65437800	1.30523300	-0.98713800
H	-0.17732800	0.87545700	-5.02136300	H	-5.68631500	-0.24164200	0.67468700
H	-0.05903500	-0.87644700	-5.05982200	H	-4.24941800	-1.74724500	2.06167900

C	-0.82806800	-2.23134700	-2.03991100	N	1.97020200	-0.03227500	-0.23934200
C	1.33320000	-2.75761100	-2.80419200	N	-1.87909600	-0.17205000	-0.03383600
H	-1.89791400	-2.18941300	-1.88323300	N	-0.29701500	-2.29545900	-0.33443900
H	2.16270500	-3.19745200	-3.33995100	N	0.25437700	0.11704600	-2.11328800
C	1.81186800	1.48872600	1.42498900	C	-0.40947800	0.22970400	-3.27138000
C	2.31118700	2.44131900	2.32167300	C	1.67046700	0.34235600	-3.85087300
C	1.41191400	3.15699300	3.13253400	N	1.60531700	0.19038300	-2.48942300
C	0.03473300	2.90112900	3.02315500	H	-1.48479600	0.21270400	-3.33527000
C	-0.41004100	1.93595900	2.10625800	H	2.58816100	0.42806400	-4.40897400
C	2.63394000	0.66734100	0.51792600	C	1.86100100	-0.30948200	2.10347700
C	4.03003400	0.65720400	0.38472100	C	2.35298100	-0.45128200	3.40927700
C	4.60833200	-0.22018500	-0.55661400	C	1.44102600	-0.58940800	4.47130200
C	3.80695100	-1.06964100	-1.34130700	C	0.06268700	-0.58134400	4.19604200
C	2.41285100	-1.02316700	-1.16591600	C	-0.36568700	-0.43712400	2.86544000
H	3.37697600	2.62391100	2.38836500	C	2.70439500	-0.15744800	0.90143200
H	1.78167400	3.89815800	3.83276200	C	4.10666700	-0.13591800	0.83301400
H	-0.69002100	3.43124000	3.62952800	C	4.72079300	0.00892600	-0.42622200
H	-1.46392600	1.71822100	2.00036700	C	3.94821500	0.12640500	-1.59788400
H	4.65435400	1.30471700	0.98778100	C	2.55824900	0.09759100	-1.44657100
H	5.68630000	-0.24115100	-0.67496800	H	3.42012200	-0.45564200	3.59876400
H	4.24941400	-1.74600900	-2.06279400	H	1.80108700	-0.70070600	5.48864100
C	-1.37951700	-1.80135000	1.84016300	H	-0.67214200	-0.68515400	4.98614000
C	0.11610600	-3.12399000	3.01737800	H	-1.42012300	-0.42889300	2.62031400
H	0.45516600	-2.94224200	4.04857500	H	4.70984300	-0.23032300	1.72717300
H	0.32444900	-4.18640600	2.81961200	H	5.80270000	0.02707500	-0.49866300
C	1.37953000	-1.80040100	-1.84116200	H	4.41661000	0.23016700	-2.56880400
C	-0.11605800	-3.12255200	-3.01896300	C	0.18439700	-3.53821300	-0.45741300
H	-0.32429700	-4.18509200	-2.82176800	C	-1.95122000	-3.83094000	-0.38482200
H	-0.45521000	-2.94026900	-4.05003700	N	-1.68391100	-2.48481700	-0.28811200
[Z5]2+				H	1.23936200	-3.74871100	-0.52175600
Co	0.07447900	-0.08389500	-0.11161700	H	-2.93903300	-4.25970200	-0.37156300
N	0.50870600	-0.30566700	1.84104700	C	-1.76198600	2.22379800	0.20515900
N	-0.41069900	2.02527100	0.13779600	C	-2.30524100	3.51160600	0.36828600
				C	-1.43410800	4.61114200	0.46458000

C	-0.04571800	4.39759000	0.39634200	C	-0.56082800	1.21012500	2.54427500
C	0.42604100	3.08306500	0.23174400	C	2.59209100	0.40050500	0.87056300
C	-2.58528800	0.99451600	0.09318600	C	3.99299900	0.38229100	0.82531000
C	-3.99020900	0.97148700	0.10754700	C	4.62206000	-0.18892400	-0.29950400
C	-4.65738300	-0.25949200	-0.01549900	C	3.87238800	-0.73650100	-1.36063700
C	-3.92590300	-1.44963500	-0.15237700	C	2.48167300	-0.68319400	-1.24388700
C	-2.52781500	-1.35322000	-0.15485200	H	3.19906200	1.66041700	3.30066900
H	-3.37615600	3.66542800	0.42159300	H	1.50241900	2.47884800	4.94690400
H	-1.83391700	5.61198800	0.59091400	H	-0.94810800	2.17621300	4.42761800
H	0.65717000	5.22010300	0.46745400	H	-1.60538200	1.07142200	2.30253300
H	1.48900000	2.87580800	0.17524900	H	4.58330200	0.79494000	1.63353800
H	-4.55962100	1.88600500	0.20916800	H	5.70474100	-0.21150500	-0.35218300
H	-5.74132400	-0.29268800	-0.00886100	H	4.36024900	-1.17736200	-2.22069600
H	-4.43104900	-2.40171000	-0.25652000	C	0.51668800	-2.89564000	1.38209000
N	0.42892700	0.36988800	-4.36440600	C	-1.55771800	-3.42956800	1.69665800
N	-0.80225600	-4.51470800	-0.49241900	N	-1.52225600	-2.21393300	1.06823600
				H	1.59290800	-2.94641300	1.38827500
[Z5]3+				H	-2.46407100	-3.94003800	1.97817800
Co	0.00020900	-0.12933200	-0.04186700	C	-1.70866500	1.87547200	-1.01924700
N	0.36085000	0.76588100	1.65973800	C	-2.14226600	3.06355300	-1.61644900
N	-0.36129400	1.59308100	-0.89677400	C	-1.18645800	3.97915200	-2.09406100
N	1.88728400	-0.12980100	-0.16610000	C	0.17882100	3.68058200	-1.95847500
N	-1.88688500	-0.20359300	0.05822900	C	0.55970500	2.47292800	-1.35188400
N	-0.17404000	-1.86867300	0.86377900	C	-2.59218600	0.83245700	-0.47256500
N	0.17494500	-1.00812600	-1.79459000	C	-3.99307600	0.79148000	-0.44465800
C	-0.51555400	-1.53656200	-2.81648600	C	-4.62168100	-0.32976300	0.13404100
C	1.55900500	-1.78387700	-3.38417100	C	-3.87150700	-1.39474300	0.67333900
N	1.52327600	-1.16877800	-2.16174300	C	-2.48087100	-1.28303500	0.60883600
H	-1.59178100	-1.57347000	-2.85204300	H	-3.20100500	3.27439400	-1.70788300
H	2.46541500	-2.03178800	-3.91165100	H	-1.50571900	4.90493800	-2.55977700
C	1.70794900	0.92580900	1.92397900	H	0.94535300	4.36001500	-2.31125600
C	2.14054300	1.54044100	3.10351000	H	1.60453900	2.22084100	-1.23537800
C	1.18397500	2.00043100	4.02733600	H	-4.58372800	1.59938800	-0.85743700
C	-0.18101600	1.83418000	3.74333900	H	-5.70433100	-0.37878300	0.16473000

H	-4.35885400	-2.25549000	1.11340700	C	2.20809300	2.57671400	-2.44976700
N	0.30603100	-2.02226100	-3.81035300	H	4.49090300	-1.67062900	1.65373800
N	-0.30463600	-3.87239500	1.90177400	H	5.77624700	-0.16762600	0.12233700
				H	4.56021300	1.41129700	-1.37587200
[Z6]2+				H	-1.54595000	2.11457000	-1.71097400
Co	-0.00000100	0.00000500	0.07901100	H	-0.83528400	3.81759200	-3.39841500
C	-2.60419100	-0.75697900	-0.70523000	H	1.62736200	4.10107900	-3.87250700
C	-2.56716100	0.94189100	0.96612100	H	3.26912200	2.68344300	-2.64102300
C	-3.97670500	0.99175400	0.98371000	N	1.91663600	-0.08863900	0.12049400
C	-4.69169600	0.14445500	0.12548900	N	0.39380300	1.49783300	-1.26638800
C	-4.00679900	-0.74621800	-0.72509400	C	-1.71732700	1.75018800	1.82203500
C	-1.73673600	-1.64428800	-1.51113000	C	-1.88910100	2.73833900	2.76667100
C	0.49727600	-2.26589600	-1.93599600	C	-0.57744800	3.10327400	3.25190400
C	0.09155300	-3.21971300	-2.88418000	H	-2.82795300	3.16639500	3.08537000
C	-1.28172700	-3.37474900	-3.14429200	C	0.34261300	2.32761900	2.58915400
C	-2.20803700	-2.57665300	-2.44987500	H	-0.35589100	3.84948100	3.99992000
H	-4.49094300	1.67059500	1.65367800	H	1.41675400	2.24024700	2.61295600
H	-5.77625400	0.16757200	0.12226800	C	1.71728500	-1.75021500	1.82204400
H	-4.56018400	-1.41131200	-1.37595500	C	1.88904600	-2.73835900	2.76669000
H	1.54598800	-2.11454600	-1.71096200	C	0.57737400	-3.10340100	3.25179300
H	0.83536400	-3.81749800	-3.39849300	H	2.82789200	-3.16642100	3.08539800
H	-1.62727000	-4.10095000	-3.87267300	C	-0.34266400	-2.32762100	2.58915700
H	-3.26905900	-2.68336000	-2.64118000	H	0.35579800	-3.84969100	3.99972100
N	-1.91664100	0.08863400	0.12046200	H	-1.41680300	-2.24022900	2.61296500
N	-0.39377600	-1.49782400	-1.26640500	O	-0.33235700	1.47831000	1.69777800
C	2.60420500	0.75697400	-0.70518100	O	0.33232100	-1.47830300	1.69780300
C	2.56713600	-0.94191400	0.96614900				
C	3.97667900	-0.99178600	0.98376100	[Z6]3+			
C	4.69168900	-0.14450400	0.12553900	Co	0.00000000	-0.00000200	-0.10135800
C	4.00681300	0.74620500	-0.72502200	C	-2.60562100	0.63663700	0.66509900
C	1.73676800	1.64430400	-1.51107900	C	-2.46176400	-1.06142500	-1.02284300
C	-0.49723300	2.26592400	-1.93597900	C	-3.86659600	-1.16212200	-1.07093300
C	-0.09148600	3.21978200	-2.88411200	C	-4.62641000	-0.33678400	-0.22585600
C	1.28180100	3.37483900	-3.14417400	C	-4.00329400	0.57798900	0.65206600

C	-1.73513700	1.50015100	1.47786700	C	-1.47998400	-2.78436500	-2.77133100
C	0.53343200	2.05475900	1.91719900	C	-0.09503500	-3.03471000	-3.11174700
C	0.14081300	3.00851700	2.86774400	H	-2.33820800	-3.28076200	-3.19967100
C	-1.22691600	3.20237400	3.12202700	C	0.69174400	-2.20942400	-2.35739100
C	-2.17447900	2.43739600	2.41836500	H	0.26245300	-3.74926500	-3.83753100
H	-4.34490100	-1.86015600	-1.74697800	H	1.75265600	-2.04323300	-2.27201900
H	-5.70873500	-0.40067000	-0.24936400	C	1.50481000	1.80678700	-1.81122800
H	-4.59680800	1.21487200	1.29577100	C	1.47996500	2.78429400	-2.77141000
H	1.57942700	1.88337800	1.70775200	C	0.09501300	3.03461600	-3.11183500
H	0.90130500	3.57662200	3.38961500	H	2.33818400	3.28069100	-3.19975900
H	-1.55364100	3.93269000	3.85403000	C	-0.69175800	2.20934000	-2.35745900
H	-3.23434400	2.56985800	2.59914200	H	-0.26248100	3.74914800	-3.83763800
N	-1.88691800	-0.17690100	-0.15938000	H	-1.75266900	2.04314000	-2.27208600
N	-0.38447000	1.32409500	1.24046300	O	-0.14823700	-1.42052400	-1.52927300
C	2.60562500	-0.63661200	0.66510800	O	0.14823000	1.42047400	-1.52931700
C	2.46175900	1.06139800	-1.02288700				
C	3.86659100	1.16209000	-1.07099000	[Z7]2+			
C	4.62640900	0.33677600	-0.22589400	Co	0.16533500	-0.47705700	0.04115100
C	4.00329800	-0.57796800	0.65206200	C	2.12072200	-0.35453500	-2.08291500
C	1.73514500	-1.50010100	1.47790700	C	0.06129800	0.71502400	-2.59248600
C	-0.53342100	-2.05470600	1.91725900	C	0.51739100	1.06981300	-3.87364100
C	-0.14079500	-3.00843900	2.86782800	C	1.81735200	0.69175800	-4.25154800
C	1.22693500	-3.20228300	3.12211500	C	2.62804000	-0.02368100	-3.35556900
C	2.17449300	-2.43731700	2.41843200	C	2.87870800	-1.10349200	-1.04865800
H	4.34489200	1.86010100	-1.74706100	C	2.80186300	-2.00671200	1.11904200
H	5.70873400	0.40065700	-0.24941400	C	4.12199500	-2.48119800	1.01648400
H	4.59681700	-1.21483000	1.29578300	C	4.83056300	-2.24583300	-0.17563000
H	-1.57941700	-1.88333200	1.70781500	C	4.20292100	-1.54828900	-1.22280900
H	-0.90128400	-3.57653500	3.38971400	H	-0.11340200	1.62010600	-4.56214000
H	1.55366500	-3.93257900	3.85413400	H	2.19360300	0.95236600	-5.23505400
H	3.23435800	-2.56976300	2.59921600	H	3.62909700	-0.31499900	-3.64646400
N	1.88691800	0.17690000	-0.15939400	H	2.22043100	-2.16630400	2.02087600
N	0.38447700	-1.32405800	1.24050100	H	4.57239300	-3.01514000	1.84592100
C	-1.50482100	-1.80683500	-1.81117200	H	5.85134100	-2.59610300	-0.29017300

H	4.74139200	-1.36019400	-2.14399000	C	-2.90850100	1.07766000	-0.59638800
N	0.85728300	0.01548200	-1.72778700	C	-3.34513000	1.79296100	-1.75582700
N	2.19711700	-1.33588500	0.11323400	C	-4.62030500	2.37920600	-1.84163000
C	-0.33651100	-0.13616300	2.81047100	C	-5.45661800	2.22967900	-0.72490200
C	-1.15721700	-2.16596900	1.87928200	C	-5.03424800	1.51960000	0.43703100
C	-1.66957500	-2.55901500	3.13017800	C	-3.76238800	0.93722800	0.51769400
C	-1.49902800	-1.69949000	4.23115600	C	-1.25851300	1.02877800	-2.04590300
C	-0.82711400	-0.46984400	4.08187500	H	-4.94441700	2.92009100	-2.72504500
H	-2.18649800	-3.50343300	3.24925000	H	-6.45201200	2.66483800	-0.74376900
H	-1.88858200	-1.98504500	5.20247100	H	-5.71772200	1.43067300	1.27680100
H	-0.69624500	0.19538600	4.92764900	H	-3.44367700	0.39777800	1.40387900
C	-0.64870200	-2.84902000	-1.67391800	H	-2.25521600	2.16038400	-3.57339500
C	-1.24966000	-4.09930200	-1.89764400	N	-1.60365300	0.61642100	-0.81440200
C	-1.86117800	-4.76378600	-0.82020100	N	-2.27373600	1.74098600	-2.65234000
C	-1.85297400	-4.15936200	0.44948700	H	3.08989200	5.86086200	1.41450900
C	-1.23460500	-2.90956900	0.60615500	H	3.06366200	4.76609400	-0.81051100
H	-0.17092600	-2.31189300	-2.48303000				
H	-1.23395000	-4.53057500	-2.89211100	[Z7]3+			
H	-2.33428900	-5.72983400	-0.96232800	Co	0.00000000	0.46168600	0.00000000
H	-2.31916900	-4.65273400	1.29448800	C	-2.06150000	1.32903900	-1.69223300
N	-0.63877400	-2.26345200	-0.45370500	C	-0.65048300	-0.36955900	-2.60960500
N	-0.50990400	-0.97940400	1.75314500	C	-1.37001500	-0.37605500	-3.81264800
C	1.43388600	3.02797200	2.23190700	C	-2.46273700	0.50813100	-3.93248700
C	1.41118100	2.38501000	0.95441500	C	-2.82021500	1.36814000	-2.87587500
C	2.00228100	3.00835900	-0.16363700	C	-2.23667600	2.12298800	-0.46373600
C	2.59986600	4.26004000	0.03136600	C	-1.36049300	2.50399200	1.69871100
C	2.61515600	4.88943500	1.30959700	C	-2.34458300	3.47191800	1.95742600
C	2.03213000	4.28391300	2.43235000	C	-3.29571400	3.76290600	0.96627700
C	0.38336300	1.05988500	2.38907600	C	-3.24003100	3.07719500	-0.26095500
H	1.99634500	2.53867600	-1.13996900	H	-1.09918200	-1.03647100	-4.62763900
H	2.04250000	4.76236300	3.40637000	H	-3.03690200	0.52497400	-4.85215500
H	0.62084000	2.31540200	4.09802100	H	-3.66067200	2.04319800	-2.97842800
N	0.77522900	2.15884200	3.10912200	H	-0.61763700	2.26247100	2.44575500
N	0.74670000	1.15778400	1.09146600	H	-2.35284100	3.97617200	2.91636900

H	-4.06656600	4.50559700	1.14048800	N	-1.01851200	-0.91291700	0.96451000
H	-3.96487000	3.28315900	-1.03942900	C	2.11193100	-1.77586700	-0.79539400
N	-1.01438300	0.47282600	-1.60249400	C	2.23712800	-2.54747900	-1.99309800
N	-1.30666500	1.84680500	0.51801000	C	3.23753000	-3.51895200	-2.16522200
C	0.65048100	-0.36955600	2.60960500	C	4.12367000	-3.70311300	-1.09634900
C	2.06150200	1.32903800	1.69223200	C	4.01149600	-2.94039400	0.10187700
C	2.82021600	1.36814000	2.87587400	C	3.01388300	-1.97386700	0.26994700
C	2.46273600	0.50813300	3.93248700	C	0.50827100	-1.14966200	-2.19945700
C	1.37001300	-0.37605100	3.81265000	H	3.31821700	-4.09644300	-3.07986300
H	3.66067400	2.04319700	2.97842600	H	4.91482800	-4.44205700	-1.18018800
H	3.03690200	0.52497600	4.85215600	H	4.72058000	-3.11493100	0.90545500
H	1.09917900	-1.03646600	4.62764100	H	2.95166000	-1.40549000	1.18893500
C	1.36049700	2.50398600	-1.69871400	H	1.02671400	-2.47556200	-3.77517800
C	2.34458800	3.47191100	-1.95742900	N	1.01851000	-0.91292000	-0.96450900
C	3.29571800	3.76290000	-0.96628100	N	1.21133900	-2.12008200	-2.84341800
C	3.24003500	3.07719200	0.26095200	H	-4.91483200	-4.44205100	1.18019100
C	2.23667900	2.12298600	0.46373400	H	-4.72058300	-3.11492700	-0.90545200
H	0.61764100	2.26246500	-2.44575800				
H	2.35284700	3.97616500	-2.91637400	[Z8]2+			
H	4.06657100	4.50559100	-1.14049200	Co	-0.00011200	0.49946100	0.00001100
H	3.96487300	3.28315600	1.03942700	C	1.72770100	1.35673700	2.08767200
N	1.30666800	1.84680100	-0.51801200	C	0.18005600	-0.32753700	2.72979700
N	1.01438300	0.47282600	1.60249300	C	0.67576700	-0.34820700	4.04072900
C	-2.23713100	-2.54747500	1.99310000	C	1.73449100	0.52169900	4.36598900
C	-2.11193300	-1.77586400	0.79539500	C	2.26685100	1.37923500	3.38993900
C	-3.01388500	-1.97386400	-0.26994500	C	2.18053300	2.18821700	0.95076900
C	-4.01149900	-2.94039100	-0.10187500	C	1.83562500	2.66387200	-1.32665100
C	-4.12367400	-3.70310800	1.09635200	C	2.86254600	3.62451800	-1.32111100
C	-3.23753400	-3.51894600	2.16522500	C	3.56148500	3.86218700	-0.12445000
C	-0.50827300	-1.14965900	2.19945900	C	3.21628000	3.13424000	1.02848700
H	-2.95166100	-1.40548900	-1.18893400	H	0.26195800	-1.01517700	4.78814600
H	-3.31822200	-4.09643600	3.07986700	H	2.13984100	0.52740400	5.37185300
H	-1.02671800	-2.47555700	3.77518100	H	3.08336700	2.04523000	3.63918200
N	-1.21134200	-2.12007800	2.84342000	H	1.27509700	2.45470100	-2.23021900

H	3.09982800	4.16459300	-2.23078400	C	-2.55241400	-2.61103000	1.88586900
H	4.35872100	4.59726700	-0.08625500	C	-4.19418200	-3.81340200	0.90042100
H	3.74488600	3.30600500	1.95875800	C	-3.06071200	-2.26015500	-0.44660200
N	0.70383900	0.51218400	1.78764300	C	-0.89875700	-1.15022800	2.18595200
N	1.50189900	1.96272500	-0.21945600	H	-4.96954000	-4.56830600	0.96099100
C	-0.17993200	-0.32800200	-2.72966800	H	-2.93957800	-1.79961500	-1.42096800
C	-1.72834400	1.35565100	-2.08778800	H	-1.60259400	-2.39309300	3.79570400
C	-2.26752600	1.37768300	-3.39005200	N	-1.66422900	-2.10547700	2.82516500
C	-1.73478900	0.52023500	-4.36597400	H	4.97173600	-4.56614200	-0.96062400
C	-0.67565400	-0.34912200	-4.04058800	N	-3.49653500	-3.55865100	2.03557800
H	-3.08435800	2.04325700	-3.63938700	N	-4.01742500	-3.21302000	-0.31575100
H	-2.14016600	0.52558200	-5.37182900	N	-1.23979600	-1.00939900	0.89086800
H	-0.26155000	-1.01605300	-4.78787800	N	3.49820100	-3.55730100	-2.03525000
C	-1.83687800	2.66335200	1.32630600	N	4.01900100	-3.21121100	0.31603200
C	-2.86424700	3.62351800	1.32059000				
C	-3.56328800	3.86064900	0.12388200	[Z8]3+			
C	-3.21773500	3.13265900	-1.02892300	Co	0.00000900	0.44296600	-0.00000600
C	-2.18155400	2.18712500	-0.95102700	C	-1.93758600	1.32349700	-1.82471600
H	-1.27624900	2.45460900	2.22991300	C	-0.47594200	-0.37108200	-2.66229600
H	-3.10178600	4.16364700	2.23016400	C	-1.10816500	-0.36339900	-3.91091700
H	-4.36086600	4.59535000	0.08555000	C	-2.18953700	0.52626700	-4.09654700
H	-3.74640700	3.30401900	-1.95923200	C	-2.61342600	1.37633000	-3.05917400
N	-1.50282500	1.96215500	0.21924100	C	-2.18919000	2.11537400	-0.60907900
N	-0.70408400	0.51162400	-1.78763500	C	-1.45744600	2.48554200	1.60915400
C	2.55363300	-2.61011700	-1.88559800	C	-2.44773100	3.46273400	1.80142900
C	2.27892600	-1.91405200	-0.66807800	C	-3.32503100	3.76553900	0.74828300
C	3.06183500	-2.25879400	0.44682900	C	-3.19254300	3.08061500	-0.47383200
C	4.19600200	-3.81162200	-0.90009100	H	-0.78326100	-1.01309800	-4.71457300
C	0.89927500	-1.15012600	-2.18575000	H	-2.69816400	0.55468400	-5.05357000
H	2.94051100	-1.79822500	1.42115700	H	-3.44141500	2.05706200	-3.21300100
H	1.60366000	-2.39276600	-3.79543100	H	-0.77069100	2.23763000	2.40580700
N	1.66518000	-2.10506600	-2.82490900	H	-2.51571300	3.96533700	2.75876100
N	1.24028400	-1.00902000	-0.89069300	H	-4.09748300	4.51675300	0.87066700
C	-2.27800200	-1.91494100	0.66829800	H	-3.85914000	3.29703500	-1.29981900

N	-0.90706800	0.45737900	-1.66876800	C	0.65840000	-1.15499200	-2.18595900
N	-1.33017800	1.82897900	0.43372800	H	4.90618600	-4.38612700	-1.06897200
C	0.47592300	-0.37103500	2.66230500	H	2.99206400	-1.55507200	1.32299900
C	1.93762400	1.32347800	1.82469100	H	1.29648800	-2.45736500	-3.75463500
C	2.61345600	1.37632200	3.05915300	N	1.40853000	-2.11166900	-2.80610900
C	2.18953100	0.52630300	4.09654700	H	-4.90633500	-4.38594200	1.06907000
C	1.10813200	-0.36333400	3.91093200	N	3.32864800	-3.46560300	-2.07353800
H	3.44146500	2.05703300	3.21296800	N	4.01259500	-2.98801400	0.20617700
H	2.69815000	0.55473100	5.05357300	N	1.08226800	-0.93285000	-0.91596600
H	0.78319800	-1.01299700	4.71460500	N	-3.32877700	-3.46543500	2.07361900
C	1.45754600	2.48544700	-1.60921200	N	-4.01267400	-2.98791400	-0.20612400
C	2.44786600	3.46259900	-1.80150800				
C	3.32516600	3.76540800	-0.74836100	[Z9]2+			
C	3.19264400	3.08052300	0.47377200	Co	0.07769100	-0.00000300	0.00000100
C	2.18925800	2.11531800	0.60903700	C	2.63444900	0.13542700	-1.18127500
H	0.77078800	2.23753800	-2.40586400	C	2.63442300	-0.13543300	1.18133300
H	2.51587600	3.96517000	-2.75885400	C	4.03882900	-0.13716900	1.21303000
H	4.09764300	4.51659400	-0.87075900	C	4.73965600	-0.00001200	0.00005200
H	3.85924100	3.29694500	1.29975900	C	4.03885600	0.13715200	-1.21294200
N	1.33024300	1.82892400	-0.43376800	C	1.71909800	0.27020000	-2.33037600
N	0.90708300	0.45738400	1.66875700	C	-0.53143800	0.34730500	-2.98141900
C	-2.37329800	-2.53739000	1.89936100	C	1.08212000	0.54347800	-4.62757600
C	-2.16570800	-1.78954500	0.70216500	C	2.10423000	0.43065600	-3.66801100
C	-3.04398300	-2.05688300	-0.36483600	H	4.57620400	-0.24246900	2.14778600
C	-4.11720300	-3.64819300	0.98730800	H	5.82400600	-0.00001700	0.00006300
C	-0.65843700	-1.15492700	2.18597900	H	4.57625100	0.24244600	-2.14768700
H	-2.99207100	-1.55506200	-1.32299400	H	-1.57778600	0.31537000	-2.70861800
H	-1.29660700	-2.45719800	3.75470600	H	1.31276000	0.66846700	-5.67990100
N	-1.40862400	-2.11153700	2.80616400	H	3.14397800	0.46885000	-3.96622200
N	-1.08227900	-0.93282000	0.91597100	C	-0.53150400	-0.34729800	2.98141000
C	2.16565400	-1.78962200	-0.70213300	C	1.08201800	-0.54345400	4.62760400
C	2.37320600	-2.53751600	-1.89930400	C	2.10414900	-0.43064000	3.66806000
C	4.11708000	-3.64834800	-0.98722800	C	1.71904600	-0.27019800	2.33041500
C	3.04393500	-2.05694600	0.36486700	H	-1.57784600	-0.31536700	2.70858600

H	1.31263500	-0.66843300	5.67993500			
H	3.14389000	-0.46882700	3.96629500	[Z9]3+		
N	0.38401400	-0.22969800	1.99172900	Co	-0.00002900	0.00000000 0.00000000
N	1.97391400	-0.00000200	0.00002200	C	-2.53528000	0.87684500 0.81134700
N	0.38405900	0.22969800	-1.99171900	C	-2.53527700	-0.87685100 -0.81135000
C	-2.55014400	-1.18002500	-0.12783900	C	-3.93841800	-0.89953300 -0.83196200
C	-2.55014600	1.18002100	0.12780200	C	-4.63454800	-0.00000600 -0.00000300
C	-3.95622000	1.20715700	0.13176200	C	-3.93842200	0.89952300 0.83195700
C	-4.66137900	-0.00000400	-0.00001600	C	-1.59633500	1.70987500 1.58170800
C	-3.95621900	-1.20716400	-0.13179600	C	0.68200000	2.14983900 1.98594300
C	-1.69756100	-2.38657300	-0.25984700	C	-0.89525900	3.39300900 3.13885100
C	0.48651000	-3.21175700	-0.35808300	C	-1.94405900	2.70301800 2.50156000
C	-1.24622400	-4.73259400	-0.51300400	H	-4.47765900	-1.58922100 -1.46945700
C	-2.18929600	-3.69609900	-0.39744400	H	-5.71859000	-0.00000700 -0.00000400
H	-4.49317200	2.14147200	0.23565700	H	-4.47766500	1.58921000 1.46945100
H	-5.74571300	-0.00000500	-0.00001400	H	1.72217000	1.93537500 1.78637200
H	-4.49317000	-2.14147900	-0.23568900	H	-1.09682500	4.17471500 3.86249600
H	1.55188800	-3.01608900	-0.34284000	H	-2.97628500	2.94062100 2.72323900
H	-1.56085400	-5.76498300	-0.62159300	C	0.68200700	-2.14983600 -1.98594400
H	-3.24729200	-3.92207600	-0.41689300	C	-0.89524700	-3.39301100 -3.13885300
C	0.48650400	3.21175600	0.35807300	C	-1.94404900	-2.70302300 -2.50156300
C	-1.24623400	4.73259500	0.51293600	C	-1.59632900	-1.70987900 -1.58171000
C	-2.18930400	3.69609800	0.39737400	H	1.72217700	-1.93537000 -1.78637100
C	-1.69756500	2.38657000	0.25980900	H	-1.09681000	-4.17471800 -3.86249800
H	1.55188200	3.01608800	0.34285800	H	-2.97627400	-2.94062900 -2.72324300
H	-1.56086600	5.76498600	0.62150200	N	-0.26465300	-1.43785700 -1.32839300
H	-3.24730000	3.92207400	0.41679800	N	-1.88880100	-0.00000300 -0.00000100
N	-0.34872100	2.15581700	0.24111900	N	-0.26465800	1.43785700 1.32839200
N	-1.87616800	-0.00000200	-0.00001800	C	2.53527600	-0.81145200 0.87672600
N	-0.34871700	-2.15581900	-0.24112800	C	2.53527400	0.81145700 -0.87672400
N	-0.23402900	-0.50191000	4.29020600	C	3.93841800	0.83206100 -0.89943300
N	0.09357600	-4.50005400	-0.49423800	C	4.63455800	0.00000400 0.00000100
N	0.09356600	4.50005600	0.49420000	C	3.93842000	-0.83205400 0.89943500
N	-0.23393500	0.50192800	-4.29020700	C	1.59633800	-1.58180200 1.70974100

C	-0.68199600	-1.98595800	2.14982200	H	-5.76526700	-0.07404800	-0.06333400
C	0.89527900	-3.13904100	3.39280900	H	-4.60672900	-0.03153700	2.16380900
C	1.94407500	-2.50178500	2.70276500	H	1.60132800	0.06502200	2.71875300
H	4.47764800	1.46961700	-1.58907000	H	-1.24582300	0.07296900	5.75132000
H	5.71859900	0.00000500	0.00000100	H	-3.10427300	0.02112600	4.05073500
H	4.47765000	-1.46960900	1.58907300	C	0.42831600	-0.03282500	-3.03341300
H	-1.72217100	-1.78614400	1.93556000	C	-1.25109600	-0.07909000	-4.63248400
H	1.09685900	-3.86282400	4.17438400	C	-2.23708400	-0.07511700	-3.62665200
H	2.97629600	-2.72361500	2.94024000	C	-1.79028500	-0.04867500	-2.30363500
C	-0.68199900	1.98595700	-2.14982100	H	1.48559400	-0.01710800	-2.80470500
C	0.89527500	3.13904400	-3.39280700	H	-1.51827900	-0.09923300	-5.68325000
C	1.94407100	2.50179000	-2.70276200	H	-3.29473100	-0.09203200	-3.85693500
C	1.59633600	1.58180500	-1.70973900	N	-0.44760400	-0.02752500	-2.00164100
H	-1.72217300	1.78614100	-1.93555900	N	-1.97375900	-0.01615900	0.04783600
H	1.09685300	3.86282800	-4.17438100	N	-0.36976400	0.02877600	2.02077500
H	2.97629200	2.72362200	-2.94023700	C	2.55595800	-1.14552800	-0.02819300
N	0.26464000	1.32839900	-1.43785500	C	2.54516200	1.20987500	-0.05965700
N	1.88878800	0.00000200	0.00000100	C	3.94872500	1.19693500	-0.07977300
N	0.26464200	-1.32839800	1.43785700	C	4.59152500	-0.05562300	-0.07210700
N	0.40916600	-3.11812700	-2.88243300	C	1.73820500	-2.37964700	-0.00052100
N	-0.40913500	-2.88252400	3.11804700	C	-0.40556600	-3.28310800	0.04398600
N	-0.40913900	2.88252500	-3.11804500	C	1.39115500	-4.74693600	0.02738300
N	0.40915500	3.11812900	2.88243300	C	2.29305900	-3.66624300	0.00245300
				H	4.53270900	2.10703200	-0.09996300
[Z10]2+				H	5.67310000	-0.12837100	-0.08619600
Co	-0.08545700	0.00570500	0.00624800	H	-1.47809800	-3.13398100	0.06046100
C	-2.62764900	-0.01143400	1.24177000	H	1.74224700	-5.77311900	0.03097400
C	-2.66667100	-0.04240900	-1.11790600	H	3.36521900	-3.81176100	-0.01440300
C	-4.68303700	-0.05760300	-0.00371400	C	-0.47798600	3.26127200	-0.04372900
C	-4.03022100	-0.03334000	1.24797400	C	1.26297500	4.78457400	-0.09973400
C	-1.69972100	0.01606700	2.38761700	C	2.20220300	3.73570200	-0.09683800
C	0.55832700	0.05556900	3.00445900	C	1.69986000	2.42643500	-0.06493100
C	-1.03101900	0.05959800	4.68854800	H	-1.54437700	3.07369300	-0.02449800
C	-2.06866600	0.03064100	3.73627100	H	1.58109000	5.82110900	-0.12350800

H	3.26224900	3.95291100	-0.11921100	N	-1.88230200	0.00316200	0.02173000
N	0.35078300	2.19409700	-0.03773500	N	-0.27322600	1.39236500	1.39033100
N	1.86255800	0.02615600	-0.03293600	C	2.54563300	-0.83650200	0.80785700
N	0.38515000	-2.18663000	0.02114600	C	2.54101200	0.84104700	-0.86730400
N	0.07530300	-0.05787600	-4.33845200	C	3.94203500	0.82096400	-0.86611900
N	0.04434300	-4.56116100	0.04776800	C	4.57371300	-0.07837000	0.02549700
N	-0.07550800	4.55466600	-0.07381300	C	1.62768600	-1.64498800	1.62788600
N	3.90212800	-1.22361200	-0.04720800	C	-0.63127900	-2.07853800	2.09436900
N	0.27707800	0.07184300	4.32696900	C	0.98651600	-3.26611600	3.26155000
N	-4.01034200	-0.06275200	-1.18581900	C	2.01655900	-2.59287100	2.57146100
				H	4.53121500	1.45870000	-1.51218700
[Z10]3+				H	5.65471500	-0.13897300	0.07298800
Co	0.00000300	0.00561600	-0.00002500	H	-1.67905500	-1.88390900	1.91431000
C	-2.54122500	0.83995900	0.86752400	H	1.20832200	-4.01704600	4.01122400
C	-2.54540900	-0.83670400	-0.80852800	H	3.06406300	-2.79348000	2.75744900
C	-4.57368800	-0.07923700	-0.02599100	C	-0.67135100	2.08682900	-2.06764700
C	-3.94223900	0.81982300	0.86606200	C	0.90613800	3.28109500	-3.27556900
C	-1.60583000	1.65087000	1.66511100	C	1.95688000	2.60672900	-2.61854900
C	0.67085800	2.08501700	2.06931100	C	1.60540000	1.65218500	-1.66442700
C	-0.90692100	3.27857400	3.27758700	H	-1.71279900	1.88893800	-1.85786800
C	-1.95752700	2.60468600	2.61985700	H	1.10763000	4.03533300	-4.02763200
H	-5.65467700	-0.13986300	-0.07374400	H	2.99057600	2.82799800	-2.85090200
H	-4.53156500	1.45736300	1.51219200	N	0.27285300	1.39344900	-1.38955200
H	1.71234800	1.88733100	1.85946700	N	1.88231100	0.00393300	-0.02166700
H	-1.10857900	4.03216100	4.03025800	N	0.29255900	-1.38565800	1.38723300
H	-2.99128100	2.82576300	2.85212700	N	0.32421300	-3.00754900	-3.02330400
C	0.63178000	-2.07790000	-2.09518800	N	-0.32352200	-3.00856400	3.02205000
C	-0.98577200	-3.26502600	-3.26314600	N	-0.39519200	3.02129200	-3.00082500
C	-2.01594000	-2.59207700	-2.57296100	N	3.88504800	-0.90494800	0.85963700
C	-1.62725100	-1.64459500	-1.62889700	N	0.39447900	3.01876600	3.00314500
H	1.67952700	-1.88348100	-1.91481600	N	-3.88481100	-0.90525700	-0.86051600
H	-1.20743000	-4.01546200	-4.01335900				
H	-3.06340900	-2.79263800	-2.75920600	[Z11]2+			
N	-0.29217400	-1.38520400	-1.38799500	Co	-0.08033200	0.00319700	0.00478000

C	-2.64428400	-0.05985400	-1.14245600	H	4.51187900	2.13922700	-0.08283000
C	-2.62082500	-0.03117900	1.22456200	H	-1.59679000	2.98303100	-0.00940500
C	-4.02571800	-0.06095900	1.21837300	H	1.64415900	5.84717100	-0.09031600
C	-4.66736200	-0.08822900	-0.03617100	H	3.24754500	3.93385500	-0.08934900
C	-1.76089200	-0.05673300	-2.32168000	C	-0.42111100	-3.25535400	0.04508600
C	0.48259100	-0.02038800	-3.01337000	C	0.07989100	-4.57171400	0.05260600
C	0.09288800	-0.04331900	-4.36524800	C	1.47269200	-4.77070600	0.03672400
C	-1.27583000	-0.07427000	-4.68608900	C	2.32385400	-3.65062200	0.01332100
C	-2.22112600	-0.08115700	-3.64341800	C	1.74611000	-2.37063400	0.00672600
H	-4.60938600	-0.06284700	2.12955100	H	-1.48915800	-3.06713200	0.05723400
H	-5.74953700	-0.11100200	-0.10257900	H	-0.60850600	-5.40948500	0.07054500
H	1.52990900	0.00333600	-2.74020300	H	1.88737200	-5.77348500	0.04231600
H	0.85274900	-0.03701000	-5.13853200	H	3.40261000	-3.75065200	0.00031300
H	-1.60039200	-0.09257200	-5.72119400	N	0.39344700	-2.17693000	0.02279800
H	-3.28769800	-0.10447300	-3.83532400	N	1.85962200	0.03785300	-0.02318800
C	0.56670300	0.05343400	2.99180100	N	0.32613300	2.18693800	-0.02694500
C	-1.12711300	0.04353300	4.72621600	N	3.90674900	-1.19791100	-0.03527500
C	-2.10919700	0.01023600	3.71887400	C	-0.10490100	4.56310000	-0.04994100
C	-1.70401800	0.00061500	2.37742900	H	-0.83291900	5.36671700	-0.04958800
H	1.60284400	0.06944900	2.67910100	C	0.22834500	0.06551400	4.35739200
H	-1.41668100	0.05197200	5.77163100	N	-3.98983500	-0.08829900	-1.21699400
H	-3.16156500	-0.00722400	3.97764500	H	1.01542200	0.09126800	5.10235000
N	-0.37274000	0.02197200	2.01997100				
N	-1.96336900	-0.03104700	0.03226600	[Z11]3+			
N	-0.42200800	-0.02689300	-2.00767600	Co	0.00318200	-0.01384000	0.00825400
C	2.52718300	1.23060200	-0.04618500	C	-2.54030400	-0.96945900	-0.63856500
C	2.55737400	-1.13317900	-0.01850300	C	-2.49906900	0.73710100	1.02266100
C	4.58298200	-0.02084800	-0.05787300	C	-3.89802000	0.70815000	1.06419000
C	3.93340900	1.22568000	-0.06449900	C	-4.55252300	-0.19800300	0.20312100
C	1.67118100	2.43835100	-0.04896000	C	-1.64278400	-1.74454500	-1.50787700
C	-0.53948700	3.22390600	-0.02733400	C	0.60999200	-2.01051300	-2.16529500
C	1.27594100	4.82671700	-0.07262000	C	0.22549800	-2.94099400	-3.14525400
C	2.17996300	3.74878700	-0.07213500	C	-1.12751800	-3.27248600	-3.28903500
H	5.66565600	-0.08421400	-0.07087900	C	-2.07370000	-2.67346700	-2.44683800

H	-4.47023800	1.36176000	1.71145500	H	-1.47033000	-1.86327400	2.08363800
H	-5.63539200	-0.24732000	0.18002800	H	-0.67243000	-3.63910600	3.61773900
H	1.65620500	-1.78223800	-2.01038000	H	1.79004000	-4.07985200	3.81729300
H	0.98697400	-3.39496000	-3.76828000	H	3.38371900	-2.68018600	2.45206500
H	-1.44299000	-3.98142600	-4.04653400	N	0.44362900	-1.39326000	1.35792500
H	-3.13043700	-2.90708400	-2.51027700	N	1.87107300	0.07985100	-0.14124400
C	0.74858700	2.06371100	2.03798700	N	0.10211100	1.39217500	-1.38601600
C	-0.88063400	3.20198900	3.42304900	N	3.97761600	-0.72901900	0.59712000
C	-1.89521300	2.48190400	2.77097100	C	-0.73839500	3.05772800	-2.91754400
C	-1.54756400	1.56572300	1.77550300	H	-1.59609300	3.54332800	-3.36503900
H	1.77204600	1.91944300	1.71521800	C	0.45050500	2.99821000	3.04821100
H	-1.13189100	3.90581900	4.20868800	N	-3.89027500	-1.03932400	-0.64859000
H	-2.93649000	2.63789000	3.02930900	H	1.25984300	3.53951600	3.52094400
N	-0.22620100	1.35162500	1.42239000				
N	-1.86546200	-0.09932200	0.15538500	[Z12]2+			
N	-0.30844700	-1.40969900	-1.36746500	Co	-0.08210200	-0.00001300	-0.00000600
C	2.42534000	0.96259400	-1.03305500	C	-2.62486300	0.16291100	1.17592500
C	2.62461500	-0.74159700	0.63817700	C	-2.62504000	-0.16293600	-1.17557700
C	4.56139800	0.15312400	-0.28370100	C	-4.03536200	-0.15727400	-1.15817800
C	3.82427400	1.00808800	-1.13356300	C	-1.72266000	0.32585400	2.32760200
C	1.39589700	1.75262000	-1.72558500	C	0.54417200	0.41456800	2.95759800
C	-0.94267600	2.01876500	-1.99374300	C	0.19440600	0.60739800	4.30569200
C	0.56557300	3.44579300	-3.23204600	C	-1.16494000	0.66014900	4.65797400
C	1.64682700	2.76903500	-2.64292500	C	-2.13882700	0.51792000	3.65269500
H	5.64552200	0.17478800	-0.29456600	H	-4.61960200	-0.27779200	-2.06232100
H	4.33414100	1.67017100	-1.82362000	H	1.58326700	0.37228500	2.65753500
H	-1.94338200	1.68249200	-1.76835200	H	0.97500900	0.71318500	5.05033400
H	0.74724000	4.25365500	-3.93187700	H	-1.46387200	0.80898600	5.69016000
H	2.66655500	3.03095800	-2.90101400	H	-3.19343000	0.55774800	3.90027500
C	-0.41666400	-2.09978500	2.13488700	C	0.54373500	-0.41455800	-2.95772200
C	0.04546400	-3.08230900	3.02666600	C	-1.16562600	-0.66014400	-4.65785100
C	1.41722400	-3.32200100	3.13709300	C	-2.13935500	-0.51794700	-3.65241500
C	2.30904500	-2.56446300	2.36815600	C	-1.72299000	-0.32588000	-2.32738100
C	1.80035300	-1.61189600	1.49338100	H	1.58287400	-0.37228700	-2.65781900

H	-1.46472400	-0.80897500	-5.68998800	N	-4.72334400	0.00001200	0.00032700
H	-3.19400100	-0.55780100	-3.89981600	C	-4.03519200	0.15729400	1.15873200
N	-0.38829800	-0.27594600	-1.98733000	H	4.53114600	2.05757200	-0.27205300
N	-1.96357400	-0.00001700	0.00012500	H	-4.61928800	0.27782200	2.06294300
N	-0.38800000	0.27593400	1.98736000				
C	2.53588400	-1.17488600	0.15385400	[Z12]3+			
C	2.53584700	1.17489200	-0.15415900	Co	0.00011800	-0.00000400	0.00000000
C	3.94809500	-1.15338700	0.15142900	C	-2.52482700	1.08226900	0.50061200
C	1.70099200	-2.38619200	0.31374600	C	-2.52484500	-1.08221900	-0.50064400
C	-0.49978500	-3.19567500	0.42770900	C	-3.93663500	-1.06437400	-0.49378800
C	1.33671800	-4.76063300	0.62136300	C	-1.60034100	2.11794800	0.97909300
C	2.22648600	-3.68082900	0.47823100	C	0.68969300	2.64741400	1.22658100
H	4.53122400	-2.05754500	0.27152900	C	0.36544900	3.88907500	1.79984300
H	-1.56034500	-2.97026200	0.40367400	C	-0.98357500	4.24063800	1.96007800
H	1.71941700	-5.76786400	0.74930500	C	-1.98151300	3.33968300	1.54263000
H	3.29601600	-3.85426200	0.49581000	H	-4.52393400	-1.88930400	-0.87739100
C	-0.49986500	3.19566200	-0.42768800	H	1.72372800	2.36188400	1.09581300
C	-0.04804100	4.51781200	-0.59640800	H	1.16442100	4.55286100	2.10763500
C	1.33660600	4.76063800	-0.62148900	H	-1.25896000	5.19302200	2.39929400
C	2.22640500	3.68084400	-0.47846500	H	-3.02999400	3.58859200	1.65585600
C	1.70094200	2.38619900	-0.31395200	C	0.68965500	-2.64742900	-1.22658800
H	-1.56042200	2.97023700	-0.40355700	C	-0.98363900	-4.24062000	-1.96010100
H	-0.76486400	5.32424400	-0.70373800	C	-1.98156300	-3.33965200	-1.54264900
H	1.71927000	5.76788200	-0.74944800	C	-1.60037400	-2.11791900	-0.97911300
H	3.29592800	3.85429700	-0.49614900	H	1.72369200	-2.36191800	-1.09580500
N	0.35242100	2.15624100	-0.28977000	H	-1.25903200	-5.19299800	-2.39932100
N	1.86127300	-0.00000200	-0.00012200	H	-3.03004800	-3.58854600	-1.65587900
N	0.35248200	-2.15623900	0.28969200	N	-0.26737100	-1.78120300	-0.82500100
C	-0.04792700	-4.51782100	0.59641100	N	-1.88028000	0.00001700	-0.00001100
H	-0.76478200	-5.32418300	0.70381700	N	-0.26734200	1.78120300	0.82499200
C	0.19376100	-0.60737200	-4.30577300	C	2.52503100	-0.50064500	1.08228300
H	0.97431300	-0.71311700	-5.05044200	C	2.52505900	0.50060000	-1.08224100
C	3.94806100	1.15341900	-0.15190200	C	3.93681000	-0.49382300	1.06441100
N	4.64044000	0.00002000	-0.00026600	C	1.60043000	-0.97915000	2.11791800

C	-0.68975800	-1.22663300	2.64687500	H	3.02977800	1.65586900	-3.58889400
C	0.98311400	-1.96028500	4.24040300	N	0.26759400	0.82493100	-1.78095800
C	1.98127000	-1.54274400	3.33975400	N	1.88050000	-0.00001800	0.00001500
H	4.52409800	-0.87748400	1.88930700	N	0.26754900	-0.82494200	1.78096300
H	-1.72369700	-1.09577200	2.36111300	C	-0.36583000	-1.80009400	3.88851700
H	1.25825300	-2.39956400	5.19283000	H	-1.16499000	-2.10806700	4.55203400
H	3.02968200	-1.65592200	3.58895000	C	0.36539100	-3.88907700	-1.79986200
C	-0.68968700	1.22663800	-2.64688600	H	1.16440700	-4.55285600	-2.10764100
C	-0.36572900	1.80010200	-3.88852200	C	3.93683800	0.49375400	-1.06434600
C	0.98322500	1.96027000	-4.24038200	N	4.61629500	-0.00004100	0.00003700
C	1.98135800	1.54270800	-3.33971600	N	-4.61609500	0.00005400	-0.00003200
C	1.60048500	0.97911800	-2.11789100	C	-3.93661700	1.06446100	0.49373300
H	-1.72363300	1.09578100	-2.36114700	H	4.52417600	0.87738500	-1.88925300
H	-1.16482600	2.10808200	-4.55207000	H	-4.52392500	1.88942300	0.87732600
H	1.25839400	2.39954100	-5.19280500				

Part 2

Cartesian coordinates of the optimized structures for classic and new designed redox mediators in vacuum at B3LYP/LANL2DZ level.

[C1]2+				H	0.98608000	-0.01400600	5.11208000
Co	-0.07444500	-0.00000600	0.00000100	H	-1.45207600	-0.01553900	5.75724200
C	-2.62761200	-0.00326400	1.19348900	H	-3.17989900	-0.01066000	3.95253700
C	-2.62763600	0.00322500	-1.19343700	C	0.55238800	0.00828700	-2.99532700
C	-4.03392900	0.00330400	-1.22127000	C	0.20681300	0.01193300	-4.35758100
C	-4.73472500	-0.00002700	0.00004600	C	-1.15355800	0.01277700	-4.71363400
C	-4.03390500	-0.00335800	1.22134900	C	-2.12590500	0.00997300	-3.69713300
C	-1.71354600	-0.00639600	2.35505700	C	-1.71359200	0.00637200	-2.35502200
C	0.55244600	-0.00827700	2.99531900	H	1.59033400	0.00758700	-2.68500600
C	0.20689700	-0.01192200	4.35757900	H	0.98598200	0.01403200	-5.11209700
C	-1.15346700	-0.01278800	4.71365800	H	-1.45218700	0.01552800	-5.75721200
C	-2.12583400	-0.01000000	3.69717600	H	-3.17997500	0.01061800	-3.95247500
H	-4.57503700	0.00589000	-2.16048100	N	-0.37976400	0.00551000	-2.01351300
H	-5.82020100	-0.00003200	0.00005700	N	-1.96951600	-0.00001800	0.00002000
H	-4.57499500	-0.00594700	2.16057100	N	-0.37972400	-0.00551500	2.01352300
H	1.59038600	-0.00756100	2.68497800	C	2.54662600	-1.19235500	-0.00306300

C	2.54660700	1.19239100	0.00303100	C	4.63837100	0.00008200	0.00042300
C	3.95473900	1.21545700	0.00306200	C	3.94088900	-0.86711400	0.86797500
C	4.65917800	0.00003400	-0.00001500	C	1.59667500	-1.65364100	1.65347800
C	3.95475900	-1.21540000	-0.00309000	C	-0.69675000	-2.06554800	2.06619100
C	1.69327600	-2.40915000	-0.00617000	C	-0.38116500	-3.03392100	3.03429100
C	-0.51249200	-3.21697900	-0.00793700	C	0.96963800	-3.31069000	3.31069800
C	-0.07361000	-4.55311400	-0.01153200	C	1.96941600	-2.60900300	2.60873300
C	1.31026500	-4.80572500	-0.01253400	H	4.48647500	1.52981000	-1.52996000
C	2.20560800	-3.72110000	-0.00981600	H	5.72424000	0.00009800	0.00051300
H	4.49580800	2.15373700	0.00541200	H	4.48626600	-1.52964200	1.53078500
H	5.74468500	0.00004300	-0.00001200	H	-1.72841700	-1.83336300	1.83499600
H	4.49584200	-2.15367100	-0.00543400	H	-1.17954500	-3.55298500	3.55377600
H	-1.57163100	-2.97912000	-0.00708700	H	1.24124000	-4.05398400	4.05391400
H	-0.79437500	-5.36382100	-0.01350000	H	3.01661300	-2.80947300	2.80875700
H	1.68594800	-5.82420900	-0.01531300	C	-0.69647000	2.06568700	-2.06608500
H	3.27349000	-3.90728500	-0.01057300	C	-0.38075800	3.03413300	-3.03407100
C	-0.51254100	3.21696900	0.00793000	C	0.97008100	3.31091200	-3.31029200
C	-0.07368000	4.55311100	0.01150200	C	1.96976800	2.60918400	-2.60824000
C	1.31019300	4.80574300	0.01246200	C	1.59690100	1.65376200	-1.65309200
C	2.20555200	3.72113100	0.00975500	H	-1.72816500	1.83347600	-1.83504700
C	1.69323800	2.40917300	0.00613800	H	-1.17907000	3.55323700	-3.55362200
H	-1.57167700	2.97909400	0.00710800	H	1.24178000	4.05424700	-4.05343200
H	-0.79445600	5.36380800	0.01347600	H	3.01699200	2.80967100	-2.80810800
H	1.68586000	5.82423200	0.01522100	N	0.26467700	1.39029200	-1.38996200
H	3.27343100	3.90733100	0.01048800	N	1.89034100	0.00004800	0.00020100
N	0.34603100	2.17223700	0.00529400	N	0.26448300	-1.39020000	1.39014400
N	1.87595800	0.00001300	-0.00001600	C	-2.53518000	0.84785200	0.84762500
N	0.34606500	-2.17223400	-0.00529900	C	-2.53488300	-0.84819900	-0.84818400
				C	-3.94079800	-0.86790700	-0.86758700
[C1]3+				C	-4.63837100	-0.00031700	-0.00050300
Co	-0.00000100	-0.00002100	0.00000500	C	-3.94109900	0.86737200	0.86672600
C	2.53497200	-0.84787400	0.84825100	C	-1.59707400	1.65322700	1.65346800
C	2.53509100	0.84799000	-0.84774300	C	0.69625800	2.06622100	2.06562200
C	3.94100900	0.86726300	-0.86724100	C	0.38044900	3.03425900	3.03398300

C	-0.97041900	3.31049700	3.31061000	H	1.29915900	-3.69717200	-0.24510700
C	-1.97003600	2.60842200	2.60880600	H	-0.66457400	-5.62572000	-0.23726100
H	-4.48610400	-1.53072800	-1.53016100	H	-3.00647100	-4.23083800	-0.11922300
H	-5.72424000	-0.00038800	-0.00062200	C	-1.78332900	2.23184200	0.04951800
H	-4.48663500	1.53013100	1.52917500	C	-2.34122400	3.52343700	0.11097600
H	1.72797600	1.83516000	1.83353400	C	-1.48509800	4.63903500	0.12615800
H	1.17870900	3.55383000	3.55314800	C	-0.09374800	4.43665600	0.08091800
H	-1.24219000	4.05366700	4.05388800	C	0.39193300	3.11816900	0.02039100
H	-3.01728000	2.80830600	2.80917300	C	-2.59567300	0.98847000	0.02748200
C	0.69696300	-2.06601100	-2.06565600	C	-4.00025200	0.95843300	0.05116500
C	0.38147500	-3.03406400	-3.03410900	C	-4.66076700	-0.28433800	0.02188600
C	-0.96930000	-3.31052800	-3.31095600	C	-3.92131900	-1.47448200	-0.03227600
C	-1.96914800	-2.60863900	-2.60929400	C	-2.51815900	-1.37756000	-0.05387200
C	-1.59650200	-1.65340900	-1.65386800	H	-3.41454700	3.67064000	0.14667000
H	1.72860600	-1.83479400	-1.83339200	H	-1.89628500	5.64260000	0.17253600
H	1.17990800	-3.55347600	-3.55316600	H	0.59770300	5.27241900	0.09144500
H	-1.24082800	-4.05372500	-4.05429600	H	1.45863800	2.92026700	-0.01480400
H	-3.01632500	-2.80869700	-2.80983500	H	-4.57633300	1.87431100	0.08946800
N	-0.26433800	-1.39004600	-1.39032100	H	-5.74531700	-0.32402000	0.03882500
N	-1.89033900	-0.00013700	-0.00020600	H	-4.42222300	-2.43450000	-0.05938400
N	-0.26482300	1.39007300	1.39015700	C	-0.42719800	-0.00148000	-3.26662800
				C	0.45108400	0.05496100	-4.39105100
[C2]2+				C	1.73878100	0.06545200	-3.86992300
Co	0.07922600	-0.09643600	-0.10488600	N	1.62022800	0.01702900	-2.49273800
N	-0.42910400	2.04355600	0.00377200	H	-1.50650300	-0.02444300	-3.25964500
N	0.51659900	-0.16234100	1.86804300	H	0.17486800	0.08324600	-5.43336900
N	-1.87900500	-0.18073700	-0.02156600	H	2.69458900	0.10301700	-4.36997300
N	1.97707900	-0.04231600	-0.22809700	C	1.86917600	-0.13867700	2.13096900
N	0.26952900	-0.02520900	-2.11609200	C	2.36058600	-0.17395100	3.44530200
N	-0.29442400	-2.31835800	-0.15286700	C	1.45050600	-0.23445300	4.51657300
C	0.22902000	-3.55577100	-0.20598500	C	0.07180200	-0.25709700	4.24080800
C	-0.79395800	-4.55530500	-0.20180900	C	-0.35497600	-0.21922700	2.90219000
C	-1.99286800	-3.86239100	-0.14242300	C	2.71371900	-0.07658600	0.91994300
N	-1.68130000	-2.50972900	-0.11281800	C	4.11618500	-0.05748300	0.85083200

C	4.73051500	-0.00619900	-0.41799900	C	-3.83263100	-1.14843900	1.17947500
C	3.95673900	0.02285600	-1.59339300	C	-2.44056000	-1.05169100	1.04010900
C	2.56182200	0.00166600	-1.44639500	H	-3.31833100	2.62387500	-2.50680300
H	3.42790200	-0.15499200	3.63696600	H	-1.68156700	3.93831700	-3.86628500
H	1.81035600	-0.26311700	5.54021400	H	0.78451400	3.51219900	-3.55636400
H	-0.66080900	-0.30357300	5.03923200	H	1.51760900	1.79091500	-1.90819400
H	-1.40957900	-0.23500000	2.65423500	H	-4.65379400	1.25391100	-1.13962700
H	4.72240900	-0.08446500	1.74854900	H	-5.70287700	-0.34462200	0.45939900
H	5.81332700	0.00825100	-0.49206600	H	-4.29381800	-1.84648500	1.86936300
H	4.42759000	0.05773800	-2.56897300	C	-0.63114400	-2.27748300	-2.20398900
				C	0.19413500	-3.06768700	-3.05351100
[C2]3+				C	1.50735300	-2.71741700	-2.75727000
Co	0.00003100	-0.12353400	-0.00160000	N	1.46212800	-1.75359700	-1.76720000
N	-0.42258900	1.27678600	-1.32393200	H	-1.70945800	-2.26788500	-2.14282600
N	0.42233300	1.24223500	1.35645900	H	-0.13226200	-3.79396200	-3.78231300
N	-1.88567500	-0.17199200	0.17419700	H	2.43594300	-3.08013200	-3.17419700
N	1.88574600	-0.16709100	-0.17850000	C	1.77972900	1.46177500	1.51765000
N	0.12668300	-1.48035800	-1.42297300	C	2.25251800	2.39276500	2.45260200
N	-0.12634000	-1.51667000	1.38427600	C	1.33044600	3.11392900	3.23693800
C	0.63164300	-2.33362300	2.14438100	C	-0.04557700	2.88283400	3.06094100
C	-0.19348100	-3.14570400	2.97316900	C	-0.46464300	1.93741700	2.10917200
C	-1.50676600	-2.78814500	2.68608000	C	2.62927000	0.64027100	0.63339700
N	-1.46172700	-1.79895100	1.72135400	C	4.02913100	0.59861600	0.54493400
H	1.70995200	-2.32230800	2.08343500	C	4.62105300	-0.28657700	-0.38541700
H	0.13305400	-3.89055700	3.68290700	C	3.83291100	-1.11705300	-1.20843100
H	-2.43528600	-3.16173300	3.09345000	C	2.44081400	-1.02407300	-1.06678200
C	-1.78004200	1.50012200	-1.47935900	H	3.31771300	2.55930100	2.57351600
C	-2.25309000	2.45462400	-2.39015800	H	1.68058500	3.83812700	3.96612900
C	-1.33122700	3.19582300	-3.15583100	H	-0.78539100	3.41945700	3.64535400
C	0.04485400	2.96063200	-2.98584200	H	-1.51801200	1.74075200	1.95355900
C	0.46418600	1.99126800	-2.05860300	H	4.65356200	1.22473500	1.17199400
C	-2.62938400	0.65599300	-0.61648500	H	5.70298700	-0.33191600	-0.46761100
C	-4.02922900	0.61187900	-0.52900900	H	4.29425300	-1.79701400	-1.91605000
C	-4.62095500	-0.29707100	0.37827400				

[C3]2+	H	4.06048500	1.24343900	-3.35718600	
Co	0.00001600	0.00231000	-0.00002700	H	1.68376600 1.31797000 -2.55844000
C	0.40173800	2.75811300	0.61934300	H	3.92239700 -3.06738100 1.00812000
C	0.83430300	3.92121100	1.28198100	H	2.82152000 -4.32945900 2.84756900
C	1.59324900	3.80545700	2.45829100	H	0.46734400 -3.70257400 3.52004700
C	1.90060400	2.52241600	2.94655000	H	-0.66422000 -1.83252300 2.30231500
C	1.44257400	1.40078700	2.23880100	N	1.95575600 -0.10538200 -1.06440200
C	-0.40177700	2.75807800	-0.61944000	N	0.94282300 -1.43520700 1.04298200
C	-0.83437900	3.92113700	-1.28212200	C	-2.81742500 -0.95816700 0.43329400
C	-1.59333300	3.80531400	-2.45842000	C	-4.16993000 -1.04870800 0.82069200
C	-1.90066000	2.52224500	-2.94662500	C	-4.63479600 -0.25350900 1.88263900
C	-1.44259200	1.40065800	-2.23883600	C	-3.73952100 0.61686200 2.53184200
H	0.58722000	4.90253900	0.89412100	C	-2.40736000 0.66138200 2.08638600
H	1.93463500	4.69372400	2.98049200	C	-2.22537200 -1.75792700 -0.67090000
H	2.48205300	2.38761700	3.85214600	C	-2.91686800 -2.80438400 -1.31369400
H	1.65989000	0.40015900	2.58734900	C	-2.29585800 -3.52121300 -2.34874000
H	-0.58731900	4.90248700	-0.89430500	C	-0.98451800 -3.17705900 -2.72461800
H	-1.93474700	4.69355100	-2.98065500	C	-0.34365600 -2.13178300 -2.04525500
H	-2.48211500	2.38739500	-3.85220900	H	-4.85682000 -1.71321800 0.30965900
H	-1.65988000	0.40000700	-2.58733800	H	-5.67319100 -0.31112600 2.19410100
N	0.71098500	1.50900200	1.09941200	H	-4.06057200 1.24364200 3.35697300
N	-0.71099300	1.50894100	-1.09945900	H	-1.68383300 1.31812300 2.55828200
C	2.81743300	-0.95812800	-0.43328300	H	-3.92231300 -3.06761100 -1.00788200
C	4.16992700	-1.04869200	-0.82071000	H	-2.82139600 -4.32985000 -2.84719500
C	4.63476000	-0.25358100	-1.88273800	H	-0.46724100 -3.70296100 -3.51974100
C	3.73946100	0.61672700	-2.53199200	H	0.66426200 -1.83274200 -2.30221000
C	2.40731100	0.66127500	-2.08650700	N	-1.95577200 -0.10536000 1.06436000
C	2.22541200	-1.75779100	0.67099600	N	-0.94279400 -1.43534400 -1.04291600
C	2.91694300	-2.80415600	1.31390300		
C	2.29595600	-3.52089200	2.34902600	[C3]3+	
C	0.98460500	-3.17674000	2.72486800	Co	0.00025000 -0.00022400 -0.00031900
C	0.34370800	-2.13155900	2.04539400	C	-0.59007100 2.70390800 0.57560700
H	4.85683500	-1.71315500	-0.30964100	C	-0.53488000 3.97153500 1.17974800
H	5.67314600	-0.31121800	-2.19422400	C	0.31832800 4.17973000 2.27826900

C	1.09874600	3.10724800	2.74968900	H	0.09182700	-1.88882000	2.45220500
C	1.00689900	1.86408600	2.10614000	N	1.57467400	0.57068600	-1.04476500
C	-1.44282400	2.36181200	-0.57634000	N	1.35220300	-0.98947000	1.04356900
C	-2.35969100	3.23952300	-1.17972600	C	-2.04684500	-1.86293000	0.57746500
C	-3.12027900	2.80028700	-2.27821300	C	-3.17228100	-2.44825400	1.18218500
C	-2.94223000	1.48619200	-2.75030700	C	-3.77850200	-1.81280700	2.28075700
C	-2.01595400	0.65151300	-2.10742300	C	-3.23946500	-0.60063800	2.75127700
H	-1.14074700	4.78888900	0.80593300	C	-2.11695200	-0.05928400	2.10711500
H	0.37168100	5.15417200	2.75410700	C	-1.32518100	-2.43065200	-0.57497600
H	1.76625000	3.22520500	3.59660100	C	-1.62859900	-3.66268700	-1.17900400
H	1.59170700	1.02252300	2.45008500	C	-0.86891100	-4.10217000	-2.27797400
H	-2.48715000	4.24865200	-0.80525600	C	0.18122900	-3.29226100	-2.74973800
H	-3.83288100	3.46739200	-2.75358100	C	0.44268200	-2.07343300	-2.10619500
H	-3.50604500	1.11017600	-3.59734900	H	-3.57784600	-3.38138900	0.80849400
H	-1.85664100	-0.36042500	-2.45237900	H	-4.64900600	-2.25336200	2.75712800
N	0.18187800	1.66495700	1.04297000	H	-3.67475600	-0.08110000	3.59823700
N	-1.28210800	1.07767900	-1.04412800	H	-1.68047300	0.86803400	2.45052000
C	2.76738800	0.06768500	-0.57746500	H	-2.43927700	-4.27711400	-0.80458600
C	3.98548100	0.42207900	-1.18209400	H	-1.09178400	-5.05229700	-2.75376800
C	3.98476500	1.29989800	-2.28095200	H	0.78817700	-3.59276100	-3.59710700
C	2.75761400	1.80326400	-2.75209800	H	1.24037600	-1.43050800	-2.45067700
C	1.57199900	1.41919800	-2.10809800	N	-1.53240900	-0.67492100	1.04420800
C	2.63781900	-0.84063400	0.57566200	N	-0.29269300	-1.65027900	-1.04283100
C	3.70831700	-1.52151700	1.18010600				
C	3.46256200	-2.36335500	2.27960400	[Z1]2+			
C	2.14380900	-2.50288300	2.75147000	Co	-0.07674400	-0.01350700	-0.00120300
C	1.11274300	-1.80273000	2.10750400	C	-2.66924500	-0.16935900	-1.09693900
H	4.92342700	0.02824200	-0.80790000	C	-2.58720200	-0.16674800	1.28634000
H	4.91855700	1.58314900	-2.75697800	C	-3.98716600	-0.24008400	1.36955900
H	2.71350400	2.47955300	-3.59910700	C	-4.73153400	-0.27838900	0.17304500
H	0.61578300	1.78806400	-2.45160900	C	-4.07545600	-0.24341900	-1.07134600
H	4.71890500	-1.40594400	0.80559800	C	-1.79982000	-0.11727600	-2.29105800
H	4.28002300	-2.89619000	2.75568000	C	0.43785200	0.01489200	-3.01329600
H	1.91256100	-3.13898300	3.59919300	C	0.04288400	-0.00982500	-4.36206700

C	-1.32706700	-0.09037000	-4.66846200	C	-0.26059900	-3.25358800	-0.00292200
C	-2.26025600	-0.14543500	-3.61680900	C	0.28108700	-4.55177000	-0.01807700
H	-4.49184400	-0.26464400	2.32886300	C	1.67963900	-4.69612000	-0.05267700
H	-5.81485300	-0.33295400	0.21197300	C	2.48761000	-3.54480300	-0.07241900
H	-4.64965900	-0.27053700	-1.99036600	C	1.87528200	-2.27702000	-0.05597300
H	1.48507400	0.07649600	-2.74235000	H	-1.33493500	-3.10030100	0.02346800
H	0.79257200	0.03375000	-5.14468100	H	-0.37430800	-5.41603800	-0.00232400
H	-1.66293700	-0.10991200	-5.70043400	H	2.13344400	-5.68215400	-0.06367800
H	-3.32103600	-0.20821000	-3.83366300	H	3.56633800	-3.64840600	-0.09872900
C	0.63973000	0.01206100	2.98158600	N	0.51348600	-2.14461200	-0.02044300
C	-0.90080000	-0.07744900	4.70192100	N	1.87343900	0.13862700	-0.05923300
C	-1.95996500	-0.13527800	3.77328900	N	0.18458400	2.18642700	-0.01073600
C	-1.62970100	-0.11346500	2.41031100	N	0.39651800	-0.00547900	4.30781700
H	1.67505500	0.06869000	2.66979500	N	-0.44152200	4.50519400	-0.00364800
H	-1.08179300	-0.08859400	5.77207100				
H	-2.98607700	-0.19324500	4.11669500	[Z1]3+			
N	-0.31039400	-0.03643600	2.01584100	Co	-0.00001700	0.01040200	0.00003600
N	-1.96977700	-0.13438800	0.07093300	C	-2.60054000	0.83004700	0.65728500
N	-0.45623800	-0.03625600	-1.99788100	C	-2.46792100	-0.86906400	-1.02731200
C	2.45605700	1.37676900	-0.06828900	C	-3.86655600	-0.91481500	-1.13953200
C	2.63203500	-0.99828000	-0.07363100	C	-4.63409900	-0.05532800	-0.32135800
C	4.03957200	-0.91186200	-0.09877600	C	-4.00738500	0.82440400	0.58424000
C	4.65081000	0.35174900	-0.10809700	C	-1.73246100	1.64929200	1.52561900
C	3.85511100	1.51148200	-0.09292000	C	0.52148900	2.09310100	2.09798300
C	1.51195900	2.52379600	-0.04613500	C	0.12466100	3.05957600	3.03835100
C	-0.72876700	3.18537400	0.00775400	C	-1.24576800	3.31768400	3.21870800
C	0.87287800	4.84534100	-0.03603100	C	-2.18441700	2.60133000	2.44945900
C	1.89658000	3.87661400	-0.05923400	H	-4.35654300	-1.59153400	-1.83120500
H	4.65015900	-1.80644500	-0.10752700	H	-5.71771200	-0.07531700	-0.38927200
H	5.73299900	0.43372300	-0.12445400	H	-4.60539100	1.47739700	1.21031900
H	4.32102800	2.48965500	-0.09711700	H	1.57047300	1.87640600	1.94045200
H	-1.77756700	2.91078000	0.03335600	H	0.87712500	3.59137100	3.61097700
H	1.09731100	5.90736200	-0.04337200	H	-1.57912600	4.05794900	3.93956100
H	2.93341300	4.18892500	-0.08547200	H	-3.24563100	2.78815200	2.57537200

C	0.84288000	-2.06072200	-2.02572200	N	0.38004600	1.39583600	-1.36560300
C	-0.62549000	-3.28853400	-3.32950800	N	1.88825400	-0.00569600	0.14406800
C	-1.72965500	-2.63269200	-2.73920600	N	0.15723000	-1.37609900	1.40968600
C	-1.46480000	-1.66561800	-1.76150100	N	0.65088800	-2.99781700	-2.97075300
H	1.86628700	-1.83955000	-1.75055000	N	-0.64930500	-2.98399900	2.98494300
H	-0.75433100	-4.05006300	-4.09291200				
H	-2.73999400	-2.88147500	-3.04336600	[Z2]2+			
N	-0.15637600	-1.38267300	-1.40330700	Co	-0.07975200	0.00638500	0.00300300
N	-1.88825100	-0.00749900	-0.14389300	C	-2.62824200	-0.29044300	1.18149100
N	-0.38079100	1.40202900	1.35912200	C	-2.64774400	-0.01527600	-1.17857900
C	2.46843800	-0.86292900	1.03137200	C	-4.04478600	-0.10448000	-1.23430600
C	2.60009600	0.82820300	-0.66129400	C	-4.74144500	-0.29447800	-0.02123900
C	4.00695800	0.82336200	-0.58856200	C	-4.03574300	-0.38888900	1.19353300
C	4.63418700	-0.05179300	0.32109900	C	-1.71015700	-0.36894500	2.33738500
C	3.86711200	-0.90766000	1.14349500	C	0.55730700	-0.30964200	2.97507000
C	1.46577000	-1.65654400	1.76938100	C	0.21885300	-0.48204100	4.32870000
C	-0.84171600	-2.05168100	2.03527000	C	-1.13696200	-0.60063000	4.68146000
C	0.62721700	-3.27233400	3.34512000	C	-2.11406500	-0.54250700	3.66999700
C	1.73107100	-2.61871200	2.75177900	H	-4.55341600	-0.02907500	-2.18918900
H	4.60457000	1.47352800	-1.21795700	H	-5.82419800	-0.36991800	-0.02464400
H	5.71782200	-0.07109900	0.38884900	H	-4.57370800	-0.53783000	2.12306000
H	4.35746300	-1.58095800	1.83824700	H	1.59264800	-0.21385900	2.67009500
H	-1.86521800	-1.83248100	1.75890100	H	1.00097700	-0.52190200	5.07908600
H	0.75643100	-4.02993900	4.11235500	H	-1.42910400	-0.73530700	5.71811100
H	2.74152100	-2.86542700	3.05725900	H	-3.16498300	-0.63128000	3.92315200
C	-0.52265700	2.08300800	-2.10759900	C	0.45083400	0.38902000	-3.04508600
C	-0.12639300	3.04531600	-3.05246800	C	-1.28424300	0.47369700	-4.55459600
C	1.24389500	3.30329000	-3.23411700	C	-1.74458100	0.17430000	-2.32633500
C	2.18296700	2.59097400	-2.46165000	H	1.51415500	0.42736500	-2.84082400
C	1.73155400	1.64300900	-1.53337100	H	-1.63068700	0.57734100	-5.57663400
H	-1.57152000	1.86644800	-1.94912000	N	-0.40374300	0.20889100	-2.00428900
H	-0.87915500	3.57406300	-3.62752100	N	-1.97676100	-0.10674000	0.00232600
H	1.57683000	4.04035600	-3.95843700	N	-0.37867800	-0.25466700	1.99791100
H	3.24408200	2.77770800	-2.58854200	C	2.60754700	-1.04021200	-0.15329600

C	2.48458500	1.31477600	0.10272400	C	4.65237500	-0.06919000	-0.07641800
C	3.89459300	1.39783700	0.07983100	C	3.97916800	0.80683400	0.79998800
C	4.65817400	0.22753100	-0.06291700	C	1.65332100	1.62803100	1.63600600
C	4.00982000	-1.01726300	-0.18158400	C	-0.63161800	2.06782500	2.08394600
C	-0.23119300	-3.33489800	-0.36618800	C	-0.28804300	3.03362400	3.04614600
C	1.69828100	-4.57606200	-0.49739400	C	1.07000500	3.29522300	3.30026100
H	4.39154900	2.35636500	0.17042400	C	2.05127000	2.58007000	2.58382700
H	5.74196500	0.28302000	-0.08277500	H	4.41651100	-1.61849100	-1.61395800
H	4.55384300	-1.94809500	-0.29462100	H	5.73808400	-0.07812200	-0.09948700
H	-1.31468700	-3.28898800	-0.35658700	H	4.54601700	1.46796500	1.44677200
H	2.18786900	-5.53842000	-0.59540600	H	-1.67051600	1.84864700	1.87151700
C	-0.67172200	3.16393200	0.35900600	H	-1.07200900	3.56288300	3.57750100
C	-0.30042700	4.51299900	0.50486500	H	1.36195300	4.03707500	4.03736200
C	1.06820800	4.83643200	0.51990200	H	3.10376400	2.76897200	2.76778900
C	2.01809600	3.80657300	0.39029000	C	-0.67671000	-2.12707200	-2.09237300
C	1.57377900	2.47881100	0.24726100	C	0.98893100	-3.26735300	-3.20965200
H	-1.71783400	2.87464900	0.34366800	C	1.57002500	-1.68156700	-1.65117700
H	-1.06159600	5.27970000	0.60222900	H	-1.73237300	-1.95225600	-1.92125100
H	1.39134400	5.86687900	0.62978100	H	1.28305300	-4.01208600	-3.94204100
H	3.07506200	4.04732500	0.40175100	N	0.23786900	-1.40492400	-1.38538800
N	0.23885600	2.17124800	0.23208900	N	1.89585500	-0.03388700	-0.01129400
N	1.87002400	0.10084900	-0.01470500	N	0.31154300	1.38115600	1.39256300
N	0.46577900	-2.17350200	-0.25784900	C	-2.52664000	0.88556600	-0.86637100
N	0.05470200	0.52469700	-4.32898100	C	-2.56760700	-0.80740600	0.81616300
N	0.33861100	-4.55470200	-0.48695000	C	-3.97957700	-0.80619300	0.79885300
C	1.82873900	-2.29268600	-0.27437800	C	-4.65236000	0.06928200	-0.07842400
N	2.48149400	-3.47132600	-0.39299100	C	-3.92461400	0.93488400	-0.93052300
N	-2.21756200	0.30166700	-3.58019800	C	0.67772500	2.12578600	-2.09304800
				C	-0.98728700	3.26544800	-3.21189000
[Z2]3+				H	-4.54673200	-1.46681700	1.44589200
Co	0.00001300	-0.00009900	0.00945600	H	-5.73805900	0.07829100	-0.10193400
C	2.56718400	0.80791100	0.81673800	H	-4.41571500	1.61758400	-1.61685700
C	2.52705500	-0.88618400	-0.86469400	H	1.73330600	1.95111800	-1.92127900
C	3.92505100	-0.93542000	-0.92825100	H	-1.28105100	4.00967000	-3.94494200

C	0.63058300	-2.06655700	2.08561300	H	-0.27440100	3.68474400	3.78150700
C	0.28658100	-3.03172400	3.04830200	H	-2.60034100	2.72252800	4.41414600
C	-1.07158100	-3.29311100	3.30201900	H	-4.03252500	1.70360300	2.55103800
C	-2.05253300	-2.57841700	2.58470000	C	1.25138500	-1.96831700	-2.13974300
C	-1.65416800	-1.62702300	1.63641800	C	1.19898500	-3.01105100	-3.07987000
H	1.66957500	-1.84758300	1.87345800	C	-0.03825800	-3.62946000	-3.33589700
H	1.07030300	-3.56067700	3.58032000	C	-1.18076600	-3.18860700	-2.64468500
H	-1.36387000	-4.03449200	4.03945900	C	-1.05839400	-2.14148900	-1.71476800
H	-3.10511200	-2.76720200	2.76831700	H	2.18592400	-1.46653200	-1.91621200
N	-0.31228900	-1.38033100	1.39339300	H	2.10214400	-3.32487100	-3.59194200
N	-1.89585000	0.03372300	-0.01221500	H	-0.11341000	-4.43731800	-4.05702100
N	-0.23722100	1.40406100	-1.38619000	H	-2.14036500	-3.65668500	-2.83299800
N	-0.33894100	-3.05830600	-3.00440200	N	0.15246200	-1.54182600	-1.47332700
N	0.34045700	3.05655200	-3.00578600	N	-1.83314200	-0.57114900	-0.07799900
C	-1.56924900	1.68053700	-1.65284800	C	2.74856900	-0.01804400	0.74801700
N	-1.97010700	2.59269900	-2.54881400	C	2.18196400	1.59914900	-0.91649600
N	1.97137000	-2.59426200	-2.54641300	C	3.50472900	2.06279800	-0.96116800
				C	4.46558200	1.45926700	-0.12556600
[Z3]2+				C	4.09138200	0.41991900	0.73699500
Co	0.00000000	0.00001400	-0.10626100	C	2.24428700	-1.09016600	1.62481100
C	-2.74864100	0.01780200	0.74779100	C	0.18175200	-2.20370600	2.31578800
C	-2.18187500	-1.59891800	-0.91712500	C	0.84410300	-2.98253500	3.18063700
C	-3.50462200	-2.06259600	-0.96201400	C	2.34767600	-2.92171900	3.36061000
C	-4.46555000	-1.45932000	-0.12631500	C	2.95911700	-1.85476100	2.47977300
C	-4.09144600	-0.42017900	0.73653900	H	3.79016700	2.87414000	-1.61983300
C	-2.24444400	1.08969700	1.62491100	H	5.49434800	1.80501100	-0.14398900
C	-0.18197500	2.20306600	2.31635600	H	4.82492800	-0.03486800	1.39172900
C	-0.84439400	2.98162000	3.18139900	H	-0.88581300	-2.19643800	2.14489500
C	-2.34798600	2.92077000	3.36120700	H	0.27406400	-3.68587000	3.78045400
C	-2.95934200	1.85401800	2.48006100	H	2.59991800	-2.72370900	4.41362100
H	-3.78999000	-2.87376500	-1.62092300	H	4.03230700	-1.70443100	2.55081700
H	-5.49430900	-1.80507600	-0.14491700	C	-1.25119800	1.96900100	-2.13925800
H	-4.82505300	0.03441900	1.39133400	C	-1.19870400	3.01201900	-3.07906500
H	0.88560600	2.19584000	2.14556000	C	0.03858000	3.63045000	-3.33483900

C 1.18102400 3.18936600 -2.64367000
 C 1.05855400 2.14198100 -1.71406500
 H -2.18576400 1.46716700 -1.91594600
 H -2.10181700 3.32601700 -3.59111000
 H 0.11380500 4.43852100 -4.05571600
 H 2.14065100 3.65746600 -2.83178400
 N -0.15233300 1.54227600 -1.47289900
 N 1.83314700 0.57115300 -0.07768200
 O -0.83316900 1.24080400 1.48165100
 O 0.83300900 -1.24116300 1.48145500
 H 2.80216700 -3.89922800 3.13597700
 H -2.80244700 3.89833400 3.13674100

[Z3]3+

Co 0.00000000 -0.00000300 0.07950400
 C 2.66214400 0.40504900 -0.79862600
 C 2.34303400 -1.30239500 0.86215000
 C 3.70985700 -1.60258200 0.86856000
 C 4.56335000 -0.86823900 0.01071800
 C 4.04948500 0.13544400 -0.82653800
 C 1.95429500 1.40779900 -1.59703100
 C -0.33353400 2.21923600 -2.10033400
 C 0.15823700 3.12856600 -2.94810100
 C 1.63313700 3.30699700 -3.22818700
 C 2.46551100 2.31942000 -2.45090200
 H 4.11603900 -2.37752100 1.50871200
 H 5.62707800 -1.08607200 -0.00228900
 H 4.70944300 0.68760000 -1.48602600
 H -1.37359800 2.03460600 -1.88018800
 H -0.55021700 3.76369800 -3.47327300
 H 1.83427600 3.19390200 -4.30461100
 H 3.54275200 2.34696200 -2.59722300
 C -1.06353300 -1.87856200 2.09179400
 C -0.93982900 -2.91468700 3.03048000

C 0.33035900 -3.46553700 3.28102500
 C 1.44592300 -2.96173300 2.58510400
 C 1.27062200 -1.92547800 1.65778000
 H -2.02732100 -1.43544600 1.88085300
 H -1.82236800 -3.27498100 3.54813400
 H 0.45188800 -4.26817200 4.00202000
 H 2.43270500 -3.37412600 2.76625600
 N 0.01351800 -1.39779400 1.42055900
 N 1.86707100 -0.31766300 0.03849700
 C -2.66213800 -0.40510100 -0.79862800
 C -2.34304600 1.30240600 0.86208600
 C -3.70987200 1.60257600 0.86849000
 C -4.56335900 0.86818900 0.01067800
 C -4.04948400 -0.13551800 -0.82654200
 C -1.95427900 -1.40786500 -1.59700700
 C 0.33355400 -2.21930800 -2.10027400
 C -0.15820300 -3.12861700 -2.94807200
 C -1.63309900 -3.30704300 -3.22818200
 C -2.46548200 -2.31946500 -2.45090800
 H -4.11606200 2.37753300 1.50861600
 H -5.62709000 1.08600600 -0.00233100
 H -4.70943800 -0.68771000 -1.48600200
 H 1.37361400 -2.03469300 -1.88009800
 H 0.55025900 -3.76373600 -3.47324900
 H -1.83422300 -3.19394500 -4.30460800
 H -3.54271800 -2.34698300 -2.59726900
 C 1.06351800 1.87865900 2.09170000
 C 0.93980600 2.91482500 3.03034000
 C -0.33038700 3.46567400 3.28086400
 C -1.44594800 2.96182800 2.58496900
 C -1.27063900 1.92553400 1.65768900
 H 2.02730900 1.43554100 1.88077900
 H 1.82234300 3.27515100 3.54797500
 H -0.45192200 4.26833900 4.00182300

H	-2.43273400	3.37421900	2.76610500	H	4.71685800	-0.00536900	1.74657200
N	-0.01353000	1.39785100	1.42048800	H	5.82716100	0.16174000	-0.48000000
N	-1.86707200	0.31765200	0.03846700	H	4.44532700	0.21774200	-2.56652700
O	0.52434200	1.30975100	-1.36033500	C	0.38500600	-3.48900700	-0.27608800
O	-0.52433400	-1.30985200	-1.36025500	C	-1.91218900	-3.91335000	-0.15586500
H	-1.95189900	-4.33399200	-2.99132500	H	1.46297900	-3.58540700	-0.34281000
H	1.95193100	4.33394600	-2.99132400	H	-2.87560100	-4.40428400	-0.11404500
				C	-1.78466900	2.22571100	0.11931400
[Z4]2+				C	-2.34560800	3.51391000	0.22405400
Co	0.08064900	-0.10461800	-0.12050000	C	-1.49413000	4.63272800	0.24517400
N	0.52369100	-0.19487500	1.84888800	C	-0.10321400	4.43852600	0.16153100
N	-0.43151700	2.04617800	0.03671000	C	0.38557800	3.12405000	0.05809400
N	1.98466700	-0.00823700	-0.25116600	C	-2.59222000	0.97757500	0.09275600
N	-1.88056400	-0.18914600	0.00115200	C	-3.99796100	0.95039400	0.15801500
N	-0.21569300	-2.32869700	-0.20048500	C	-4.66530900	-0.28771900	0.12891900
N	0.20339500	0.00875100	-2.11008000	C	-3.92428000	-1.47506400	0.03590900
C	-0.57392900	0.03537600	-3.16250500	C	-2.51814300	-1.39998100	-0.02736400
C	1.64305700	0.18024900	-3.91960300	H	-3.41817400	3.65599100	0.28989900
H	-1.65393200	-0.01640900	-3.09522300	H	-1.90842900	5.63286100	0.32621400
H	2.52109400	0.25803500	-4.54731300	H	0.58495000	5.27695700	0.17619600
C	1.87502200	-0.14441500	2.10973500	H	1.45164400	2.93026200	-0.00787400
C	2.36813400	-0.18886500	3.42380500	H	-4.56844500	1.86813200	0.23059400
C	1.46159500	-0.28654400	4.49474100	H	-5.74915500	-0.32272500	0.17845300
C	0.08311000	-0.33754100	4.22016100	H	-4.42232800	-2.43790600	0.01217700
C	-0.34555200	-0.28932200	2.88306400	C	1.58855700	0.09855600	-2.56259100
C	2.71572700	-0.04126900	0.89835000	C	0.22323200	0.14717000	-4.43895500
C	4.11932400	0.01971300	0.84254300	H	-0.04165100	1.05007400	-5.01144300
C	4.74449000	0.11391500	-0.41732200	H	0.03605600	-0.69956500	-5.11784900
C	3.97222500	0.14570400	-1.59320100	C	-1.64586500	-2.57511600	-0.12453900
C	2.57137100	0.08188600	-1.47937200	C	-0.59291200	-4.64061400	-0.25762800
H	3.43485900	-0.14736300	3.61504700	H	-0.51492700	-5.26552500	-1.16101900
H	1.82345800	-0.32119000	5.51755700	H	-0.41319100	-5.32072000	0.58984300
H	-0.64726300	-0.41238300	5.01854100				
H	-1.39933900	-0.32602200	2.63460000	[Z4]3+			

Co	-0.00006900	-0.00032400	-0.14565500	C	1.28470600	-3.18380500	3.17152100
N	-0.40384300	1.34926000	1.24171600	C	-0.08747800	-3.02519000	2.90591600
N	0.40414000	-1.34820300	1.24309700	C	-0.49210800	-2.09633600	1.93283700
N	-1.89673600	-0.17887900	-0.16432600	C	2.61681200	-0.61669000	0.67721100
N	1.89674200	0.17798000	-0.16529600	C	4.01875600	-0.52602700	0.68520000
N	0.09932800	1.39332300	-1.51814900	C	4.64245400	0.39339000	-0.18724900
N	-0.09975400	-1.39484900	-1.51715900	C	3.87505100	1.20204200	-1.04892600
C	0.71359700	-2.09690100	-2.26712300	C	2.47387800	1.07289200	-1.01929800
C	-1.48654900	-2.76584400	-2.75932600	H	3.27739500	-2.51499400	2.64824100
H	1.79149300	-1.98945900	-2.24254500	H	1.62459800	-3.89417100	3.91888500
H	-2.34261300	-3.27115200	-3.18860900	H	-0.83428400	-3.60502600	3.43765700
C	-1.75539200	1.49436200	1.49452500	H	-1.54134700	-1.95366900	1.70776100
C	-2.21468400	2.40741900	2.45449900	H	4.61899200	-1.14332400	1.34415300
C	-1.28362000	3.18589100	3.16930200	H	5.72508200	0.47746300	-0.19321000
C	0.08835400	3.02864400	2.90184400	H	4.35408800	1.90814600	-1.71882100
C	0.49265200	2.09911100	1.92925900	C	-1.47702300	-1.79436900	-1.80609800
C	-2.61657700	0.61652800	0.67772600	C	-0.05411200	-3.04967800	-3.14302200
C	-4.01854500	0.52631300	0.68569300	H	0.23707800	-4.09848100	-2.96455500
C	-4.64251500	-0.39335200	-0.18629800	H	0.14664700	-2.88137800	-4.21422400
C	-3.87536500	-1.20272400	-1.04749000	C	1.47647400	1.79287900	-1.80747700
C	-2.47416300	-1.07403300	-1.01789200	C	0.05314700	3.04825800	-3.14389000
H	-3.27637600	2.51467200	2.64943000	H	-0.14783700	2.87974900	-4.21501300
H	-1.62320400	3.89642200	3.91666500	H	-0.23811800	4.09706600	-2.96556400
H	0.83521400	3.61002100	3.43183500				
H	1.54168700	1.95736100	1.70265500	[Z5]2+			
H	-4.61864900	1.14443300	1.34397100	Co	0.07983800	-0.08007100	-0.10781400
H	-5.72518600	-0.47690600	-0.19238600	N	0.53358900	-0.25467600	1.85137800
H	-4.35460000	-1.90900800	-1.71703300	N	-0.45529000	2.03486400	0.10713400
C	-0.71427800	2.09544800	-2.26778500	N	1.97883700	-0.00574400	-0.24591000
C	1.48568300	2.76460500	-2.76047700	N	-1.87894700	-0.20163700	-0.02226200
H	-1.79211800	1.98778000	-2.24281900	N	-0.26189000	-2.32010300	-0.27907200
H	2.34163100	3.26990600	-3.19000800	N	0.25032800	0.08842900	-2.11788300
C	1.75583900	-1.49395100	1.49480400	C	-0.41364800	0.17494000	-3.28214600
C	2.21553100	-2.40673800	2.45485600	C	1.65708100	0.29431700	-3.87438800

N	1.60263800	0.16654200	-2.50088500	C	-2.50680000	-1.39957300	-0.11846500
H	-1.48889500	0.14927500	-3.35529200	H	-3.45898800	3.61734400	0.35451100
H	2.56737400	0.37519600	-4.44771400	H	-1.96354500	5.60206300	0.48062100
C	1.88852900	-0.23647800	2.10541300	H	0.53377100	5.26649700	0.36758100
C	2.39042500	-0.34196900	3.41166100	H	1.42224500	2.93514100	0.12922000
C	1.48910400	-0.46856900	4.48499100	H	-4.60206100	1.81122500	0.17982300
C	0.10858200	-0.48400700	4.21878900	H	-5.74486500	-0.39400200	0.01122300
C	-0.32946900	-0.37384700	2.88760200	H	-4.39324600	-2.48323500	-0.19165000
C	2.72334000	-0.10242300	0.89360500	N	0.41755900	0.30190500	-4.37822100
C	4.12620300	-0.07735100	0.81345500	N	-0.75307200	-4.54960600	-0.40759500
C	4.73241500	0.04326000	-0.45359700				
C	3.94943800	0.13323700	-1.62167400	[Z5]3+			
C	2.55867500	0.10209800	-1.46179000	Co	0.00000600	-0.00014300	-0.11957200
H	3.45898900	-0.32720700	3.59664300	N	0.44161600	-1.33203800	1.26140000
H	1.85714500	-0.55315500	5.50254500	N	-0.44142400	1.33503900	1.25832000
H	-0.61727300	-0.58005800	5.01898800	N	1.88765700	0.19953000	-0.17434500
H	-1.38620900	-0.38142700	2.64847300	N	-1.88766200	-0.19993300	-0.17363200
H	4.73915600	-0.15361800	1.70380300	N	-0.10711200	-1.41021400	-1.49841400
H	5.81467100	0.06233800	-0.53421500	N	0.10691100	1.40661700	-1.50177700
H	4.41271700	0.21851900	-2.59820900	C	-0.62079000	2.19408100	-2.31861300
C	0.22345600	-3.56719900	-0.38394500	C	1.42511800	2.74224500	-2.75438300
C	-1.90405400	-3.88042600	-0.31382900	N	1.44397100	1.76205700	-1.78263000
N	-1.65156500	-2.52015000	-0.23290800	H	-1.69889400	2.18473000	-2.36468200
H	1.27779500	-3.78546600	-0.44386300	H	2.30221300	3.21260700	-3.17489600
H	-2.88536400	-4.32727100	-0.30093000	C	1.80237700	-1.47850900	1.47597400
C	-1.81208700	2.20505500	0.17009500	C	2.28772200	-2.39794600	2.41561300
C	-2.38430400	3.48415100	0.30538800	C	1.37610400	-3.18163900	3.15166600
C	-1.54090500	4.60754600	0.37757400	C	-0.00257200	-3.01929900	2.92681500
C	-0.14783900	4.42432700	0.31477700	C	-0.43533000	-2.08274000	1.97193700
C	0.35331900	3.11698700	0.17943800	C	2.64023000	-0.59812700	0.63878800
C	-2.60943600	0.95549000	0.08329900	C	4.04086800	-0.50250500	0.58515900
C	-4.01468500	0.90524500	0.09904200	C	4.62366500	0.41684000	-0.31549400
C	-4.66081800	-0.34076900	0.00300200	C	3.82491400	1.22565900	-1.15345700
C	-3.90557900	-1.51888100	-0.10946700	C	2.43754400	1.07634700	-1.04581100

H	3.35474400	-2.50899900	2.57783800	C	2.58307400	0.83871900	-0.71608900
H	1.73658600	-3.89971100	3.88197800	C	2.60850000	-0.86687100	0.95284700
H	-0.73450400	-3.60310400	3.47496000	C	4.02098000	-0.87638400	0.95479000
H	-1.49143800	-1.93813400	1.78105500	C	4.70518100	-0.00819900	0.09249400
H	4.67260800	-1.11908100	1.21461200	C	3.98568600	0.86511700	-0.74966900
H	5.70502100	0.50227600	-0.37027100	C	1.68585400	1.70591800	-1.51326800
H	4.27858700	1.92453000	-1.84818800	C	-0.56473900	2.27034500	-1.92544400
C	0.62048500	-2.19988700	-2.31321000	C	-0.19068800	3.24180300	-2.86897000
C	-1.42548700	-2.74908300	-2.74738000	C	1.17685900	3.43679400	-3.13415600
N	-1.44421500	-1.76632700	-1.77822200	C	2.12634100	2.65845100	-2.44771400
H	1.69858300	-2.19066500	-2.35943800	H	4.56210700	-1.54144000	1.61850700
H	-2.30264100	-3.22047300	-3.16661900	H	5.79058500	-0.00119500	0.07914100
C	-1.80216400	1.48203700	1.47267400	H	4.51529400	1.54660200	-1.40448400
C	-2.28742000	2.40368100	2.41019700	H	-1.60851900	2.08976800	-1.69578100
C	-1.37573300	3.18908000	3.14433700	H	-0.95149600	3.82471800	-3.37662400
C	0.00292000	3.02620000	2.91974100	H	1.49860200	4.17828600	-3.85869700
C	0.43558800	2.08741200	1.96701500	H	3.18364500	2.79784600	-2.64300300
C	-2.64012300	0.59972500	0.63763100	N	1.92449000	-0.02717500	0.11641600
C	-4.04077400	0.50413200	0.58427400	N	0.34789200	1.51981900	-1.26317300
C	-4.62370700	-0.41730200	-0.31415000	C	-2.58308300	-0.83868200	-0.71612500
C	-3.82507100	-1.22819600	-1.15021700	C	-2.60850000	0.86681700	0.95290500
C	-2.43768200	-1.07876900	-1.04298200	C	-4.02098000	0.87631900	0.95486700
H	-3.35442700	2.51514000	2.57223900	C	-4.70518500	0.00818400	0.09252300
H	-1.73614200	3.90886200	3.87299900	C	-3.98569400	-0.86508000	-0.74969700
H	0.73490300	3.61128500	3.46645100	C	-1.68586400	-1.70583300	-1.51335600
H	1.49168000	1.94241500	1.77635200	C	0.56472900	-2.27023600	-1.92556800
H	-4.67242200	1.12228200	1.21227400	C	0.19067700	-3.24164100	-2.86914700
H	-5.70507400	-0.50275700	-0.36868100	C	-1.17687100	-3.43661800	-3.13434300
H	-4.27884200	-1.92866900	-1.84326800	C	-2.12635200	-2.65831400	-2.44785500
N	0.15830400	3.01860900	-3.09350900	H	-4.56210400	1.54133000	1.61863200
N	-0.15873100	-3.02609300	-3.08619400	H	-5.79058900	0.00117500	0.07918200
				H	-4.51530500	-1.54653100	-1.40454600
[Z6]2+				H	1.60851000	-2.08967200	-1.69589600
Co	-0.00000300	-0.00000200	0.08043800	H	0.95148400	-3.82452800	-3.37683500

H	-1.49861400	-4.17807000	-3.85892400	H	-5.71512100	-0.51092700	-0.26332100
H	-3.18365600	-2.79769900	-2.64314900	H	-4.64415300	1.12218600	1.29071500
N	-1.92449500	0.02716800	0.11642300	H	1.52562600	1.93306300	1.72143100
N	-0.34790200	-1.51974600	-1.26325400	H	0.80485200	3.62796000	3.39929500
C	1.79631600	-1.70312300	1.81668400	H	-1.65795700	3.93377300	3.85165400
C	2.01897000	-2.68142000	2.76217100	H	-3.30488100	2.52944300	2.59842700
C	0.73211000	-3.09119700	3.27326800	N	-1.88891800	-0.21152400	-0.15259400
H	2.97604900	-3.07733400	3.07072700	N	-0.42265400	1.32453100	1.25357000
C	-0.22550900	-2.35138800	2.62540100	C	2.63072500	-0.58836900	0.67148900
H	0.55261200	-3.84102200	4.02957900	C	2.44502100	1.10342600	-1.02570800
H	-1.30150400	-2.30475100	2.67661400	C	3.85070900	1.23061600	-1.08072900
C	-1.79630800	1.70301700	1.81678400	C	4.63292200	0.42530900	-0.23444900
C	-2.01894800	2.68123700	2.76235300	C	4.02866300	-0.49956800	0.65153200
C	-0.73207000	3.09111400	3.27332300	C	1.77995700	-1.47312100	1.48816100
H	-2.97602300	3.07713100	3.07095000	C	-0.47551500	-2.08102800	1.93465100
C	0.22552800	2.35121300	2.62553200	C	-0.06161300	-3.03225900	2.88041200
H	-0.55255300	3.84098200	4.02958800	C	1.31298500	-3.19953000	3.12988200
H	1.30152300	2.30455600	2.67674500	C	2.24081300	-2.40895600	2.42368500
O	0.39864300	-1.47893700	1.71397700	H	4.31540900	1.93325000	-1.76421300
O	-0.39863700	1.47881900	1.71406200	H	5.71519900	0.51027000	-0.26336900
				H	4.64396400	-1.12059700	1.29285700
[Z6]3+				H	-1.52590900	-1.93060500	1.72372200
Co	0.00000800	-0.00004100	-0.08841800	H	-0.80549200	-3.62321900	3.40406700
C	-2.63081000	0.58918300	0.67036200	H	1.65723600	-3.92852800	3.85724800
C	-2.44482900	-1.10492800	-1.02450200	H	3.30442900	-2.52600200	2.60233400
C	-3.85050200	-1.23229800	-1.07949200	N	1.88896600	0.21124300	-0.15265200
C	-4.63285100	-0.42587200	-0.23440400	N	0.42246600	-1.32278200	1.25539800
C	-4.02873900	0.50029000	0.65033700	C	-1.47304500	-1.82801100	-1.81689900
C	-1.78018900	1.47510800	1.48593100	C	-1.43017800	-2.79240100	-2.79232900
C	0.47519500	2.08370500	1.93197100	C	-0.04053600	-3.01675500	-3.13688500
C	0.06109300	3.03621500	2.87635600	H	-2.27575900	-3.30126900	-3.23581900
C	-1.31355100	3.20376800	3.12537100	C	0.73242300	-2.19002600	-2.37070000
C	-2.24123100	2.41219000	2.42011300	H	0.32465400	-3.71651800	-3.87578800
H	-4.31508500	-1.93587700	-1.76208300	H	1.79196000	-2.00904200	-2.28554300

C	1.47334300	1.82558300	-1.81908700	C	-1.70912800	-1.71184100	4.14779700
C	1.43063000	2.78879700	-2.79568900	C	-1.01540900	-0.49029400	4.03398400
C	0.04104000	3.01275000	-3.14071100	H	-2.37593400	-3.50197200	3.12716400
H	2.27627200	3.29718000	-3.23961600	H	-2.14888800	-1.99542200	5.09885500
C	-0.73205000	2.18697200	-2.37363100	H	-0.92046200	0.16850300	4.89107700
H	-0.32403500	3.71169400	-3.88044400	C	-0.60440000	-2.84938100	-1.71989700
H	-1.79160600	2.00617500	-2.28835500	C	-1.20902000	-4.09149000	-1.97799800
O	-0.11998000	-1.42124100	-1.52482500	C	-1.87227200	-4.75622000	-0.93163300
O	0.12021500	1.41920200	-1.52669700	C	-1.91028900	-4.15779300	0.34066000
				C	-1.28639600	-2.91491500	0.53187800
[Z7]2+				H	-0.08577600	-2.31083500	-2.50366700
Co	0.16330500	-0.48939100	0.04140800	H	-1.15804600	-4.51958400	-2.97327600
C	2.20629400	-0.33043000	-2.00689600	H	-2.34922800	-5.71652700	-1.10043400
C	0.16982100	0.76616800	-2.56346100	H	-2.41776300	-4.65343100	1.16109800
C	0.68411500	1.16623600	-3.81083700	N	-0.63809200	-2.26922400	-0.49745600
C	1.99761100	0.79740800	-4.14856200	N	-0.58806600	-0.99825500	1.72161700
C	2.76784200	0.04572300	-3.24467200	C	1.35674100	3.00398700	2.29471900
C	2.92148500	-1.11566300	-0.96780500	C	1.39597100	2.35551300	1.02072100
C	2.76535600	-2.08069000	1.16648600	C	2.04623400	2.97430300	-0.06735500
C	4.08485300	-2.56337700	1.09687500	C	2.63691200	4.22269400	0.15479300
C	4.83640200	-2.29940800	-0.06226300	C	2.58918500	4.85619400	1.43022200
C	4.24810100	-1.56630000	-1.10822400	C	1.94840900	4.25792800	2.52290400
H	0.08537900	1.74713600	-4.50465000	C	0.28973400	1.03441800	2.40450600
H	2.41688800	1.09249200	-5.10536900	H	2.09061900	2.50148900	-1.04173300
H	3.78078700	-0.23666700	-3.50363500	H	1.91612400	4.74611000	3.49201200
H	2.15245400	-2.26261600	2.04377900	H	0.44225900	2.30578100	4.11839200
H	4.50427200	-3.12542200	1.92451400	N	0.64906900	2.13765600	3.14180800
H	5.85823700	-2.65485400	-0.15139600	N	0.72074800	1.13039100	1.12822400
H	4.82100000	-1.35678100	-2.00441000	C	-2.87438200	1.09045300	-0.67608400
N	0.92827600	0.03028500	-1.69263300	C	-3.26106000	1.85045700	-1.82446100
N	2.19712000	-1.37548400	0.16274400	C	-4.52549500	2.45394000	-1.93782300
C	-0.45809200	-0.15595500	2.78828000	C	-5.40295500	2.27413100	-0.86006300
C	-1.25829200	-2.17688600	1.81188400	C	-5.03275900	1.51782600	0.29061500
C	-1.83777300	-2.56562500	3.03550100	C	-3.77284900	0.91975300	0.39836400

C	-1.16722500	1.07175000	-2.06229900	C	-2.85547900	1.34021300	-2.86508400
H	-4.81839400	3.03095500	-2.80957200	C	-2.50227100	0.47383200	-3.92120400
H	-6.39224000	2.72046500	-0.89987500	C	-1.39944200	-0.39900700	-3.80360600
H	-5.75187900	1.40763100	1.09703800	H	-3.70647300	2.00409600	-2.96731000
H	-3.49569300	0.34278900	1.27542500	H	-3.08711100	0.47803700	-4.83611500
H	-2.09795200	2.26747600	-3.58740500	H	-1.13729200	-1.06329100	-4.62063000
N	-1.56625200	0.62351400	-0.86039100	C	-1.37437500	2.52726500	1.69251800
N	-2.15392100	1.81658400	-2.68341300	C	-2.36633500	3.48811400	1.95272000
H	3.06210200	5.82560800	1.55586000	C	-3.32842400	3.76281000	0.96501000
H	3.14709800	4.72730600	-0.66047000	C	-3.27025500	3.06725200	-0.25826800
				C	-2.25790600	2.11966400	-0.46230100
[Z7]3+				H	-0.62237000	2.29600700	2.43596800
Co	0.00003000	0.46703900	0.00000400	H	-2.37734900	4.00303300	2.90736000
C	2.08237200	1.31849000	1.68898700	H	-4.10623400	4.49962400	1.14002500
C	0.66266700	-0.37790900	2.60703900	H	-4.00440100	3.26529300	-1.03193700
C	1.39938500	-0.39904100	3.80361800	N	-1.31768300	1.85785100	0.51616700
C	2.50231400	0.47367600	3.92120400	N	-1.02266200	0.47355200	-1.60273000
C	2.85563000	1.33999000	2.86506600	C	2.24552500	-2.54555100	-1.99912100
C	2.25816200	2.11943300	0.46224400	C	2.12025700	-1.76888100	-0.80196500
C	1.37467600	2.52708000	-1.69259000	C	3.03158200	-1.96131700	0.25856500
C	2.36674400	3.48780800	-1.95281600	C	4.03257100	-2.92227400	0.08502800
C	3.32887100	3.76241700	-0.96511600	C	4.14269900	-3.68808200	-1.11337400
C	3.27062300	3.06689600	0.25818000	C	3.25042400	-3.51213700	-2.17672700
H	1.13713900	-1.06327800	4.62065000	C	0.50183600	-1.15139300	-2.20311800
H	3.08714200	0.47784200	4.83612300	H	2.97367600	-1.39203200	1.17835100
H	3.70670300	2.00377100	2.96728800	H	3.33787200	-4.09588100	-3.08781200
H	0.62264500	2.29587100	-2.43603300	H	1.03092600	-2.49002000	-3.77663400
H	2.37781100	4.00270600	-2.90746700	N	1.21077000	-2.12376500	-2.84764600
H	4.10676300	4.49913900	-1.14015700	N	1.02044800	-0.91065100	-0.96983900
H	4.00479100	3.26486900	1.03184400	C	-2.12049400	-1.76862700	0.80200800
N	1.02274000	0.47350600	1.60271600	C	-2.24582900	-2.54524200	1.99918700
N	1.31790200	1.85770300	-0.51621700	C	-3.25080300	-3.51174600	2.17682100
C	-0.66271400	-0.37794300	-2.60702600	C	-4.14308100	-3.68766900	1.11347000
C	-2.08221300	1.31865400	-1.68901600	C	-4.03288100	-2.92191500	-0.08496300

C	-3.03181800	-1.96103900	-0.25852600	C	1.84927900	1.34084600	2.00308000
C	-0.50200500	-1.15122500	2.20313400	C	2.46912700	1.33361100	3.27041400
H	-3.33828500	-4.09545300	3.08792700	C	1.99590300	0.45648000	4.26121700
H	-4.93862600	-4.42130300	1.19955100	C	0.91518900	-0.40366800	3.98336300
H	-4.75166600	-3.09529900	-0.88031200	H	3.30400900	1.99052000	3.48331800
H	-2.97385600	-1.39179000	-1.17833100	H	2.46525900	0.43870200	5.23970800
H	-1.03117200	-2.48977300	3.77666900	H	0.54934700	-1.08626100	4.74344100
N	-1.02063000	-0.91045600	0.96986700	C	1.76563300	2.71220000	-1.38779800
N	-1.21103500	-2.12350700	2.84769300	C	2.79482400	3.67028300	-1.42610900
H	4.93819300	-4.42176900	-1.19944600	C	3.56394900	3.88360900	-0.26832800
H	4.75135200	-3.09567400	0.88037300	C	3.28146700	3.13432000	0.88866900
				C	2.23808100	2.19282600	0.85554000
[Z8]2+				H	1.15191100	2.52102300	-2.26149100
Co	-0.00148700	0.50796700	0.00014900	H	2.98319300	4.22799600	-2.33721900
C	-1.85826300	1.32309300	-2.00525800	H	4.36599600	4.61497800	-0.26431000
C	-0.33297800	-0.36453100	-2.70386800	H	3.86738400	3.28846000	1.78803700
C	-0.91288800	-0.42058600	-3.98084800	N	1.49100300	1.98978200	-0.27767000
C	-1.99946400	0.43138500	-4.26089900	N	0.80244200	0.50594400	1.75024700
C	-2.47832200	1.30806300	-3.27244000	C	-2.45756200	-2.61706200	1.97471100
C	-2.25313600	2.17589100	-0.86032000	C	-2.25427100	-1.89086000	0.76393300
C	-1.78524500	2.70525400	1.38157500	C	-3.11487000	-2.21218000	-0.30548000
C	-2.82096700	3.65641300	1.41662300	C	-4.15913300	-3.79730000	1.07677200
C	-3.59096100	3.86103700	0.25785100	C	-0.77825200	-1.16517700	2.21556100
C	-3.30286800	3.11022000	-0.89676100	H	-3.06516400	-1.72968700	-1.27730600
H	-0.54257200	-1.10280000	-4.73909700	H	-1.40096800	-2.46309000	3.82983500
H	-2.46893600	0.40764400	-5.23920700	N	-1.50758100	-2.13505200	2.87598100
H	-3.31768500	1.95870100	-3.48695400	N	-1.19845300	-0.99285200	0.94651900
H	-1.17056300	2.52091100	2.25608400	C	2.26813500	-1.87876500	-0.76012700
H	-3.01356000	4.21556200	2.32597100	C	2.47525100	-2.60629200	-1.96946200
H	-4.39795500	4.58692700	0.25127300	C	4.18531800	-3.77323700	-1.07032300
H	-3.88941200	3.25776900	-1.79682000	C	3.13174600	-2.19196400	0.30926600
N	-0.80573300	0.49599000	-1.75022300	C	0.78618800	-1.16601800	-2.21199800
N	-1.50523000	1.98137900	0.27375300	H	4.96076800	-4.52458000	-1.15986000
C	0.33524000	-0.35509500	2.70610700	H	3.07966500	-1.70755800	1.28002500

H	1.41610100	-2.46342200	-3.82397800	C	-1.39076200	-0.45765200	-3.79871000
N	1.52134600	-2.13256800	-2.87095100	H	-3.72187900	1.93197400	-2.98977400
H	-4.92962000	-4.55360900	1.16733500	H	-3.09726800	0.38276800	-4.83582400
N	3.41081800	-3.54861400	-2.16176400	H	-1.12762900	-1.13464500	-4.60523700
N	4.08052100	-3.13732200	0.14001700	C	-1.38383200	2.54901800	1.66033000
N	1.20626100	-0.98814300	-0.94373000	C	-2.38051000	3.51008200	1.90446900
N	-3.38703700	-3.56512200	2.16833000	C	-3.34257000	3.76582400	0.91169500
N	-4.05749300	-3.16343200	-0.13490600	C	-3.27975800	3.05248700	-0.30207200
				C	-2.26362500	2.10617900	-0.49108800
[Z8]3+				H	-0.63159000	2.33308100	2.40847000
Co	0.00013000	0.47360600	-0.00008400	H	-2.39495100	4.03943600	2.85126800
C	2.08205600	1.28843800	1.70671200	H	-4.12398500	4.50170500	1.07477300
C	0.65119800	-0.40633600	2.60783100	H	-4.01392000	3.23757800	-1.07913300
C	1.39012100	-0.45730200	3.79896000	N	-1.32361100	1.86181300	0.49427000
C	2.50555500	0.40271600	3.92547000	N	-1.01271300	0.45707200	-1.61247700
C	2.86141200	1.28073200	2.88195100	C	2.27616700	-2.53094700	-1.96860100
C	2.26452500	2.10529600	0.49080100	C	2.13499800	-1.74705500	-0.78511500
C	1.38505100	2.54803700	-1.66078800	C	3.09120400	-1.98675500	0.22829600
C	2.38211700	3.50867300	-1.90505100	C	4.08553400	-3.61016100	-1.15416300
C	3.34420900	3.76422700	-0.91226700	C	0.52422000	-1.16831100	-2.19453300
C	3.28104300	3.05115900	0.30164800	H	3.10977700	-1.46233000	1.17822200
H	1.12654800	-1.13394500	4.60563300	H	1.09641100	-2.53304700	-3.75723600
H	3.09676200	0.38277700	4.83615700	N	1.24624400	-2.13860200	-2.83122500
H	3.72223900	1.93127300	2.98977500	N	1.02999300	-0.90540200	-0.95942900
H	0.63277300	2.33218800	-2.40891900	C	-2.13582400	-1.74609700	0.78540700
H	2.39682400	4.03782800	-2.85195800	C	-2.27693500	-2.53008000	1.96883500
H	4.12592500	4.49976700	-1.07543700	C	-4.08657300	-3.60897600	1.15458000
H	4.01524900	3.23612200	1.07869800	C	-3.09223000	-1.98558100	-0.22788400
N	1.01290700	0.45683800	1.61232800	C	-0.52480300	-1.16767400	2.19469800
N	1.32449700	1.86109900	-0.49459900	H	-4.87544800	-4.34331600	1.26766500
C	-0.65156000	-0.40662400	-2.60776800	H	-3.11081600	-1.46116800	-1.17781900
C	-2.08162700	1.28896500	-1.70684000	H	-1.09713600	-2.53226300	3.75746200
C	-2.86123900	1.28119100	-2.88191800	N	-1.24697500	-2.13779600	2.83146200
C	-2.50589200	0.40275300	-3.92524700	H	4.87430900	-4.34460300	-1.26721900

N	-3.22090200	-3.45334000	2.18661400	C	-2.55612400	-1.18911100	0.00566800
N	-4.04900100	-2.91111300	-0.02773200	C	-3.96361100	-1.21468100	0.00569300
N	-1.03060900	-0.90469900	0.95962900	C	-4.67029500	0.00001400	0.00000000
N	3.22002400	-3.45433500	-2.18631600	C	-3.96360300	1.21470600	-0.00569400
N	4.04789900	-2.91237700	0.02817200	C	-1.70394800	2.40668100	-0.01172700
				C	0.47791500	3.24290700	-0.01586900
[Z9]2+				C	-1.25069100	4.77167500	-0.02383600
Co	0.08169800	0.00000000	0.00000100	C	-2.19512500	3.72434900	-0.01858800
C	2.64386700	0.00641600	1.19123300	H	-4.50279800	-2.15453600	0.01008300
C	2.64387100	-0.00642900	-1.19122300	H	-5.75562600	0.00001800	0.00000100
C	4.04962400	-0.00658200	-1.22119900	H	-4.50278400	2.15456300	-0.01008300
C	4.75200200	-0.00001200	0.00000900	H	1.54582100	3.05375700	-0.01493600
C	4.04962000	0.00656100	1.22121400	H	-1.55812500	5.81270300	-0.02919000
C	1.72624300	0.01246500	2.34973900	H	-3.25372700	3.95348100	-0.01999600
C	-0.52523400	0.01579600	3.00216900	C	0.47789400	-3.24291100	0.01586400
C	1.07911300	0.02474500	4.66604500	C	-1.25072100	-4.77166700	0.02381900
C	2.10620600	0.01970400	3.69925900	C	-2.19514900	-3.72433600	0.01857500
H	4.58968800	-0.01173700	-2.16145600	C	-1.70396300	-2.40667100	0.01172100
H	5.83732900	-0.00001400	0.00001100	H	1.54580200	-3.05376800	0.01493600
H	4.58968100	0.01171400	2.16147300	H	-1.55816200	-5.81269400	0.02916700
H	-1.57307600	0.01430500	2.72899600	H	-3.25375200	-3.95346100	0.01997800
H	1.29871500	0.03031700	5.72899300	N	-0.35336300	-2.17419300	0.01036200
H	3.14551200	0.02138500	4.00606800	N	-1.88110000	0.00000600	-0.00000200
C	-0.52522400	-0.01579600	-3.00217000	N	-0.35334900	2.17419400	-0.01036400
C	1.07912800	-0.02475300	-4.66604000	N	-0.23303700	-0.02286000	-4.31840200
C	2.10621900	-0.01971600	-3.69925100	N	0.08645600	4.53536300	-0.02248600
C	1.72625100	-0.01247400	-2.34973200	N	0.08642700	-4.53536400	0.02247400
H	-1.57306700	-0.01430100	-2.72900000	N	-0.23305100	0.02285700	4.31840300
H	1.29873400	-0.03032700	-5.72898700				
H	3.14552500	-0.02140200	-4.00605600	[Z9]3+			
N	0.39068800	-0.01036100	-2.00263400	Co	0.00016900	0.00000000	0.00000000
N	1.98244700	-0.00000500	0.00000400	C	2.54764000	-0.00901100	1.19706800
N	0.39068100	0.01035800	2.00263600	C	2.54764400	0.00900700	-1.19705900
C	-2.55611700	1.18912700	-0.00567200	C	3.95361800	0.00903000	-1.22615700

C	4.65334100	-0.00000300	0.00000800	H	1.71328800	2.65209500	0.02216400
C	3.95361400	-0.00903500	1.22617100	H	-1.09685200	5.70932100	0.04190100
C	1.60918800	-0.01796900	2.33770100	H	-2.98815700	4.02525500	0.02899000
C	-0.66972500	-0.02331100	2.94009500	C	0.66964300	-2.94086200	-0.02352100
C	0.90378900	-0.03464700	4.64015400	C	-0.90434100	-4.64047800	-0.03468200
C	1.95544900	-0.02754100	3.69433100	C	-1.95573800	-3.69433600	-0.02729600
H	4.49838100	0.01592800	-2.16423800	C	-1.60910800	-2.33777200	-0.01772800
H	5.73932400	-0.00000300	0.00001000	H	1.71328300	-2.65209900	-0.02216100
H	4.49837400	-0.01593400	2.16425400	H	-1.09686300	-5.70931800	-0.04190900
H	-1.71327600	-0.02183300	2.65106500	H	-2.98816500	-4.02524900	-0.02900000
H	1.09602300	-0.04179800	5.70904500	N	-0.27384800	-1.96327000	-0.01583400
H	2.98781600	-0.02936800	4.02546000	N	-1.89734000	0.00000200	-0.00000300
C	-0.66971500	0.02331000	-2.94009700	N	-0.27384400	1.96327000	0.01583200
C	0.90380500	0.03464300	-4.64015100	N	-0.39795500	0.03243000	-4.25683300
C	1.95546100	0.02753700	-3.69432500	N	0.39749600	4.25751700	0.03265700
C	1.60919600	0.01796600	-2.33769600	N	0.39748800	-4.25751800	-0.03266100
H	-1.71326700	0.02183300	-2.65107100	N	-0.39797000	-0.03243200	4.25683200
H	1.09604300	0.04179300	-5.70904100				
H	2.98783000	0.02936300	-4.02545000	[Z10]2+			
N	0.27411300	0.01581200	-1.96276300	Co	-0.08623200	0.01021900	0.00898000
N	1.89760700	-0.00000200	0.00000300	C	-2.66496600	0.00800600	1.18948400
N	0.27410700	-0.01581300	1.96276400	C	-2.64592300	0.03510100	-1.17390500
C	-2.54738000	1.19705900	0.00883200	C	-4.69331200	0.02799100	-0.11267300
C	-2.54738200	-1.19705400	-0.00883800	C	-4.06967700	0.01132900	1.15751700
C	-3.95335900	-1.22616400	-0.00886200	C	-1.76365600	-0.01130900	2.36006100
C	-4.65309600	0.00000500	-0.00000500	C	0.47981300	-0.03275700	3.03100300
C	-3.95335700	1.22617200	0.00885400	C	-1.14212500	-0.04783600	4.68133300
C	-1.60910300	2.33777600	0.01772300	C	-2.16072400	-0.02974300	3.70269000
C	0.66964900	2.94086100	0.02352100	H	-5.77440900	0.03181500	-0.20735200
C	-0.90433200	4.64048000	0.03467500	H	-4.67058200	0.00095900	2.05913500
C	-1.95573000	3.69434000	0.02728800	H	1.53148600	-0.03736800	2.77247900
H	-4.49812900	-2.16422700	-0.01560600	H	-1.37168900	-0.06161100	5.74212200
H	-5.73907500	0.00000600	-0.00000500	H	-3.20416300	-0.03029300	3.99646700
H	-4.49812500	2.16423600	0.01559700	C	0.48622400	0.03668400	-3.02764900

C	-1.15698400	0.05553300	-4.66322800	N	0.03074000	4.57066500	0.04627300
C	-2.16686600	0.05234500	-3.67485400	N	3.87911000	-1.30383000	-0.01803000
C	-1.74553000	0.04206100	-2.34200900	N	0.17154500	-0.04940900	4.34464200
H	1.54122000	0.02775400	-2.78220600	N	-3.98723300	0.03929000	-1.27480900
H	-1.39429500	0.06388300	-5.72222100				
H	-3.22208100	0.05726400	-3.92311700	[Z10]3+			
N	-0.40758600	0.03446000	-2.00840300	Co	-0.00003100	0.00043500	0.01215700
N	-1.97845000	0.02144000	0.01091700	C	-2.56949800	-0.79405600	0.89179900
N	-0.42380200	-0.01219400	2.02112300	C	-2.54484900	0.78314000	-0.88275900
C	2.53503800	-1.19463000	-0.01134900	C	-4.59418600	0.07153700	-0.09705000
C	2.58067000	1.16429000	0.01195800	C	-3.97396600	-0.77564900	0.85994600
C	3.98605000	1.11473400	0.00479300	C	-1.64661200	-1.55935400	1.75514700
C	4.60023600	-0.15551100	-0.00952700	C	0.62501900	-1.96937100	2.22132000
C	1.69414600	-2.41355800	-0.02435900	C	-0.96519200	-3.09723500	3.47720400
C	-0.46415300	-3.28118900	-0.03201400	C	-2.00928100	-2.46066200	2.76074500
C	1.30279500	-4.77819200	-0.05745400	H	-5.67584500	0.13326400	-0.17458200
C	2.22715700	-3.71010300	-0.04517800	H	-4.58209800	-1.37528300	1.52804800
H	4.59413500	2.01081700	0.00965600	H	1.67287400	-1.78692700	2.01680200
H	5.68034200	-0.26195100	-0.01484200	H	-1.16756800	-3.80892000	4.27247200
H	-1.53702300	-3.12186600	-0.02993400	H	-3.04589300	-2.67605100	2.99625600
H	1.62771200	-5.81362700	-0.07296000	C	0.63795800	1.97071500	-2.21317000
H	3.29860000	-3.87106500	-0.05153100	C	-0.97365100	3.07684900	-3.47158500
C	-0.39610000	3.28805300	0.04082600	C	-2.01009600	2.43394400	-2.74894800
C	1.37158600	4.77661900	0.04041300	C	-1.62276400	1.54771200	-1.74222000
C	2.29058000	3.70442000	0.02915400	H	1.68906000	1.79707300	-2.01707600
C	1.76295400	2.40297100	0.02526700	H	-1.18241800	3.78179500	-4.27097800
H	-1.46897900	3.13001800	0.04314300	H	-3.05983300	2.61288700	-2.95814900
H	1.70382200	5.81001100	0.04433400	N	-0.28513000	1.31016500	-1.46703200
H	3.35573200	3.90327700	0.02356400	N	-1.89035300	-0.00424600	0.01003600
N	0.40632000	2.19764300	0.03155700	N	-0.30596700	-1.31128100	1.48412800
N	1.86697700	-0.00435700	0.00482900	C	2.54602100	-0.88191200	-0.78067700
N	0.34188400	-2.19264400	-0.01715400	C	2.56817000	0.89393800	0.79511600
N	0.16090500	0.04784600	-4.33724300	C	3.97267700	0.87216800	0.76759200
N	-0.03825900	-4.56402200	-0.05098800	C	4.59424700	-0.08204200	-0.08176000

C	1.62514700	-1.74279000	-1.54510600	C	0.09811200	0.08037500	-4.37472200
C	-0.63487000	-2.21786600	-1.96731300	C	-1.27141100	0.06587900	-4.69608500
C	0.97863400	-3.46404200	-3.08447600	C	-2.21635100	0.03863800	-3.65233200
C	2.01399300	-2.74120500	-2.44004700	H	-4.63702000	-0.11847100	2.09546100
H	4.57987300	1.54662500	1.36101900	H	-5.75727200	-0.08352300	-0.15800600
H	5.67601600	-0.15229700	-0.14996100	H	1.53706200	0.07774900	-2.74793400
H	-1.68625700	-2.02249000	-1.79455100	H	0.85576300	0.09911600	-5.15090700
H	1.18856000	-4.25805400	-3.79513700	H	-1.59636100	0.07411600	-5.73166500
H	3.06404000	-2.94382300	-2.62465000	H	-3.28491000	0.02449200	-3.83901600
C	-0.62810000	2.21693000	1.97316700	C	0.53134200	-0.06905700	3.01992100
C	0.96052500	3.48610200	3.08830500	C	-1.18008600	-0.14266700	4.73536600
C	2.00550500	2.77029600	2.45247800	C	-2.15022000	-0.12471200	3.71542900
C	1.64410000	1.75601900	1.56039500	C	-1.73144100	-0.07887900	2.37746900
H	-1.67569300	2.01106500	1.79070900	H	1.57130900	-0.04918400	2.71684800
H	1.16184400	4.28706800	3.79387300	H	-1.48052300	-0.17858800	5.77772200
H	3.04181300	3.01305000	2.66115200	H	-3.20595100	-0.14742200	3.96443100
N	0.30379200	1.47712100	1.31926800	N	-0.39565100	-0.04968600	2.03480100
N	1.89026000	0.00519100	0.01208400	N	-1.96519200	-0.02251500	0.02707000
N	0.28709100	-1.47457200	-1.30195300	N	-0.41331800	0.04336200	-2.01376700
N	0.33333600	2.83851300	-3.19622900	C	2.53799900	1.23364000	0.01306400
N	-0.32875700	-3.19489500	-2.84133900	C	2.55631900	-1.13208000	-0.03508600
N	-0.34215200	3.20352300	2.84341700	C	4.59087900	-0.03310500	-0.02603900
N	3.88451000	-0.95304600	-0.85129900	C	3.94595200	1.21908100	0.00251100
N	0.33785900	-2.84636300	3.20161900	C	1.68816600	2.44775100	0.03978800
N	-3.88323400	0.84564200	-0.96299900	C	-0.51660500	3.24833500	0.06783000
				C	1.30640400	4.84210300	0.06794300
[Z11]2+				C	2.20275400	3.75730500	0.04887600
Co	-0.07910800	0.00722800	0.01067100	H	5.67366900	-0.10912700	-0.03427600
C	-2.63886500	-0.00853500	-1.15508300	H	4.53138200	2.12947800	0.01562500
C	-2.63712600	-0.06246100	1.21276300	H	-1.57640900	3.01409100	0.07295000
C	-4.04349400	-0.08605600	1.19001700	H	1.68014600	5.86117600	0.07432400
C	-4.67537500	-0.06720300	-0.07324800	H	3.27162300	3.94024500	0.03988000
C	-1.75263700	0.02747500	-2.33076700	C	-0.41291300	-3.26601600	-0.07637200
C	0.48868300	0.06867700	-3.02211000	C	0.09580600	-4.57951800	-0.11904400

C	1.48982800	-4.77118200	-0.13110700	C	-0.68882100	-2.06183700	-2.09788700
C	2.33431300	-3.64524400	-0.10191000	C	0.97449300	-3.31999700	-3.33901400
C	1.74741400	-2.36947000	-0.06095500	C	1.97706200	-2.62479100	-2.63139900
H	-1.48351300	-3.08667100	-0.06796600	C	1.60454600	-1.66905300	-1.67801300
H	-0.58680600	-5.42255100	-0.14290900	H	-1.72163800	-1.82826000	-1.87209900
H	1.90972700	-5.77161200	-0.16370300	H	1.24346300	-4.06535400	-4.08117400
H	3.41490000	-3.73388600	-0.11128200	H	3.02463700	-2.83181800	-2.82510000
N	0.39226600	-2.18019900	-0.04696000	N	0.27100500	-1.39163800	-1.41741500
N	1.86126100	0.04354600	-0.00455900	N	1.88175500	-0.03090100	-0.01642900
N	0.34029400	2.20330900	0.05031200	N	0.29975000	1.37780900	1.40053100
N	3.90514000	-1.20297900	-0.04562500	C	-2.54106000	0.88863800	-0.84174400
C	-0.07622200	4.58595100	0.07690900	C	-2.54418000	-0.80968700	0.82403200
H	-0.79819700	5.39558900	0.08957600	C	-4.57871800	-0.01698400	0.07867600
C	0.18005600	-0.11528600	4.38177500	C	-3.94698400	0.88466500	-0.81478200
N	-3.98307400	-0.02943400	-1.24328400	C	-1.60770000	1.69821900	-1.64525400
H	0.95754000	-0.13044400	5.13800100	C	0.68489300	2.09972900	-2.06120400
				C	-0.98077800	3.37926500	-3.27704300
[Z11]3+				C	-1.98200400	2.67086900	-2.58064700
Co	-0.00000900	0.00004000	-0.01249900	H	-5.66128100	-0.06939800	0.14706500
C	2.54583100	0.79441900	0.83387700	H	-4.54453300	1.53583300	-1.44195100
C	2.53947200	-0.87425800	-0.86157800	H	1.71815100	1.86255000	-1.84121400
C	3.94543000	-0.87131100	-0.83666500	H	-1.25119400	4.13777900	-4.00521400
C	4.57890400	0.01411100	0.07164100	H	-3.02993900	2.88105500	-2.76891400
C	1.63917100	1.60995700	1.65581600	C	0.63414800	-2.10272000	2.06742300
C	-0.63022200	2.06680300	2.10407700	C	0.27192500	-3.06395600	3.03107100
C	-0.26631700	3.01093800	3.08381300	C	-1.08892500	-3.30896100	3.28892200
C	1.09501200	3.25067400	3.34427000	C	-2.06177000	-2.58016700	2.57267400
C	2.06660200	2.53405100	2.61423600	C	-1.63601500	-1.63920700	1.63007400
H	4.54171700	-1.51153200	-1.47619600	H	1.67734100	-1.90089400	1.85860200
H	5.66158500	0.06465900	0.13953500	H	1.04905800	-3.60247400	3.56339500
H	-1.67374000	1.86905900	1.89305800	H	-1.38796900	-4.04570300	4.02812400
H	-1.04245000	3.54060800	3.62637600	H	-3.12571200	-2.72648300	2.73214200
H	1.39530200	3.97419900	4.09592000	N	-0.29694100	-1.40214000	1.37701200
H	3.13081700	2.67686700	2.77504000	N	-1.88175400	0.03075100	-0.01260400

N	-0.27355500	1.41690400	-1.39156100	C	2.53958900	-1.18688600	-0.00065300
N	-3.88566700	-0.85957200	0.89427600	C	3.95370200	1.16291000	0.00050500
C	0.36829500	3.08873500	-3.01155100	C	1.70697100	2.41147000	0.00147300
H	1.16776700	3.61322900	-3.52430700	C	-0.48863800	3.24108100	0.00189600
C	-0.37407900	-3.03357400	-3.06644300	C	1.35392800	4.81066700	0.00323100
N	3.88742100	0.84248200	0.90300000	C	2.23744600	3.71550200	0.00250400
H	-1.17449600	-3.54831000	-3.58754400	H	4.54583000	2.07060500	0.00080200
				H	-1.55139200	3.01999900	0.00164300
[Z12]2+				H	1.74069000	5.82492400	0.00403400
Co	-0.08057400	0.00000100	0.00000000	H	3.30823800	3.88675200	0.00277500
C	-2.62925100	0.00081800	-1.18864500	C	-0.48863000	-3.24108000	-0.00189800
C	-2.62924700	-0.00081500	1.18865300	C	-0.03218600	-4.57259900	-0.00291500
C	-4.04169600	-0.00080400	1.16853400	C	1.35393700	-4.81066300	-0.00323000
C	-1.72933800	0.00160500	-2.35542400	C	2.23745200	-3.71549300	-0.00250700
C	0.53322400	0.00206400	-3.00412900	C	1.70697500	-2.41146400	-0.00147700
C	0.17894700	0.00296400	-4.36515200	H	-1.55138600	-3.02000700	-0.00163800
C	-1.18264000	0.00317500	-4.71538400	H	-0.74380500	-5.39137400	-0.00344700
C	-2.15089000	0.00249400	-3.69391500	H	1.74070800	-5.82491700	-0.00402800
H	-4.63550000	-0.00143700	2.07600500	H	3.30824500	-3.88674100	-0.00277700
H	1.57406300	0.00190900	-2.70350500	N	0.35619400	-2.18550800	-0.00119400
H	0.95444300	0.00348100	-5.12347000	N	1.86293500	0.00000300	-0.00000600
H	-1.48596200	0.00385600	-5.75756300	N	0.35619300	2.18551300	0.00119000
H	-3.20702600	0.00266600	-3.94203900	C	-0.03219800	4.57259900	0.00291700
C	0.53323500	-0.00207400	3.00412600	H	-0.74381300	5.39138000	0.00345800
C	-1.18262500	-0.00319200	4.71538400	C	0.17896400	-0.00298100	4.36514600
C	-2.15087900	-0.00250700	3.69392400	H	0.95445600	-0.00350700	5.12347200
C	-1.72933200	-0.00160900	2.35542800	C	3.95370600	-1.16289500	-0.00051300
H	1.57407100	-0.00192100	2.70349100	N	4.64496800	0.00000700	-0.00000700
H	-1.48593600	-0.00388000	5.75756700	N	-4.72845500	0.00000700	0.00000700
H	-3.20701500	-0.00268100	3.94205200	C	-4.04170000	0.00080400	-1.16852100
N	-0.39259400	-0.00138700	2.01681000	H	4.54583800	-2.07059100	-0.00079000
N	-1.96581800	0.00000100	0.00000200	H	-4.63550900	0.00141900	-2.07599200
N	-0.39259700	0.00138300	-2.01680900				
C	2.53958700	1.18689400	0.00064000				

[Z12]3+	H	1.27574700	-5.53619900	1.50286200			
Co	-0.00024500	0.00000000	-0.00000100	H	3.04226200	-3.82514400	1.03800100
C	-2.53276000	0.31311900	1.15307000	C	-0.68070500	2.83244100	-0.76912700
C	-2.53277400	-0.31311900	-1.15304400	C	-0.35467400	4.15307900	-1.12759700
C	-3.94804700	-0.30764500	-1.13320600	C	0.99787000	4.52329100	-1.22787000
C	-1.60886700	0.61317900	2.25824000	C	1.99257300	3.55904200	-0.96594800
C	0.68081700	0.76866400	2.83202600	C	1.60889500	2.25843700	-0.61282600
C	0.35499000	1.12732500	4.15265400	H	-1.71626100	2.52745500	-0.68670200
C	-0.99746800	1.22812700	4.52300200	H	-1.14874000	4.86649500	-1.32145200
C	-1.99233400	0.96646000	3.55883400	H	1.27573300	5.53620800	-1.50285600
H	-4.54824500	-0.54421200	-2.00577200	H	3.04224600	3.82514500	-1.03802600
H	1.71633300	0.68588300	2.52702800	N	0.27280500	1.90342500	-0.51652800
H	1.14916100	1.32096200	4.86601300	N	1.88502700	0.00000200	-0.00001400
H	-1.27513200	1.50328400	5.53592800	N	0.27281500	-1.90342100	0.51652300
H	-3.04198000	1.03882300	3.82495900	C	-0.35465900	-4.15306500	1.12761100
C	0.68078400	-0.76866700	-2.83203300	H	-1.14871700	-4.86649300	1.32149400
C	-0.99752100	-1.22813700	-4.52299100	C	0.35494300	-1.12733100	-4.15265400
C	-1.99237700	-0.96646900	-3.55881600	H	1.14909900	-1.32097400	-4.86603800
C	-1.60889600	-0.61318200	-2.25822400	C	3.94784500	1.13329100	-0.30745900
H	1.71630200	-0.68588200	-2.52704000	N	4.62511700	0.00000000	-0.00002200
H	-1.27518700	-1.50329800	-5.53591500	N	-4.62529100	-0.00000400	0.00002400
H	-3.04202500	-1.03883400	-3.82493300	C	-3.94803300	0.30764600	1.13324100
N	-0.27284200	-0.51644900	-1.90298400	H	4.54799500	2.00594600	-0.54383700
N	-1.88527300	-0.00000100	0.00001000	H	-4.54823000	0.54420100	2.00582200
N	-0.27281700	0.51644700	1.90298400				
C	2.53257700	-1.15310300	0.31285800				
C	2.53257100	1.15310500	-0.31289600				
C	3.94784900	-1.13329700	0.30741000				
C	1.60890700	-2.25843400	0.61280500				
C	-0.68069500	-2.83243200	0.76914000				
C	0.99788700	-4.52328300	1.22786900				
C	1.99258900	-3.55903900	0.96593000				
H	4.54799600	-2.00594100	0.54380700				
H	-1.71625100	-2.52743900	0.68673300				

