

Supporting information

Theoretical studies on the reaction mechanism of alcohol oxidation by high-valent iron-oxo complex of nonheme ligand

Lin Cheng,^{1,3} Jinping Wang,² Meiyan Wang,^{1,3} Zhijian Wu^{1,*}

¹State Key Laboratory of Rare Earth Resource Utilization, Changchun
Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun
130022, P.R. China

²Department of Applied Chemistry, Qingdao Agricultural University, Qingdao 266109,
P. R. China

³Graduate School, Chinese Academy of Sciences, Beijing 100049, P.R. China

Table S1 Cartesian coordinates all structures considered in this work (B3LYP level)

0				0			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 3			
Fe	0.11358100	-0.27048900	-0.55922000	Fe	-0.05626600	-0.30321000	-0.48952900
N	2.08833900	-0.19855100	-0.29594100	N	1.87736300	-0.12232400	-0.12894200
N	-1.83694800	-0.28237300	-0.25561000	N	-2.03227700	-0.44466400	-0.27543900
N	-0.01069600	1.75394200	-0.45261400	N	-0.17452300	1.72693000	-0.50438000
C	2.50193300	-0.44694500	0.96745400	C	2.22881300	-0.14664900	1.17530700
C	-2.21812000	-0.37701000	1.03747100	C	-2.46310700	-0.62189000	0.99390900
C	-0.02810200	2.31984900	0.76746800	C	-0.25197000	2.36397900	0.67694500
C	1.40204100	-0.76601000	1.95987200	C	1.10941300	-0.47057000	2.14245900
H	1.70347200	-0.52456100	2.98669200	H	1.32332500	-0.08865700	3.14809000
C	-1.10546200	-0.68269200	2.01261000	C	-1.37117300	-0.76212200	2.03349100
H	-0.96384100	-1.76679200	1.98996100	H	-1.06199800	-1.80962100	2.05087200
H	-1.36534600	-0.38491300	3.03553300	H	-1.72714600	-0.48405800	3.03307600
C	0.23765000	1.39999200	1.93621700	C	-0.38308800	1.49585200	1.90909400
H	-0.45380200	1.61455900	2.75913000	H	-1.38336400	1.64045200	2.33278400
N	0.16298900	-0.04223400	1.56127000	N	-0.18764300	0.04436000	1.62260400
O	0.08351000	-0.22294200	-2.18115900	O	-0.02504100	-0.36031400	-2.10457700
H	1.19205000	-1.83595700	1.90184600	H	1.02418400	-1.55866400	2.20386600
C	-2.76087500	-0.15382000	-1.21938300	C	-2.91534100	-0.40749800	-1.28579900
C	-3.55722400	-0.31125000	1.40148300	C	-3.81852200	-0.73925600	1.28512900
C	-4.11993500	-0.10687300	-0.92706700	C	-4.28352100	-0.53467800	-1.06651400
H	-2.37729100	-0.10055400	-2.23188100	H	-2.48663400	-0.28458300	-2.27416500
C	-4.52433800	-0.17969600	0.40392500	C	-4.74226400	-0.69816300	0.23937500
H	-3.83838800	-0.38516500	2.44708900	H	-4.14304200	-0.87106800	2.31253700
H	-4.83959600	-0.01453700	-1.73299200	H	-4.96803900	-0.50522200	-1.90712500
H	-5.57731000	-0.13953300	0.66504600	H	-5.80409300	-0.79416000	0.44427200
H	-0.15025500	1.99402900	-2.48823300	H	-0.03704700	1.85766200	-2.55070000
C	-0.17101000	2.52702600	-1.54420800	C	-0.10234000	2.44577400	-1.64191900
C	-0.35453500	3.90081500	-1.45332700	C	-0.10752800	3.83452400	-1.63762800
C	-0.38566800	4.49349700	-0.19044900	C	-0.18057600	4.50282800	-0.41460100
H	-0.47702300	4.48797700	-2.35692000	H	-0.04991900	4.37598800	-2.57556900
C	-0.22095300	3.69045000	0.93562000	C	-0.25281600	3.75622700	0.75878900
H	-0.53643300	5.56335500	-0.08352800	H	-0.18043400	5.58780800	-0.37472300
H	-0.23696100	4.11717000	1.93389700	H	-0.31202300	4.24302300	1.72765400
H	4.16558600	-0.65615600	2.31324400	H	3.81209200	-0.00030400	2.62304400
C	3.85497100	-0.46546100	1.29080000	C	3.55316100	0.01667100	1.56906500
C	4.79580100	-0.24901300	0.28252700	C	4.53254400	0.18574200	0.58956300
C	4.35606500	-0.01366500	-1.01887900	C	4.15870000	0.18406000	-0.75296300
H	5.85667200	-0.26573800	0.51264800	H	5.57299000	0.31043800	0.87350100
C	2.98767000	0.00618200	-1.27052900	C	2.81608900	0.02421700	-1.07766300
H	5.05528400	0.15126200	-1.83124400	H	4.89173000	0.29550500	-1.54412700
H	2.57550800	0.17280400	-2.25951000	H	2.45776300	-0.01110000	-2.09866300

H	1.24401700	1.61038800	2.31542700	H	0.32592600	1.82497700	2.67730300
C	-0.49097000	-3.12735100	-0.39111400	O	-0.00982100	-2.14320400	-0.08230400
O	0.38818700	-2.13189200	-0.37206900	C	0.82283800	-3.00732700	-0.66543600
O	-1.65489200	-3.04934900	-0.02080400	O	1.74459800	-2.70898000	-1.40381600
C	0.11622900	-4.42253600	-0.90172200	C	0.48257400	-4.44886400	-0.31808000
H	-0.58208600	-5.24735900	-0.75186800	H	0.29209300	-4.56530500	0.75345700
H	0.33818400	-4.31959000	-1.96979500	H	-0.43138200	-4.74290200	-0.84649700
H	1.06321500	-4.63291600	-0.39492100	H	1.29830800	-5.10399800	-0.62761100

0				1			
Charge=1 Multiplicity = 5				Charge=1 Multiplicity = 1			
Fe	0.09123800	-0.40386500	-0.59858800	Fe	0.13066200	-0.28394100	0.11682700
N	2.24803200	-0.24337900	-0.21293200	N	-1.57512300	0.39288100	-0.63454900
N	-2.01981500	-0.23174900	-0.02766400	N	2.04887000	-0.77450900	0.36441000
N	0.01595100	1.70211800	-0.66424200	N	0.45388000	1.59118400	0.80884500
C	2.58952500	-0.36806100	1.08394800	C	-1.50206100	0.81357200	-1.91977000
C	-2.24517800	-0.22755200	1.29817100	C	2.81460400	-0.69481900	-0.74708400
C	0.02767200	2.36148800	0.50724600	C	0.94894300	2.50004300	-0.04994100
C	1.43463800	-0.62364300	2.02983000	C	-0.19503000	0.52570500	-2.62607900
H	1.68497800	-0.33028200	3.05759500	H	-0.03937600	1.20317300	-3.47450600
C	-1.02703900	-0.49062800	2.15906200	C	2.07750000	-0.30820800	-2.01129700
H	-0.88923800	-1.57474000	2.21340500	H	1.65935500	-1.21772200	-2.44823100
H	-1.16893000	-0.11713800	3.18128800	H	2.74870700	0.15543300	-2.74468100
C	0.31504700	1.54947100	1.75158300	C	1.39796100	1.97910100	-1.39645800
H	-0.34623200	1.86467500	2.56698600	H	2.49334700	1.99527000	-1.42422600
N	0.20853600	0.07210000	1.54705000	N	0.93741500	0.58399900	-1.66104800
O	0.05423800	-0.49798300	-2.20840300	O	-0.36200400	-0.79102200	1.57326100
H	1.21960300	-1.69591600	2.01919900	H	-0.23730700	-0.49659500	-3.01085300
C	-3.05052300	-0.15997300	-0.88137900	C	2.58774100	-1.19523700	1.52021600
C	-3.53016700	-0.10623000	1.82123400	C	4.16778000	-1.01707200	-0.71683000
C	-4.36557600	-0.05104700	-0.43686000	C	3.93045100	-1.54697500	1.61743500
H	-2.79656900	-0.20674400	-1.93467200	H	1.90324200	-1.25046200	2.35932100
C	-4.60612200	-0.01527800	0.93596600	C	4.73371500	-1.45297600	0.48231100
H	-3.68761000	-0.09830200	2.89543800	H	4.76448900	-0.93650900	-1.61998500
H	-5.17786800	-0.00021100	-1.15366100	H	4.33008000	-1.88658400	2.56667300
H	-5.61917400	0.07491100	1.31631000	H	5.78635800	-1.71503000	0.52654300
H	-0.17062500	1.76936800	-2.71071400	H	-0.31133000	1.18870800	2.67434600
C	-0.16585700	2.37905400	-1.81296200	C	0.08890800	1.97761500	2.04713500
C	-0.34229000	3.75698700	-1.83415200	C	0.21250400	3.29396900	2.47311700
C	-0.34273700	4.44923500	-0.62215900	C	0.71801900	4.24413300	1.58510900
H	-0.48340200	4.27043600	-2.77893200	H	-0.09100600	3.56430000	3.47857400
C	-0.15691100	3.74266800	0.56458900	C	1.09026900	3.84081600	0.30476400
H	-0.48752100	5.52514200	-0.60019300	H	0.81917000	5.28317500	1.88329800
H	-0.15110200	4.25399400	1.52249500	H	1.48781500	4.55299100	-0.41202900

H	4.17096600	-0.42603000	2.54697600	H	-2.50928300	1.71982800	-3.58707800
C	3.91983800	-0.33263300	1.49490600	C	-2.59626800	1.38484200	-2.55821600
C	4.91694000	-0.18693900	0.52855500	C	-3.80075600	1.50215600	-1.86075500
C	4.55597900	-0.07472300	-0.81374800	C	-3.86862900	1.04449900	-0.54819900
H	5.96188900	-0.16143500	0.82258500	H	-4.67033700	1.93898800	-2.34240800
C	3.20357400	-0.10484100	-1.14396800	C	-2.73193300	0.49687800	0.04310600
H	5.30323400	0.03427500	-1.59225300	H	-4.78714800	1.09661200	0.02579900
H	2.85631700	-0.02554300	-2.16940500	H	-2.74880800	0.09337500	1.05328800
H	1.33588100	1.78031200	2.07679900	H	1.05958200	2.64728600	-2.19669700
C	-0.56750700	-3.17691200	-0.78422200	C	-2.96986500	-1.93069600	3.56379400
O	0.12502600	-2.21433000	-0.14643900	O	-3.32493800	-1.46234600	2.27249900
O	-1.54957700	-2.96149400	-1.46533000	H	-3.53564000	-1.34116200	4.29162900
C	0.00324000	-4.56114200	-0.54405100	H	-3.23439900	-2.98878900	3.70440100
H	-0.66220800	-5.31398600	-0.96868800	H	-2.82729200	-1.98028800	1.61100600
H	0.98856700	-4.63732200	-1.01744000	O	-0.03943700	-1.88979000	-0.86758900
H	0.14115300	-4.74396200	0.52653100	C	-1.02641100	-2.75970500	-0.72191200
				O	-1.99940400	-2.62105500	0.00685700
				C	-0.82837100	-4.01342300	-1.55951300
				H	-0.51711700	-3.76438200	-2.57866600
				H	-0.03464100	-4.62434500	-1.11442400
				H	-1.75211700	-4.59339200	-1.58072300
				H	-1.89699300	-1.80792600	3.77269500

1	Charge=1 Multiplicity = 3			1	Charge=1 Multiplicity = 5		
Fe	0.12502300	-0.28536700	0.12212300	Fe	0.13245800	-0.28450300	0.12343800
N	-1.56682900	0.42419500	-0.62894500	N	-1.57069900	0.39146300	-0.63259400
N	2.03452600	-0.81363000	0.36375300	N	2.05218500	-0.77486600	0.36967100
N	0.49602200	1.58374600	0.80678200	N	0.45730700	1.59372700	0.81038000
C	-1.48978000	0.84046100	-1.91554200	C	-1.49650900	0.81449400	-1.91704600
C	2.79920500	-0.74943600	-0.74971800	C	2.81785900	-0.69802700	-0.74231900
C	1.00988000	2.47905400	-0.05552700	C	0.94995200	2.50101100	-0.05195600
C	-0.19136600	0.52451500	-2.62603900	C	-0.19014000	0.52441100	-2.62333000
H	-0.02503000	1.19686600	-3.47653900	H	-0.03383900	1.20012700	-3.47313300
C	2.06520800	-0.35560400	-2.01344000	C	2.08028700	-0.31464700	-2.00738900
H	1.62664900	-1.25882900	-2.44334700	H	1.65943900	-1.22503700	-2.44003700
H	2.74325600	0.08949700	-2.75201800	H	2.75160100	0.14462700	-2.74341700
C	1.43462800	1.94821200	-1.40658100	C	1.40712200	1.97477900	-1.39399800
H	2.52967200	1.94566900	-1.44871800	H	2.50275600	1.98452300	-1.41129000
N	0.94524500	0.56215200	-1.66493800	N	0.94264500	0.58146200	-1.65922500
O	-0.37508300	-0.77623500	1.57833800	O	-0.36343100	-0.78746500	1.57735300
H	-0.25589500	-0.49742500	-3.00875400	H	-0.23433000	-0.49853700	-3.00633900
C	2.56863800	-1.23848200	1.52008200	C	2.59079400	-1.19203200	1.52670500

C	4.14742100	-1.09184500	-0.72048800	C	4.17114700	-1.01986400	-0.71087400
C	3.90609400	-1.61022900	1.61604100	C	3.93352200	-1.54337100	1.62493200
H	1.88478300	-1.28002600	2.36049500	H	1.90613300	-1.24450100	2.36584200
C	4.70876800	-1.53192900	0.47932800	C	4.73697700	-1.45218100	0.48968600
H	4.74385400	-1.02316900	-1.62481000	H	4.76805700	-0.94144100	-1.61408000
H	4.30226800	-1.95248600	2.56576400	H	4.33313300	-1.88005000	2.57521000
H	5.75750900	-1.80930300	0.52280700	H	5.78976900	-1.71344500	0.53498000
H	-0.27077800	1.20288300	2.67624800	H	-0.31135700	1.19630000	2.67516400
C	0.14566200	1.98083600	2.04588300	C	0.08620200	1.98436000	2.04533500
C	0.30322300	3.29426400	2.46953000	C	0.20109200	3.30358200	2.46486700
C	0.82922900	4.23039900	1.57847800	C	0.70397300	4.25198100	1.57348700
H	0.01015900	3.57337400	3.47569100	H	-0.10719100	3.57753000	3.46788500
C	1.18651400	3.81619700	0.29740200	C	1.08260900	3.84433400	0.29630300
H	0.95741900	5.26696200	1.87486200	H	0.79809800	5.29310300	1.86668900
H	1.59868600	4.51733100	-0.42203300	H	1.47828400	4.55496200	-0.42299400
H	-2.48633300	1.76236500	-3.58080100	H	-2.50217100	1.72553000	-3.58256600
C	-2.57552800	1.43084700	-2.55097600	C	-2.58980700	1.38867700	-2.55436200
C	-3.77545300	1.57102100	-1.84976700	C	-3.79426800	1.50638000	-1.85686600
C	-3.84783900	1.11643100	-0.53651200	C	-3.86322600	1.04582100	-0.54545200
H	-4.63849900	2.02258300	-2.32959000	H	-4.66312800	1.94523700	-2.33798000
C	-2.71938400	0.54932300	0.05217900	C	-2.72753100	0.49526200	0.04498500
H	-4.76366200	1.18486300	0.04003600	H	-4.78191600	1.09702000	0.02833300
H	-2.74104200	0.14582200	1.06220800	H	-2.74642500	0.08763600	1.05345400
H	1.09765800	2.62219600	-2.20248300	H	1.07957100	2.64275900	-2.19892700
C	-3.02524800	-1.88952000	3.54919100	C	-2.98161000	-1.94011200	3.54212800
O	-3.38340100	-1.40604500	2.26425400	O	-3.35113600	-1.47404200	2.25400300
H	-3.57451700	-1.29558300	4.28605300	H	-3.54718400	-1.35625800	4.27468800
H	-3.30660700	-2.94394200	3.68506300	H	-3.23528300	-3.00072700	3.68418200
H	-2.89956000	-1.92827800	1.59593600	H	-2.85198500	-1.98577700	1.58879300
O	-0.08078800	-1.89141700	-0.85920800	O	-0.03529800	-1.89367200	-0.85898100
C	-1.09009100	-2.73658000	-0.72035500	C	-1.02841700	-2.75885600	-0.72596500
O	-2.06954900	-2.56955500	-0.00660500	O	-2.01481200	-2.61160700	-0.01741900
C	-0.90996000	-4.00021300	-1.54715600	C	-0.81883900	-4.01758500	-1.55326300
H	-0.57356300	-3.76610800	-2.56182200	H	-0.49126700	-3.77461000	-2.56878600
H	-0.14117900	-4.62923600	-1.08379900	H	-0.03297100	-4.62708200	-1.09255200
H	-1.84831600	-4.55558600	-1.58172500	H	-1.74315800	-4.59608200	-1.58578700
H	-1.94864300	-1.78647300	3.74923200	H	-1.90832600	-1.80746100	3.74232600

1-2				1-2			
Charge=1 Multiplicity =1				Charge=1 Multiplicity = 3			
Fe	0.03165200	-0.21981900	0.22495800	Fe	0.04823000	-0.22841900	0.22095000
N	-1.59103200	0.82055600	-0.24864200	N	-1.59959400	0.76017200	-0.28322700
N	1.79854000	-1.13947100	0.19765400	N	1.84778300	-1.08838200	0.20755100

N	1.04529900	1.47008200	0.64338000	N	0.96511100	1.50443500	0.65767400
C	-1.76603800	1.01648700	-1.57604500	C	-1.74584000	0.97507900	-1.61082100
C	2.34456000	-1.26071800	-1.03171700	C	2.40306400	-1.21548400	-1.01744800
C	1.58523700	2.13451600	-0.39469500	C	1.48213100	2.19983200	-0.37132100
C	-0.74638800	0.33223500	-2.46182500	C	-0.69502900	0.32176100	-2.48103200
H	-0.66168200	0.82704500	-3.43732500	H	-0.59997900	0.82736200	-3.44996500
C	1.46008800	-0.81501200	-2.17812200	C	1.51079800	-0.80623300	-2.16919400
H	0.82388000	-1.66047500	-2.45091800	H	0.88546700	-1.66498400	-2.42442200
H	2.05161600	-0.53163000	-3.05718600	H	2.09385700	-0.52572300	-3.05488000
C	1.23655400	1.62356500	-1.77437800	C	1.27557700	1.62531200	-1.75617900
H	2.13259500	1.57720200	-2.40373100	H	2.24044000	1.54274300	-2.26918700
N	0.55997000	0.29148500	-1.74407600	N	0.59823700	0.29226400	-1.74137800
O	-0.23761100	-0.45453700	1.92608500	O	-0.22561600	-0.50794900	1.90971300
H	-1.05864800	-0.70062100	-2.62997700	H	-0.98763400	-0.71446300	-2.66515800
C	2.45028100	-1.61102400	1.27094000	C	2.51010600	-1.52152600	1.29108200
C	3.59492200	-1.84376500	-1.21396800	C	3.66985100	-1.76597000	-1.18555800
C	3.69685000	-2.22052800	1.16049800	C	3.77410600	-2.09651000	1.19508500
H	1.92945700	-1.48461500	2.21416000	H	1.98377300	-1.39419600	2.23076500
C	4.28041300	-2.33280000	-0.10050200	C	4.36510100	-2.21569000	-0.06171300
H	4.01892200	-1.92273300	-2.21016400	H	4.09895600	-1.84989800	-2.17912900
H	4.19492300	-2.59454900	2.04838700	H	4.27943300	-2.43922100	2.09145200
H	5.25519400	-2.79592900	-0.21932300	H	5.35297800	-2.65309800	-0.16912500
H	0.79239800	1.31779900	2.67218100	H	0.65406700	1.35668900	2.67860500
C	1.26042300	1.91505500	1.89695000	C	1.09524300	1.98308100	1.91099000
C	2.02859000	3.04342000	2.15642100	C	1.75039500	3.17824500	2.17923900
C	2.60118700	3.72991000	1.08531500	C	2.29254000	3.90255400	1.11691800
H	2.17595900	3.36952600	3.18028300	H	1.83289400	3.52847200	3.20242400
C	2.37615400	3.26724600	-0.20922900	C	2.15676600	3.40454600	-0.17652700
H	3.21274600	4.61103500	1.25396100	H	2.81295300	4.83924400	1.29185400
H	2.80217700	3.77828100	-1.06738100	H	2.56508800	3.94173400	-1.02741100
H	-2.94616800	1.90384500	-3.13800000	H	-2.90716200	1.85929800	-3.18849200
C	-2.83335300	1.75832800	-2.06821600	C	-2.81840200	1.69917900	-2.11853700
C	-3.75273400	2.29909500	-1.16710600	C	-3.77362600	2.20204800	-1.23351600
C	-3.56436800	2.09227400	0.19702600	C	-3.61650900	1.97361200	0.13126600
H	-4.59891600	2.87523500	-1.52865000	H	-4.62384000	2.76425500	-1.60729500
C	-2.46554200	1.35064300	0.62065900	C	-2.51134800	1.25162700	0.57118700
H	-4.25568500	2.49044000	0.93144800	H	-4.33693800	2.34028200	0.85401900
H	-2.27770800	1.14254300	1.66533900	H	-2.35144700	1.02672400	1.61695600
H	0.56258700	2.34503100	-2.24943700	H	0.67344500	2.32519300	-2.34619700
H	-1.33159800	-1.02203000	2.41840400	H	-1.24217200	-1.07188200	2.38989800
C	-2.34036000	-1.53454200	2.95895000	C	-2.27508800	-1.61212200	2.97629200
O	-3.48376500	-0.97415700	2.44477600	O	-3.42557300	-1.07975700	2.45704300
H	-2.24554600	-1.29770900	4.02153500	H	-2.17084200	-1.35331800	4.03215800
H	-2.22080100	-2.60663500	2.75078300	H	-2.12392600	-2.68050900	2.77242500

H	-3.55487300	-1.30077300	1.51809500	H	-3.48960700	-1.41879200	1.53344500
O	-0.67114700	-1.86627300	-0.46546900	O	-0.60283700	-1.90142800	-0.48121600
C	-1.87516000	-2.37691700	-0.44888400	C	-1.78807900	-2.44844700	-0.44632100
O	-2.89544300	-1.81397100	-0.04181900	O	-2.81901400	-1.91877400	-0.01849400
C	-1.93589400	-3.79608400	-0.99403000	C	-1.81868200	-3.86672500	-0.99715300
H	-1.51428600	-4.48449800	-0.25226100	H	-1.38147300	-4.54846000	-0.25812600
H	-2.97121900	-4.07897700	-1.19041600	H	-2.84795200	-4.17207100	-1.19209000
H	-1.33653100	-3.89686500	-1.90377200	H	-1.21922900	-3.95165900	-1.90836600

1-2				2			
Charge=1 Multiplicity = 5				Charge=1 Multiplicity = 1			
Fe	0.13895700	-0.40388200	0.32412600	Fe	-0.15001800	-0.23789200	-0.16656700
N	-1.80831700	0.15778300	-0.53133500	N	1.46329500	0.71681700	0.48085600
N	2.29674700	-0.40521600	0.27088900	N	-1.90286000	-1.14625400	-0.33560400
N	0.16102600	1.73033200	0.88100400	N	-1.06890500	1.44697000	-0.69349800
C	-1.78331500	0.61461900	-1.79967400	C	1.49793100	0.91149300	1.82252500
C	2.87329000	-0.19609500	-0.93031800	C	-2.57448500	-1.28289100	0.82878100
C	0.39820600	2.64322100	-0.07527900	C	-1.70120300	2.11934300	0.28554800
C	-0.46431000	0.47398000	-2.53399100	C	0.36209900	0.26855500	2.58769400
H	-0.43711900	1.13567500	-3.41092900	H	0.17245200	0.77544900	3.54154100
C	1.91980900	-0.00727600	-2.09328100	C	-1.80185800	-0.86104500	2.05999100
H	1.61469400	-0.99798400	-2.44191400	H	-1.19948000	-1.71428200	2.38319600
H	2.41614800	0.51241500	-2.92456400	H	-2.46942500	-0.58082400	2.88359300
C	0.95972400	2.13595700	-1.38905100	C	-1.52751100	1.58212400	1.68958900
H	2.04592100	2.28168800	-1.35733400	H	-2.49596800	1.52565700	2.19908900
N	0.69622500	0.69821200	-1.64404800	N	-0.85428200	0.24346800	1.72311900
O	-0.09590900	-0.85584200	1.93896400	O	0.35692900	-0.50678500	-1.85008900
H	-0.39986300	-0.55785600	-2.89303800	H	0.63125800	-0.76940900	2.79680300
C	3.06260100	-0.65285300	1.34624900	C	-2.44165000	-1.59432500	-1.48045700
C	4.25785300	-0.21327100	-1.08216600	C	-3.84066500	-1.85745700	0.87087100
C	4.45133100	-0.69809100	1.26779400	C	-3.69736900	-2.19428500	-1.50845600
H	2.52530900	-0.81894600	2.27413400	H	-1.82464300	-1.45842400	-2.36227200
C	5.05705600	-0.47235000	0.03238400	C	-4.40945100	-2.32175900	-0.31674700
H	4.70078200	-0.03244600	-2.05668700	H	-4.36623700	-1.94955900	1.81615500
H	5.03856400	-0.90325900	2.15624200	H	-4.10348300	-2.54961100	-2.44920500
H	6.13838500	-0.49393700	-0.06438800	H	-5.39451100	-2.77814800	-0.30795700
H	-0.42175800	1.33837500	2.81116900	H	-0.58938100	1.29931000	-2.68317800
C	-0.24746100	2.13588100	2.09722600	C	-1.12708500	1.90295500	-1.95997100
C	-0.43656000	3.47797000	2.40681100	C	-1.82946200	3.05537000	-2.29162100
C	-0.20696900	4.43018600	1.41320200	C	-2.49664000	3.75259700	-1.28385500
H	-0.76366000	3.76499500	3.40034400	H	-1.85241600	3.39299700	-3.32205000
C	0.21499500	4.00730900	0.15413700	C	-2.43201000	3.27681500	0.02431900
H	-0.35524900	5.48696100	1.61434200	H	-3.05837300	4.65340400	-1.51141500

H	0.40498000	4.72352400	-0.63974300	H	-2.93580800	3.79711400	0.83341500
H	-2.88322300	1.45951000	-3.44611200	H	2.54506100	1.74164400	3.50497500
C	-2.93239100	1.09018000	-2.42632300	C	2.54647500	1.58939700	2.43012400
C	-4.14157000	1.06698800	-1.72894500	C	3.60292400	2.04997800	1.63846900
C	-4.16419600	0.56787900	-0.42869500	C	3.56920300	1.82520400	0.26613500
H	-5.05105400	1.42845900	-2.19950100	H	4.44010100	2.56962600	2.09428900
C	-2.97152200	0.12557200	0.13945000	C	2.47355500	1.16282600	-0.28244300
H	-5.08481700	0.51674600	0.14242600	H	4.37803200	2.13641600	-0.38404500
H	-2.93711400	-0.29585700	1.13999200	H	2.40129000	0.95912400	-1.34457800
H	0.59107500	2.75075700	-2.22041400	H	-0.91813100	2.29092100	2.26088900
H	-0.85766300	-1.61161700	2.90934400	C	4.33165800	-0.37419900	-2.81021900
C	-1.73579300	-2.33656400	3.26046500	O	4.61148600	-0.74313700	-1.52734200
O	-2.74069600	-2.25577000	2.32642700	H	5.09673400	0.25440500	-3.25519500
H	-2.09382700	-1.98815800	4.23278700	H	3.79284400	-1.07940200	-3.44126200
H	-1.25066000	-3.32095500	3.31672100	H	3.94320300	-1.40207600	-1.24245100
H	-2.40149900	-2.67512900	1.49398200	O	0.59235000	-1.86612200	0.57322700
O	0.11081100	-2.03195600	-0.75549500	C	1.66478400	-2.46288300	0.14667200
C	-0.58141900	-3.13937500	-0.62359000	O	2.31609800	-2.10872900	-0.85262200
O	-1.53893700	-3.29325100	0.13662500	C	2.08064600	-3.69367600	0.92877400
C	-0.11284400	-4.27475600	-1.51603400	H	1.71666600	-4.58318900	0.40109400
H	0.90651100	-4.56480300	-1.23756500	H	3.17078200	-3.75906700	0.96650800
H	-0.77608200	-5.13466800	-1.41487400	H	1.66456000	-3.69787700	1.93841400
H	-0.08269500	-3.95045300	-2.56165100	H	1.18039000	-1.04266000	-1.82944700

2	Charge=1 Multiplicity = 3			2	Charge=1 Multiplicity = 5		
Fe	-0.15144600	-0.23810600	-0.16774600	Fe	0.19947900	0.11493400	0.33591000
N	1.46194400	0.71772000	0.47815000	N	-0.33383400	-1.82577700	-0.48890200
N	-1.90391900	-1.14754600	-0.33560400	N	0.26380900	2.27705200	0.14503300
N	-1.07242700	1.44598500	-0.69449600	N	-1.79708500	0.05446400	1.18331600
C	1.49700100	0.91292200	1.81984200	C	-1.04167500	-1.85817100	-1.63344300
C	-2.57480500	-1.28409700	0.82920300	C	-0.15942700	2.82043800	-1.01425600
C	-1.70444200	2.11808500	0.28492100	C	-2.83967700	0.24178800	0.35436000
C	0.36228400	0.26904400	2.58587700	C	-1.11383100	-0.55055100	-2.40051700
H	0.17307300	0.77569100	3.53993800	H	-1.95609100	-0.56631500	-3.10768700
C	-1.80174000	-0.86142000	2.05988000	C	-0.56765000	1.83670400	-2.09653100
H	-1.19890700	-1.71429400	2.38322100	H	0.33428500	1.52527600	-2.63268000
H	-2.46904700	-0.58114600	2.88366800	H	-1.23427000	2.32328300	-2.82375200
C	-1.52830500	1.58183600	1.68899800	C	-2.53610800	0.89121800	-0.98515300
H	-2.49582000	1.52562700	2.20031600	H	-2.63031600	1.97456700	-0.84734500
N	-0.85475500	0.24333900	1.72224100	N	-1.17276300	0.62362300	-1.50558500
O	0.35430800	-0.50637100	-1.85177200	O	1.15994000	-0.39627800	1.87264900
H	0.63224600	-0.76878200	2.79460400	H	-0.19494400	-0.46537700	-2.98993000
C	-2.44301800	-1.59641500	-1.47998600	C	0.68482900	3.09252300	1.12698600

C	-3.84064300	-1.85934900	0.87220100	C	-0.17811200	4.19890400	-1.21808800
C	-3.69841000	-2.19710400	-1.50707200	C	0.71145400	4.47755900	0.99612000
H	-1.82652900	-1.46052500	-2.36216900	H	1.00260400	2.60092300	2.04198900
C	-4.40979200	-2.32446300	-0.31492900	C	0.27056300	5.04157800	-0.20050800
H	-4.36566300	-1.95136900	1.81779900	H	-0.53675800	4.60386000	-2.15975600
H	-4.10481800	-2.55307300	-2.44745100	H	1.06178500	5.09447100	1.81677900
H	-5.39458900	-2.78140400	-0.30542500	H	0.26757900	6.11859300	-0.33824900
H	-0.59503200	1.29783800	-2.68463700	H	-1.13467900	-0.56095700	3.03023900
C	-1.13255700	1.90127100	-1.96112300	C	-2.02350300	-0.42088400	2.42153500
C	-1.83661300	3.05273000	-2.29254700	C	-3.30123200	-0.72068400	2.88440900
C	-2.50348400	3.74966800	-1.28437900	C	-4.38339800	-0.53886800	2.02316700
H	-1.86110000	3.38982600	-3.32311400	H	-3.43959800	-1.09561700	3.89306800
C	-2.43688600	3.27457700	0.02394900	C	-4.14776400	-0.05408400	0.73671000
H	-3.06650900	4.64971600	-1.51175300	H	-5.39402500	-0.77225700	2.34469300
H	-2.94040000	3.79466900	0.83335300	H	-4.96744700	0.09966300	0.04077300
H	2.54364200	1.74493500	3.50158300	H	-2.17667600	-3.02841800	-3.04200800
C	2.54488800	1.59233900	2.42678100	C	-1.60377500	-3.03778000	-2.11944300
C	3.60050100	2.05405300	1.63462300	C	-1.41474200	-4.22127600	-1.40544600
C	3.56670700	1.82849700	0.26247200	C	-0.67682700	-4.18511700	-0.22210700
H	4.43717700	2.57491200	2.08996400	H	-1.84140400	-5.15302500	-1.76456900
C	2.47177500	1.16436800	-0.28542300	C	-0.16110600	-2.96447400	0.20371000
H	4.37499200	2.14019000	-0.38810800	H	-0.51096500	-5.08139600	0.36645400
H	2.39942500	0.96009400	-1.34730200	H	0.40579500	-2.86297600	1.12482400
H	-0.91791600	2.29107900	2.25866300	H	-3.29690500	0.60561100	-1.72497500
C	4.36586300	-0.37613100	-2.79732200	C	4.32532600	-1.96832300	2.31671600
O	4.61905000	-0.74006500	-1.50724000	O	5.11682300	-1.49450000	1.51881100
H	5.14244500	0.24662600	-3.23041600	H	4.65802000	-2.71696000	3.05595400
H	3.83624100	-1.08212800	-3.43520800	H	3.25937100	-1.67477000	2.32908600
H	3.94498500	-1.39754700	-1.23285000	H	4.34359400	-0.26417600	0.52079700
O	0.59259300	-1.86546100	0.57153700	O	1.90876200	0.02681800	-1.26115100
C	1.66550100	-2.46089700	0.14413700	C	3.06462700	-0.22942600	-0.93866600
O	2.31610100	-2.10533700	-0.85512600	O	3.54452400	0.23937100	0.21194200
C	2.08274100	-3.69179000	0.92529200	C	4.00706400	-1.02590200	-1.80721100
H	1.71826200	-4.58123300	0.39783000	H	3.46182500	-1.47244700	-2.63872300
H	3.17293500	-3.75688400	0.96161400	H	4.78798300	-0.36432900	-2.20037600
H	1.66792000	-3.69641100	1.93545300	H	4.50708100	-1.80819400	-1.22625600
H	1.17886900	-1.04060300	-1.83176700	H	1.98620100	0.09283500	1.98891500

3	Charge=1 Multiplicity = 1			3	Charge=1 Multiplicity = 3		
Fe	-0.15467900	-0.19977900	0.08792500	Fe	-0.18942100	0.21110100	0.21259500
N	-2.08251200	0.31506900	0.07469900	N	1.72928500	0.66129500	0.02449900
N	1.71614900	-0.69378800	-0.31739700	N	-2.09267600	-0.28449100	-0.09099200

N	0.51895900	1.63927500	0.36063200	N	0.45620400	-1.89414600	0.42533800
C	-2.60648500	0.33800200	-1.17697900	C	2.18982500	0.62801200	-1.25053900
C	1.98853600	-0.68866100	-1.64346200	C	-2.44415000	-0.27364400	-1.40557200
C	0.58744200	2.38118400	-0.76864600	C	0.76907600	-2.44084300	-0.76174100
C	-1.64754100	-0.06568800	-2.27347300	C	1.12278700	0.49645300	-2.31639400
H	-1.91503000	0.38926300	-3.23577800	H	1.53181500	0.06816800	-3.24025800
C	0.78415200	-0.50861400	-2.54040400	C	-1.34926900	0.14236400	-2.36422700
H	0.35287900	-1.49582400	-2.72560600	H	-1.32990900	1.23240200	-2.42985700
H	1.06179600	-0.07307300	-3.50827400	H	-1.52656000	-0.26349500	-3.36885400
C	-0.05474600	1.77544400	-1.99327100	C	0.15632300	-1.76512500	-1.97400900
H	0.53134200	1.99709800	-2.89285400	H	-0.83450600	-2.20645900	-2.12804100
N	-0.26384900	0.29984900	-1.85160800	N	-0.03404700	-0.29331500	-1.81070600
O	-0.00992800	-0.85158500	2.00903300	O	-0.14979800	0.97329100	1.99612000
H	-1.67996800	-1.15173700	-2.37633100	H	0.75352800	1.49975500	-2.54664200
C	2.71904700	-0.92197000	0.54915000	C	-3.01791400	-0.66824300	0.81229500
C	3.27163200	-0.90998300	-2.13359000	C	-3.72302200	-0.61163400	-1.83313700
C	4.02361000	-1.16825500	0.13212000	C	-4.32050900	-1.00474300	0.45421800
H	2.44252800	-0.89573500	1.59670300	H	-2.67258600	-0.73289800	1.83867200
C	4.30710000	-1.16064800	-1.23225700	C	-4.68679000	-0.96726100	-0.88840900
H	3.45519300	-0.89166400	-3.20348200	H	-3.95845700	-0.59737900	-2.89286100
H	4.79842000	-1.35472000	0.86802700	H	-5.02636500	-1.30074600	1.22297600
H	5.31568100	-1.34137300	-1.59096200	H	-5.69376600	-1.22709000	-1.19992800
H	1.06319500	1.50762000	2.36038300	H	0.56595100	-2.01699600	2.47773000
C	1.06626100	2.14746700	1.48644000	C	0.86297600	-2.50178600	1.55213800
C	1.64923500	3.40909300	1.53506300	C	1.60454300	-3.68162800	1.53406500
C	1.69976600	4.17855700	0.37444100	C	1.94664700	-4.23937400	0.30308300
H	2.06602100	3.76725800	2.47030000	H	1.90954200	-4.14504800	2.46647500
C	1.16864900	3.64588000	-0.79864800	C	1.52129600	-3.60895000	-0.86722800
H	2.15354100	5.16471300	0.37692000	H	2.53381300	-5.15139900	0.25151000
H	1.20399200	4.20249600	-1.73042600	H	1.76353800	-4.02032800	-1.84275300
H	-4.31190200	0.68313900	-2.43742800	H	3.87466600	0.74932500	-2.58066800
C	-3.93610200	0.66638200	-1.41900600	C	3.53902500	0.78839400	-1.54889700
C	-4.77116600	0.96345000	-0.34131400	C	4.44363700	1.00522700	-0.50823400
C	-4.23771200	0.93274900	0.94490100	C	3.96546600	1.04878900	0.80023800
H	-5.81369500	1.21735500	-0.50581800	H	5.50080200	1.13579100	-0.71818800
C	-2.89373600	0.60960300	1.10579600	C	2.60534300	0.86440800	1.02651100
H	-4.84519000	1.15750900	1.81493200	H	4.63220500	1.21624900	1.63936800
H	-2.44218000	0.57983300	2.08928100	H	2.16526600	0.88426100	2.01722800
H	-1.03537900	2.24231000	-2.13623700	H	0.74054800	-1.97438900	-2.87845500
H	-0.10523800	-1.90108700	1.88186100	H	-0.01021600	2.46359000	1.64026400
C	-0.20862700	-0.44375500	3.34232500	C	-1.02377600	0.83231800	3.04652400
O	0.99520300	-0.09771800	3.98325100	O	-1.13733500	-0.56459800	3.36562700
H	-0.73343400	-1.24431700	3.88007500	H	-2.03152100	1.22494800	2.80906600
H	-0.81047500	0.46891900	3.36359300	H	-0.64164400	1.37358600	3.92787200

O	-0.72327800	-2.04171000	-0.44095100	O	-0.57495500	2.42088100	-0.62178200
C	-0.67497600	-3.13259000	0.23125400	C	-0.34728100	3.45041600	0.03271000
O	-0.31776400	-3.21723400	1.43695200	O	0.00067200	3.43832200	1.29683000
C	-1.11235800	-4.39369900	-0.48520800	C	-0.45742100	4.83001800	-0.56092600
H	-2.20594600	-4.40224900	-0.56422000	H	0.46009900	5.39445800	-0.36854900
H	-0.70837900	-4.42224400	-1.50119600	H	-0.64810500	4.77176400	-1.63296300
H	-0.79624900	-5.27724900	0.07121600	H	-1.27524700	5.37073900	-0.07226300
H	1.47315900	-0.91252800	4.20732400	H	-1.51885900	-0.64500200	4.25548500

3-4				3-4			
Charge=1 Multiplicity = 1				Charge=1 Multiplicity = 3			
Fe	-0.04593000	-0.27216200	0.11569400	Fe	0.23080200	0.15885300	0.16475800
N	-1.94347300	0.32046900	0.07260400	N	1.87721100	-0.95543400	0.05875100
N	1.86779600	-0.68579300	-0.25773200	N	-1.39843100	1.25383500	-0.20725000
N	0.52371200	1.58281400	0.51068400	N	-1.27340000	-1.44507800	0.47681700
C	-2.40742400	0.53094800	-1.18453300	C	2.24792400	-1.24806300	-1.21715400
C	2.14269900	-0.72936400	-1.58554500	C	-1.72248300	1.29750900	-1.52486600
C	0.56838500	2.39576500	-0.56784300	C	-1.63554300	-2.00458800	-0.69092900
C	-1.45520500	0.10294500	-2.27882000	C	1.41033600	-0.60130300	-2.29743900
H	-1.65674300	0.62910900	-3.22019900	H	1.45647800	-1.16971500	-3.23536000
C	0.93211300	-0.58945400	-2.48208100	C	-0.72396000	0.66728900	-2.47093700
H	0.45325100	-1.56460900	-2.59660000	H	0.01508800	1.42706400	-2.74222500
H	1.20791400	-0.22441300	-3.47942200	H	-1.21306400	0.33372700	-3.39506200
C	0.34545500	1.75087100	-1.91805600	C	-0.70512900	-1.75682600	-1.86326900
H	1.27397500	1.82018800	-2.49579200	H	-1.24316600	-1.85029400	-2.81467000
N	-0.05460900	0.31146700	-1.81286700	N	0.01216200	-0.44538600	-1.80858000
H	-1.58253800	-0.96740600	-2.46020700	H	1.80633200	0.39973600	-2.48655200
C	2.88966100	-0.76274000	0.61982300	C	-2.24460800	1.82416200	0.67381700
C	3.43510500	-0.89369800	-2.06990200	C	-2.87200000	1.93173000	-1.98496500
C	4.20780100	-0.93815900	0.20216600	C	-3.40165700	2.49080200	0.28431700
H	2.62987500	-0.66148200	1.67562100	H	-1.99992500	1.71320800	1.72324800
C	4.48717200	-1.01580900	-1.15952500	C	-3.72149900	2.55269900	-1.06962800
H	3.61512200	-0.92119200	-3.14022100	H	-3.09637500	1.93859200	-3.04716200
H	4.99585900	-1.00452300	0.94466600	H	-4.03948200	2.93784100	1.03906300
H	5.50512800	-1.15075700	-1.51224200	H	-4.62006100	3.05935300	-1.40776500
H	0.89287400	1.41414900	2.54490700	H	-1.75070100	-1.11302500	2.47046600
C	0.84754100	2.10604900	1.71337100	C	-2.03282300	-1.65920300	1.56856400
C	1.16648100	3.44717600	1.88894200	C	-3.15663900	-2.48388400	1.53561500
C	1.16256700	4.29398100	0.78214600	C	-3.52309100	-3.07729200	0.32950100
H	1.41829200	3.80934800	2.87978400	H	-3.73601800	-2.63837000	2.43973700
C	0.87012700	3.75205600	-0.46698200	C	-2.75674000	-2.82276600	-0.80897100
H	1.39900400	5.34852600	0.88457900	H	-4.39889000	-3.71641100	0.26829500
H	0.88582800	4.36984100	-1.36014100	H	-3.02412500	-3.25311100	-1.76968200
H	-4.00611200	1.21643500	-2.44826500	H	3.60716700	-2.25347600	-2.54027600

C	-3.67228600	1.05506900	-1.42788300	C	3.35750900	-2.03423400	-1.50678500
C	-4.49757500	1.36473800	-0.34520600	C	4.14023300	-2.52367700	-0.46038700
C	-4.02109500	1.14811700	0.94627900	C	3.77570900	-2.20892700	0.84608500
H	-5.49028500	1.77194000	-0.51000300	H	5.01262100	-3.13665800	-0.66397300
C	-2.73928900	0.63234300	1.11248100	C	2.64218500	-1.43152000	1.06103200
H	-4.62562800	1.37715100	1.81724400	H	4.35158900	-2.56082100	1.69514700
H	-2.32274800	0.44644300	2.09639200	H	2.32980600	-1.17247600	2.06367900
H	-0.41051800	2.30631600	-2.48367200	H	0.06026900	-2.54054900	-1.85413900
H	-1.43473400	-1.96568100	1.68501600	H	1.67275900	1.94744100	1.74729800
O	-0.62627500	-2.12336700	-0.49290700	O	1.52714700	1.90167000	-0.58921400
C	-1.40012800	-2.93498100	0.05419800	C	2.23592400	2.67644900	0.07226600
O	-1.89420600	-2.76794100	1.25472000	O	2.30433600	2.65344100	1.38412400
C	-1.82533500	-4.20338200	-0.62520200	C	3.09108600	3.73927400	-0.56085500
H	-2.90721300	-4.33452700	-0.53112500	H	2.72133700	4.72651600	-0.26315800
H	-1.52991100	-4.19905100	-1.67468600	H	4.11882500	3.65824900	-0.19407700
H	-1.35304300	-5.05376100	-0.12015300	H	3.06899500	3.65197300	-1.64733400
O	-0.26167900	-0.94341500	2.00066400	O	-0.81594300	0.44400100	3.66001900
C	0.78090700	-1.81140900	2.72152800	H	-0.41520700	1.17902100	2.60048500
O	1.37612100	-0.80508800	3.39049900	C	0.38661200	-0.03433300	3.30765300
H	0.20576300	-2.53327300	3.32676100	O	0.52978800	0.82006100	2.01952200
H	1.37513400	-2.34678800	1.96135900	H	1.24552300	0.23187400	3.94717400
H	0.24391700	-0.29633900	2.81959600	H	0.43588600	-1.09863400	3.01337700

4	Charge=1 Multiplicity =1			4	Charge=1 Multiplicity =3		
Fe	0.01781900	0.13813300	0.03063800	Fe	0.02383800	0.24642500	-0.05407000
N	1.72952500	-0.79255100	-0.38346800	N	1.77163500	-0.41199500	-0.71201000
N	-1.79145000	0.92983800	0.07233000	N	-1.89696100	0.65364200	0.20707300
N	-0.72246400	-1.46071100	0.88224000	N	-0.27577700	-1.52881600	0.98622700
C	1.80753200	-1.17572600	-1.68322400	C	1.71293300	-0.98732000	-1.94076400
C	-2.45751700	0.78821700	-1.09901500	C	-2.68801700	0.23852700	-0.81392800
C	-1.28049200	-2.35518500	0.03770900	C	-0.76014400	-2.57525100	0.29467900
C	0.64401900	-0.73556900	-2.54196600	C	0.37357000	-0.91196200	-2.65296000
H	0.51757200	-1.38481900	-3.41780600	H	0.31953000	-1.66875500	-3.44813300
C	-1.62491400	0.23464400	-2.23349500	C	-1.97761100	-0.29860200	-2.04625900
H	-1.09714600	1.06837500	-2.70351900	H	-1.68212900	0.55864700	-2.65824000
H	-2.24773600	-0.24932700	-2.99625700	H	-2.66503000	-0.91447500	-2.64305400
C	-1.11538700	-2.06689500	-1.43869100	C	-0.96697900	-2.40248700	-1.20573900
H	-2.06551200	-2.21074300	-1.96571400	H	-1.98110700	-2.73219300	-1.46571400
N	-0.58440700	-0.68933900	-1.69704000	N	-0.74247300	-1.02771200	-1.69033400
O	0.49752000	1.00987100	1.78503100	O	0.55107400	1.39609800	1.73944600
H	0.83614200	0.28329300	-2.88509100	H	0.30121600	0.07464400	-3.11925300
C	-2.43234300	1.48377700	1.11751600	C	-2.47161000	1.21162200	1.28873000
C	-3.77991500	1.19169100	-1.24948500	C	-4.07284200	0.36817300	-0.76339600

C	-3.74910700	1.92718300	1.03602000	C	-3.84758100	1.38627000	1.39778300
H	-1.85464000	1.56751400	2.03122500	H	-1.78934800	1.52097800	2.07196300
C	-4.43739000	1.77673000	-0.16607800	C	-4.66481800	0.95490700	0.35549300
H	-4.28443300	1.05535600	-2.20111300	H	-4.67796500	0.01823100	-1.59417700
H	-4.22002000	2.37590000	1.90404300	H	-4.26173500	1.84903400	2.28706000
H	-5.46790800	2.10472700	-0.26102700	H	-5.74313000	1.06889000	0.41039200
H	-0.37062600	-0.92438600	2.84199200	H	0.28878400	-0.77241700	2.82025400
C	-0.80926800	-1.68769600	2.20978600	C	-0.07711400	-1.65919700	2.31386600
C	-1.43400400	-2.81115700	2.73724500	C	-0.33817500	-2.84000100	2.99660600
C	-2.00884100	-3.73561200	1.86510500	C	-0.83625200	-3.93027900	2.28130400
H	-1.47288500	-2.94958700	3.81245100	H	-0.16024400	-2.89823100	4.06506000
C	-1.93289100	-3.49799200	0.49401000	C	-1.05292100	-3.79182300	0.91328200
H	-2.51011000	-4.62103100	2.24346100	H	-1.05673700	-4.86870600	2.78090400
H	-2.37328200	-4.19117400	-0.21667600	H	-1.44629400	-4.61645400	0.32551300
H	2.91312300	-2.17871700	-3.22861600	H	2.74667500	-2.01629800	-3.51683000
C	2.89483200	-1.88342500	-2.18398700	C	2.83395600	-1.55597000	-2.53742300
C	3.95244600	-2.19997500	-1.32999600	C	4.05897600	-1.51932900	-1.87029800
C	3.87432700	-1.80664500	0.00367600	C	4.11848100	-0.91737300	-0.61601300
H	4.81379600	-2.74759200	-1.69971400	H	4.94516200	-1.95412900	-2.32223100
C	2.74761700	-1.11255400	0.43578700	C	2.95530700	-0.38097200	-0.07202400
H	4.66782200	-2.03241500	0.70790500	H	5.04675900	-0.86232700	-0.05762600
H	2.65783600	-0.79398700	1.46726000	H	2.96487500	0.09600600	0.90099300
H	-0.41417500	-2.79450500	-1.86199300	H	-0.28432000	-3.08340700	-1.72868600
C	3.42046300	2.45288000	2.62374300	C	3.61234200	2.69538000	3.28358200
O	3.11389500	1.28298000	2.76944900	O	3.23026000	1.70895800	2.68661000
H	2.75413900	3.17003600	2.11438000	H	2.92559400	3.51367700	3.56363000
H	4.38812200	2.83258700	2.99683900	H	4.67079100	2.81532900	3.57387400
H	0.53399100	1.98394800	1.46323600	H	0.33135100	2.28475100	1.29651800
O	0.66666400	1.71483600	-1.00015900	O	0.18474700	1.81111300	-1.26587400
C	0.89757500	2.90024200	-0.56299600	C	0.04741200	3.04778600	-0.91359600
O	0.81500900	3.25409300	0.64164600	O	-0.00732800	3.45173200	0.26791200
C	1.31950500	3.92193500	-1.60276800	C	-0.02737600	4.04880800	-2.05183600
H	0.63462600	3.90350000	-2.45618500	H	-0.85956500	3.79931800	-2.71905500
H	1.34533300	4.92272100	-1.16931300	H	-0.15775400	5.06028700	-1.66493100
H	2.31632000	3.66859800	-1.98216600	H	0.89013000	3.99939100	-2.64819900
H	1.39574400	0.89216000	2.16625500	H	1.46049900	1.49667000	2.08781100

4				5			
	Charge=1 Multiplicity =5				Charge=1 Multiplicity =1		
Fe	0.17831600	0.38569200	0.03149700	N	-1.71150800	0.72940700	-0.32421700
N	1.99929800	-0.78186900	-0.54119500	H	-1.90028500	-1.93486600	1.68977600
N	-1.98608300	0.91913100	-0.05797400	N	1.85500900	-0.85447100	0.12780500
N	-0.64827200	-1.39368500	1.11341900	N	0.64497000	1.63465200	0.91959500

C	1.88817800	-1.31800000	-1.77445600	C	-1.75923300	1.23669300	-1.57729900
C	-2.59173100	0.43737500	-1.16003500	C	2.49221900	-0.74876100	-1.06069700
C	-1.21214000	-2.33576900	0.33895900	C	1.13075800	2.55010000	0.06328500
C	0.62307200	-0.98262700	-2.54601500	C	-0.57413200	0.90752600	-2.45972800
H	0.48267900	-1.69306500	-3.37355000	H	-0.45673900	1.63917100	-3.26813100
C	-1.68321300	-0.16437100	-2.22068400	C	1.65431600	-0.19371900	-2.19307000
H	-1.25078500	0.66653800	-2.78827000	H	1.08525100	-1.01864200	-2.62770400
H	-2.27164500	-0.77258500	-2.92305500	H	2.27733400	0.25126400	-2.97843100
C	-0.94014500	-2.27137100	-1.15614800	C	1.30845600	2.10313000	-1.36938700
H	-1.80973000	-2.65300000	-1.70833000	H	2.38145500	2.02286300	-1.57652800
N	-0.55433600	-0.92992300	-1.64988400	N	0.66877200	0.78323400	-1.64729700
O	0.48062500	1.47753800	1.83330100	O	-0.42083800	-0.66445100	1.63441200
H	0.74578900	0.01593700	-2.97792100	H	-0.76576200	-0.07066100	-2.90810300
C	-2.72149200	1.54985200	0.86891100	C	2.46466600	-1.44429400	1.16834500
C	-3.96606300	0.56281100	-1.35764900	C	3.79567600	-1.20550300	-1.22372600
C	-4.09640600	1.73404200	0.73815000	C	3.76347500	-1.93288100	1.06947300
H	-2.17718900	1.91158600	1.73637700	H	1.87189200	-1.52770900	2.07071200
C	-4.72866100	1.22579100	-0.39502400	C	4.44075200	-1.80702700	-0.14157200
H	-4.42934500	0.15676200	-2.25185900	H	4.29092100	-1.10239000	-2.18406500
H	-4.65218400	2.25812400	1.50840700	H	4.22458300	-2.40758200	1.92841500
H	-5.80013700	1.34083900	-0.52960200	H	5.45633100	-2.17586300	-0.24765100
H	-0.36899500	-0.64612200	3.01345500	H	0.11298800	1.16273500	2.84894700
C	-0.82006200	-1.45380900	2.44564900	C	0.51621500	1.95113900	2.22335500
C	-1.54549900	-2.46613400	3.06423500	C	0.87252300	3.19914100	2.71760200
C	-2.13234000	-3.44621900	2.26300300	C	1.36870000	4.15705100	1.83243000
H	-1.65439300	-2.47787500	4.14345500	H	0.75532800	3.41236500	3.77448700
C	-1.96854200	-3.37665900	0.88140100	C	1.49862000	3.82709400	0.48566800
H	-2.71494200	-4.24837900	2.70622600	H	1.64933700	5.14499500	2.18449500
H	-2.41985200	-4.11921100	0.22977200	H	1.88317400	4.54595500	-0.23154100
H	2.77710600	-2.51817900	-3.32694200	H	-2.89347500	2.32063800	-3.04649900
C	2.90194900	-2.09376100	-2.33534600	C	-2.88228600	1.91260900	-2.04070800
C	4.07244200	-2.30815700	-1.60753900	C	-3.99203800	2.03484200	-1.20196400
C	4.18902700	-1.74693500	-0.33767600	C	-3.94590300	1.47024000	0.06987100
H	4.87634300	-2.90670800	-2.02560500	H	-4.88182600	2.55343800	-1.54566200
C	3.12627800	-0.99421900	0.15746100	C	-2.78318300	0.82366400	0.48042100
H	5.08090900	-1.88921700	0.26328100	H	-4.79495800	1.51881100	0.74252400
H	3.17618200	-0.53700500	1.14165300	H	-2.70203600	0.33188400	1.44209100
H	-0.11495800	-2.96116200	-1.36887000	H	0.91827700	2.86292900	-2.05606200
C	3.68459300	2.06811300	3.52086100	C	-3.17979100	-3.28483700	2.29751200
O	3.08968600	1.19103500	2.92653000	O	-2.85315000	-2.10484700	1.57373500
H	3.19456900	3.01333300	3.81345800	H	-4.22671900	-3.51869800	2.08339800
H	4.74770800	1.95493100	3.79591300	H	-2.55902900	-4.13740300	1.99038600
H	0.51368900	2.39659400	1.39445600	Fe	0.00920700	-0.14146800	0.15719200
O	0.70960800	1.90016400	-1.15753600	H	-3.07406200	-3.14973400	3.38456500

C	0.78753800	3.15069700	-0.82588800	O	-0.56473800	-1.57984900	-0.90532200
O	0.66005200	3.58498400	0.33833600	C	-0.53614200	-2.84833800	-0.49931600
C	1.05577200	4.11816600	-1.96225700	O	0.00487800	-3.24374000	0.52116000
H	0.25450300	4.04870400	-2.70610800	C	-1.30252200	-3.77034400	-1.43068500
H	1.12190800	5.14147100	-1.59047300	H	-1.18419500	-3.48108300	-2.47857800
H	1.98865800	3.84616600	-2.46754900	H	-0.97757700	-4.80158000	-1.28161800
H	1.33853100	1.38534100	2.29765800	H	-2.36638600	-3.69450300	-1.17814100

5	Charge=1 Multiplicity =3			5	Charge=1 Multiplicity =5		
N	0.01973500	0.41337000	0.08077400	N	1.91639700	-0.22753600	-0.54160200
H	-0.47939100	-0.97226700	3.09773500	H	1.53886700	2.38347800	1.65416500
N	3.41705800	0.17751700	2.03707600	N	-2.28387900	0.21352700	0.19319200
N	1.73920500	2.36012600	1.14749400	N	-0.02671600	-1.59727800	1.08685500
C	0.31216200	0.26238500	-1.23118400	C	1.91100400	-0.82844300	-1.74688100
C	4.37765300	-0.12601000	1.13424900	C	-2.82298400	-0.12480300	-0.99306600
C	2.36452000	2.86404300	0.06905800	C	-0.24269200	-2.65943900	0.29062800
C	1.74399200	-0.11815600	-1.54256400	C	0.58185900	-0.80676700	-2.47091200
H	2.02573100	0.17185900	-2.56194700	H	0.54167000	-1.56621700	-3.26213000
C	3.88062800	-0.38480400	-0.27220100	C	-1.82322700	-0.39466100	-2.09811800
H	3.56590700	-1.42906200	-0.33259100	H	-1.56843400	0.55940000	-2.56846400
H	4.66629600	-0.21383400	-1.01818800	H	-2.24071200	-1.05679700	-2.86764900
C	3.05609300	1.86745800	-0.83229900	C	-0.76258000	-2.37063400	-1.09891300
H	4.13815900	1.97347300	-0.69590700	H	-1.83838100	-2.57878300	-1.10232500
N	2.67677900	0.45545900	-0.53221300	N	-0.56299400	-0.95259300	-1.52949900
O	0.78154600	0.46773700	2.70322800	O	0.20063200	1.02491300	1.62591000
H	1.81366600	-1.20624200	-1.46512500	H	0.48193500	0.17646600	-2.94091000
C	3.72997800	0.30769500	3.33604000	C	-3.07881900	0.58956100	1.20537400
C	5.70725700	-0.26771700	1.51637800	C	-4.20077900	-0.13487900	-1.19340500
C	5.03877100	0.16743300	3.78635800	C	-4.46498400	0.61807900	1.07904400
H	2.89715700	0.50709600	3.99870200	H	-2.57412500	0.88185800	2.11979200
C	6.04243900	-0.11877800	2.86344500	C	-5.03280600	0.24429300	-0.13816200
H	6.46326900	-0.50236900	0.77372700	H	-4.61330900	-0.42014900	-2.15630900
H	5.25634900	0.27497700	4.84314200	H	-5.07949300	0.93125000	1.91594000
H	7.07332400	-0.23064600	3.18507100	H	-6.11065400	0.25123900	-0.26918300
H	0.66804800	2.71616600	2.86566000	H	0.51056300	-0.87360500	2.93441600
C	1.15735800	3.19878300	2.02704900	C	0.35362000	-1.78305100	2.36387800
C	1.18354300	4.57730500	1.85894500	C	0.53353000	-3.05243500	2.89950500
C	1.82211100	5.10642800	0.73675500	C	0.32508000	-4.16069700	2.07738500
H	0.70535300	5.21759800	2.59212700	H	0.83686000	-3.16505200	3.93459400
C	2.42015900	4.23628200	-0.17164400	C	-0.06686500	-3.96235500	0.75454800
H	1.85344700	6.17889700	0.57069800	H	0.46606100	-5.16697600	2.46015500
H	2.92797300	4.61217800	-1.05471900	H	-0.24009700	-4.80473300	0.09184400
H	-0.41844800	0.22566800	-3.25226600	H	3.04439800	-1.80963200	-3.29475000

C	-0.67784200	0.33884800	-2.20434700	C	3.07684900	-1.32138000	-2.32556000
C	-2.00174300	0.53941500	-1.80815700	C	4.28475800	-1.15462700	-1.64397800
C	-2.29436600	0.64869900	-0.45129600	C	4.28777200	-0.49434500	-0.41736100
H	-2.79136500	0.59613700	-2.55116900	H	5.20991600	-1.52612600	-2.07439700
C	-1.25411500	0.58397300	0.47181000	C	3.07680800	-0.04495000	0.10719900
H	-3.31192800	0.77764100	-0.09966700	H	5.20878700	-0.32280400	0.12913000
H	-1.42297200	0.62405900	1.54100300	H	3.02335500	0.51490500	1.03561800
H	2.85385000	2.09815700	-1.88448300	H	-0.31090100	-3.05461100	-1.82700500
C	-1.71893800	-2.17331600	4.01943600	C	2.71777300	3.77534000	2.38546400
O	-1.32178100	-1.41362400	2.88435600	O	2.41255700	2.75965400	1.43607600
H	-2.61254200	-2.73745200	3.73698000	H	3.69284000	4.18875700	2.11365500
H	-0.93905500	-2.88180000	4.32977900	H	1.98020900	4.58963700	2.37107100
Fe	1.58566600	0.33469700	1.30232800	Fe	-0.09931100	0.31050400	0.20146800
H	-1.97361000	-1.53552500	4.87932900	H	2.78382100	3.38151500	3.41043300
O	1.53694300	-1.52619600	1.03304200	O	-0.09107200	1.78181200	-0.91569500
C	1.58369300	-2.41672000	2.02311700	C	-0.38825900	3.04728200	-0.54218300
O	1.83382200	-2.15501900	3.18861600	O	-1.19948100	3.30952600	0.32116800
C	1.24299300	-3.81925200	1.55168900	C	0.41408000	4.08120400	-1.30004400
H	1.64196000	-4.02241000	0.55399400	H	0.48566800	3.83202600	-2.36250200
H	1.61871500	-4.55212700	2.26793800	H	-0.03085000	5.06884600	-1.16867800
H	0.15118600	-3.90084300	1.50088300	H	1.42850400	4.07918800	-0.88362200

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Charge=1 Multiplicity =1				Charge=1 Multiplicity =3			
Fe	0.11275100	0.12375800	0.13223400	Fe	-0.02770900	0.01986800	0.04556600
N	1.89456200	-0.75420700	-0.10418600	N	-0.01025500	0.00491800	2.04277200
N	-1.72142300	0.81713600	-0.10888000	N	0.46469600	0.01128900	-1.86792900
N	-0.75981200	-1.54660200	0.87099800	N	-0.13066100	-1.99669400	-0.09745200
C	2.14471300	-1.16618200	-1.36890800	C	1.22281200	0.12539100	2.58773700
C	-2.24767900	0.59019400	-1.33135900	C	1.79387500	-0.00001000	-2.10548100
C	-1.18341900	-2.45689000	-0.02497600	C	1.02881800	-2.67095000	0.01048600
C	1.06554500	-0.83677600	-2.37688900	C	2.34506300	0.32234500	1.59324600
H	1.07725500	-1.52862500	-3.22784700	H	3.31007900	-0.01113600	1.99356200
C	-1.28314600	0.02044600	-2.35012800	C	2.66374800	0.18473800	-0.88099100
H	-0.75179600	0.85703200	-2.81186200	H	2.77229000	1.25879500	-0.70753700
H	-1.80726300	-0.52647800	-3.14289700	H	3.66481200	-0.23860300	-1.02529500
C	-0.73983300	-2.23092400	-1.45082100	C	2.22216100	-1.86098300	0.45962100
H	-1.54044200	-2.48081200	-2.15620700	H	3.12592100	-2.15900200	-0.08369300
N	-0.25691800	-0.83562600	-1.68424100	N	1.99803400	-0.38818400	0.32646400
O	0.34960500	0.70563700	1.73914900	O	-1.73108600	0.12435300	-0.17941600
H	1.24243400	0.17696900	-2.74153100	H	2.40605500	1.38765000	1.36156500
C	-2.44147400	1.45267300	0.82752000	C	-0.40287400	0.00322000	-2.89140900
C	-3.55127000	0.96611200	-1.63989600	C	2.29795100	-0.06363100	-3.40058200
C	-3.74796100	1.86348500	0.58435900	C	0.03237200	-0.05141000	-4.21143600

H	-1.92734500	1.62995700	1.76397500	H	-1.44778100	0.05781100	-2.61296500
C	-4.31327600	1.61118100	-0.66451300	C	1.40139000	-0.09216300	-4.46994600
H	-3.95583400	0.76909500	-2.62769000	H	3.37038800	-0.07703700	-3.56752800
H	-4.30289500	2.37727200	1.36150100	H	-0.69427900	-0.05425100	-5.01630200
H	-5.33178900	1.91787600	-0.88209100	H	1.76994000	-0.13801700	-5.49014700
H	-0.66406300	-0.94732100	2.83294000	H	-2.14754300	-2.04905900	-0.47839900
C	-1.03755200	-1.72568600	2.17645800	C	-1.25774500	-2.66487300	-0.40751000
C	-1.75516500	-2.82492100	2.63304200	C	-1.26366800	-4.03777300	-0.62469700
C	-2.21016500	-3.76386600	1.70712900	C	-0.06211000	-4.73994300	-0.52907300
H	-1.95621800	-2.93339900	3.69327100	H	-2.19328600	-4.53945600	-0.87045600
C	-1.91972800	-3.57640800	0.35708500	C	1.10227700	-4.04530900	-0.20668200
H	-2.78180900	-4.62873400	2.02961700	H	-0.03062800	-5.81129300	-0.70225900
H	-2.25348400	-4.28927700	-0.39077400	H	2.05419000	-4.56016000	-0.11902400
H	3.50989100	-2.12112500	-2.72730600	H	2.41254800	0.21857500	4.37546900
C	3.33952700	-1.79198500	-1.70704300	C	1.41147100	0.13052600	3.96518200
C	4.30995600	-1.97558100	-0.72026000	C	0.29690300	0.03442100	4.80065300
C	4.04932600	-1.53545700	0.57502900	C	-0.96923300	-0.06994400	4.23038100
H	5.25308700	-2.45545500	-0.96298400	H	0.41953500	0.04314700	5.87934300
C	2.82481100	-0.93199800	0.84766100	C	-1.08501900	-0.08635100	2.84309400
H	4.77771900	-1.65201600	1.36986600	H	-1.86196900	-0.13634900	4.84233500
H	2.57339200	-0.56096200	1.83325000	H	-2.04541500	-0.14616200	2.34648400
H	0.08764300	-2.91733600	-1.66215700	H	2.40626700	-2.08315900	1.51662100
C	1.93058600	3.16884500	2.75570600	C	-3.71949500	2.53284700	0.18815400
O	2.28887000	1.97913800	2.11493000	O	-2.85751500	1.85543700	1.04379900
H	2.83865900	3.79074600	2.80310600	H	-4.09743700	3.40715600	0.74840300
H	1.19069700	3.72704400	2.16246500	H	-3.18832700	2.92787900	-0.69117400
H	1.31545300	1.27248000	1.99283400	H	-2.23619000	0.91166500	0.37399600
H	1.55428600	3.01172600	3.77730000	H	-4.58780500	1.93137400	-0.12347800
O	0.86471500	1.54737800	-0.85030500	O	0.37741300	1.85575000	0.21688000
C	0.65136400	2.83470900	-0.60813700	C	-0.13754500	2.81833700	-0.53964700
O	-0.15867100	3.28139100	0.19227300	O	-0.82127800	2.64543900	-1.53856600
C	1.56051300	3.73565900	-1.42887000	C	0.19300300	4.20552500	-0.01254700
H	1.64592800	3.38472400	-2.46169400	H	1.23232100	4.26973200	0.32326200
H	1.18476300	4.76009100	-1.40947800	H	-0.00002800	4.95221500	-0.78474200
H	2.56514600	3.71579600	-0.99102300	H	-0.44626400	4.41426700	0.85296700

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Charge=1 Multiplicity =5

Fe	0.10673200	0.12100300	0.12303600
N	1.85810100	-0.80487600	-0.13154900
N	-1.70824500	0.86832300	-0.10361600
N	-0.79721900	-1.52111500	0.88716800
C	2.07708800	-1.24028700	-1.39425100
C	-2.25616500	0.65322100	-1.31884700

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Charge=1 Multiplicity =1

Fe	0.10936500	0.04160100	0.12654900
N	1.60108400	-1.26306800	-0.08099400
N	-1.46805900	1.19601900	-0.13031400
N	-1.15447200	-1.29569700	0.93374400
C	1.72550900	-1.77207500	-1.32823200
C	-2.05078000	1.07775200	-1.34268300

C	-1.26196700	-2.42266000	0.00292300	C	-1.81217600	-2.09736100	0.07576900
C	0.99645300	-0.88328700	-2.39025900	C	0.75518700	-1.21086300	-2.34564700
H	0.97426400	-1.57942400	-3.23738300	H	0.57685000	-1.91274300	-3.16956900
C	-1.32093200	0.04941300	-2.34400300	C	-1.28561100	0.23427400	-2.34189900
H	-0.76715300	0.86709500	-2.81324900	H	-0.55853900	0.88309200	-2.83749700
H	-1.86839000	-0.48452700	-3.12973000	H	-1.94725500	-0.18229500	-3.11089500
C	-0.84275000	-2.21306600	-1.43310100	C	-1.34147800	-2.04877900	-1.35959900
H	-1.66778400	-2.43486200	-2.11933200	H	-2.18816400	-2.10483800	-2.05326800
N	-0.31695600	-0.83500800	-1.68128600	N	-0.51132000	-0.83856700	-1.64886300
O	0.37778700	0.71487700	1.71579200	O	0.53306700	0.59866000	1.76584400
H	1.20132400	0.12247100	-2.76274900	H	1.18520600	-0.29232600	-2.74972800
C	-2.39633600	1.53181000	0.83796200	C	-1.97818600	2.03146700	0.78652400
C	-3.55053200	1.06909700	-1.61395700	C	-3.20894200	1.78013300	-1.66010800
C	-3.69181600	1.98298500	0.60760200	C	-3.12787000	2.77280300	0.53171600
H	-1.86649800	1.69842500	1.76740000	H	-1.42222100	2.08556700	1.71474300
C	-4.27996900	1.74273500	-0.63298400	C	-3.75587700	2.63982800	-0.70557500
H	-3.97251900	0.88061000	-2.59608300	H	-3.66573500	1.66603200	-2.63819300
H	-4.22038500	2.51823300	1.38860400	H	-3.51555700	3.44237500	1.29158400
H	-5.29072600	2.08072600	-0.84004500	H	-4.65715400	3.20185500	-0.93066000
H	-0.64749800	-0.91699200	2.84377100	H	-0.87753900	-0.66006000	2.86247700
C	-1.05389400	-1.68788700	2.19835900	C	-1.45330700	-1.34168200	2.24559800
C	-1.79112400	-2.76646600	2.67293100	C	-2.42858500	-2.19667800	2.74671900
C	-2.28842800	-3.69629900	1.75968100	C	-3.12393900	-3.02009300	1.86114700
H	-1.97433000	-2.86611600	3.73725200	H	-2.63972000	-2.20682200	3.81055500
C	-2.01970000	-3.52122400	0.40344200	C	-2.81101000	-2.96914200	0.50369000
H	-2.87606400	-4.54480600	2.09657300	H	-3.89803700	-3.69168000	2.21975400
H	-2.38667100	-4.22771100	-0.33486900	H	-3.32871400	-3.59867100	-0.21367200
H	3.39231200	-2.25449100	-2.75869800	H	2.78852200	-3.09806900	-2.64560800
C	3.24677300	-1.90725000	-1.74061900	C	2.71603100	-2.69747000	-1.63932300
C	4.22539800	-2.10710000	-0.76498500	C	3.61254500	-3.08888800	-0.64298200
C	3.99881500	-1.63854200	0.52664800	C	3.48285300	-2.55047800	0.63552700
H	5.14957100	-2.61944300	-1.01417500	H	4.39764700	-3.80524400	-0.86470500
C	2.79765200	-0.99396700	0.80943600	C	2.45732700	-1.64184300	0.88067600
H	4.73639300	-1.76349100	1.31165700	H	4.16033700	-2.82568900	1.43636800
H	2.57700300	-0.59278900	1.79072600	H	2.29890600	-1.18589200	1.85104000
H	-0.04517100	-2.92829800	-1.66292400	H	-0.72541700	-2.93537000	-1.54659600
C	2.16133600	3.08461200	2.76127400	C	2.93673600	3.10390600	2.52086100
O	2.42960400	1.91024900	2.06634500	O	3.11438400	1.84054100	2.02352300
H	3.09889700	3.66949900	2.76604800	H	3.87814900	3.64678600	2.68603400
H	1.40970000	3.69869500	2.24228400	H	2.34042400	3.63100700	1.74043400
H	1.30658900	1.25817100	1.86881600	H	1.41720500	1.01989000	1.82209400
H	1.86485600	2.91479700	3.80822600	H	2.29584800	3.11287200	3.41880200
O	0.88773400	1.52383300	-0.86995900	O	1.20653500	1.21297000	-0.91165500
C	0.73338000	2.81609900	-0.60479300	C	1.38223100	2.50202000	-0.70533800

O	-0.04491200	3.28352100	0.21435400	O	0.83827800	3.16196300	0.17691500
C	1.66813300	3.68933700	-1.42642600	C	2.38881900	3.12657400	-1.66165100
H	1.72886900	3.34650000	-2.46365600	H	2.27560300	2.73449500	-2.67660500
H	1.33305300	4.72742400	-1.39196800	H	2.27774500	4.21249600	-1.66447900
H	2.67535900	3.62545800	-0.99891500	H	3.40252400	2.87729100	-1.32583900

6				6			
Charge=1 Multiplicity =3				Charge=1 Multiplicity =5			
Fe	0.03745900	0.01421400	0.03155600	Fe	0.15121400	0.23735500	0.20104800
N	0.06850800	0.00565300	2.02392400	N	2.25865600	-0.46421600	-0.09892700
N	0.49502300	-0.01483500	-1.88575600	N	-2.03517600	0.23269700	-0.32403600
N	-0.22722900	-1.97119900	-0.12774000	N	-0.32050800	-1.47595500	1.19572700
C	1.30954300	0.04128500	2.56126000	C	2.50424400	-0.95100300	-1.32677900
C	1.81646200	-0.12834900	-2.13932400	C	-2.32244400	-0.34309800	-1.50189100
C	0.87566000	-2.73592300	-0.02652200	C	-0.48384200	-2.58355300	0.44753800
C	2.43669500	0.14538000	1.55615400	C	1.32080800	-0.91357600	-2.26933700
H	3.37493600	-0.26263300	1.95178000	H	1.41999500	-1.65939700	-3.06934600
C	2.71388500	-0.02080300	-0.92343600	C	-1.11796200	-0.69048300	-2.35003300
H	2.91468000	1.03991600	-0.75089400	H	-0.82216700	0.21315000	-2.89196900
H	3.67423200	-0.52569700	-1.08304000	H	-1.35872800	-1.46259000	-3.09254300
C	2.12844600	-2.02338700	0.42846800	C	-0.08338100	-2.49572000	-1.01007500
H	3.00861000	-2.39226400	-0.11045900	H	-0.78801000	-3.05985500	-1.63246400
N	2.02186000	-0.53733600	0.29522100	N	0.04706700	-1.09374000	-1.51733300
O	-1.72019000	0.24183000	-0.15777200	O	0.41108100	1.04216200	1.76087700
H	2.58118700	1.20160500	1.32076100	H	1.28046300	0.07969600	-2.72572400
C	-0.38442200	0.04941900	-2.89634300	C	-3.02795500	0.70065900	0.44481800
C	2.29757700	-0.22256500	-3.44127900	C	-3.63393200	-0.50389500	-1.94431100
C	0.02882700	-0.02749400	-4.22284200	C	-4.36518200	0.59188500	0.07052600
H	-1.41743500	0.17601300	-2.59557200	H	-2.72464700	1.18105000	1.36884000
C	1.38737500	-0.17287200	-4.49883300	C	-4.67107200	-0.02783100	-1.14073600
H	3.36319700	-0.32003500	-3.62370400	H	-3.83826700	-0.97883200	-2.89914400
H	-0.70514400	0.03006400	-5.01908300	H	-5.14401700	0.98534200	0.71482500
H	1.73846700	-0.24059900	-5.52400900	H	-5.70325200	-0.13597300	-1.46030400
H	-2.23803800	-1.85276900	-0.50626700	H	-0.40324200	-0.57295100	3.03385000
C	-1.40418100	-2.54366900	-0.44296700	C	-0.57516200	-1.51146100	2.51611300
C	-1.51787700	-3.91063200	-0.67065200	C	-1.01343000	-2.67029700	3.14602700
C	-0.37610800	-4.70695200	-0.58132600	C	-1.20245600	-3.81976200	2.37800600
H	-2.48401400	-4.33569900	-0.92030200	H	-1.20663300	-2.66595200	4.21321500
C	0.84038900	-4.10979600	-0.25452900	C	-0.93429500	-3.77655300	1.01058800
H	-0.42989000	-5.77602600	-0.76311200	H	-1.55306300	-4.73957500	2.83643600
H	1.74851400	-4.69923300	-0.17205000	H	-1.06623200	-4.65674100	0.38873200
H	2.51149300	0.05842900	4.34416800	H	3.94022600	-1.78943800	-2.70102100
C	1.50491600	0.03914000	3.93824400	C	3.77061500	-1.39149800	-1.70506400
C	0.39040500	0.02206400	4.77920000	C	4.81282000	-1.29913900	-0.78057900

C	-0.88372800	-0.00351600	4.21597400	C	4.55552100	-0.77995700	0.48778100
H	0.51887900	0.02640200	5.85724800	H	5.81152300	-1.63019800	-1.04919200
C	-1.00486700	-0.01721100	2.82941000	C	3.25718900	-0.37486200	0.79062000
H	-1.77494600	-0.01422500	4.83378100	H	5.34113900	-0.69014900	1.23030800
H	-1.96436500	-0.03802100	2.32589700	H	2.98722000	0.03997000	1.75697800
H	2.28901300	-2.25833100	1.48656300	H	0.88933900	-2.98866700	-1.11797800
C	-3.41145500	3.37361500	-0.04083500	C	0.51379500	4.66971700	2.38343400
O	-2.78823200	2.67268800	0.95687100	O	1.36694400	3.76061100	1.81224800
H	-3.87638000	4.30806800	0.30406900	H	0.96777500	5.66103800	2.52444500
H	-2.59837000	3.61301900	-0.76463900	H	-0.31469900	4.76101000	1.64827100
H	-2.05370200	1.07895900	0.22983900	H	0.66554400	1.98948300	1.72075400
H	-4.12101300	2.74908500	-0.60963400	H	0.05339200	4.29497500	3.31202700
O	0.58959400	1.83741100	0.19290400	O	0.44621200	1.67822600	-0.96325000
C	0.15124800	2.84965600	-0.52689900	C	-0.09885500	2.87707300	-0.79908500
O	-0.66318500	2.77063500	-1.44355800	O	-0.94936000	3.13899900	0.04320400
C	0.72674000	4.18820200	-0.08544600	C	0.45529700	3.92042300	-1.75130300
H	1.78625400	4.10425600	0.17347300	H	0.60668600	3.50747300	-2.75238300
H	0.59085400	4.93162700	-0.87312200	H	-0.21527400	4.78053400	-1.79477400
H	0.19610600	4.52608800	0.81275000	H	1.43213800	4.25146000	-1.37927500

6-4	Charge=1 Multiplicity =1			6-4	Charge=1 Multiplicity =3		
Fe	0.16280700	-0.27882800	0.12961800	Fe	0.16280700	-0.27882800	0.12961800
N	-1.62956700	-0.92790600	-0.46445900	N	-1.62956700	-0.92790600	-0.46445900
N	2.00966600	0.47398500	0.23056300	N	2.00966600	0.47398500	0.23056300
N	-0.71511300	1.52872500	0.21874900	N	-0.71511300	1.52872500	0.21874900
C	-1.72720400	-1.06756600	-1.80743100	C	-1.72720400	-1.06756600	-1.80743100
C	2.63397900	0.57327300	-0.96638000	C	2.63397900	0.57327300	-0.96638000
C	-0.74237000	2.21892900	-0.93972200	C	-0.74237000	2.21892900	-0.93972200
C	-0.45344800	-0.81508200	-2.58595300	C	-0.45344800	-0.81508200	-2.58595300
H	-0.66990500	-0.50415900	-3.61514300	H	-0.66990500	-0.50415900	-3.61514300
C	1.85745200	0.01717100	-2.14068400	C	1.85745200	0.01717100	-2.14068400
H	2.05129200	-1.05558200	-2.20806500	H	2.05129200	-1.05558200	-2.20806500
H	2.16169500	0.48507500	-3.08481300	H	2.16169500	0.48507500	-3.08481300
C	-0.03200800	1.60145700	-2.12609400	C	-0.03200800	1.60145700	-2.12609400
H	0.85669100	2.19961700	-2.35497300	H	0.85669100	2.19961700	-2.35497300
N	0.39884200	0.19009100	-1.88415900	N	0.39884200	0.19009100	-1.88415900
O	0.05355800	-0.60706200	1.96352900	O	0.05355800	-0.60706200	1.96352900
H	0.11537500	-1.74745700	-2.62214200	H	0.11537500	-1.74745700	-2.62214200
C	2.63737700	0.89098500	1.34284000	C	2.63737700	0.89098500	1.34284000
C	3.91455500	1.10459500	-1.07646400	C	3.91455500	1.10459500	-1.07646400
C	3.92350800	1.42048300	1.30749100	C	3.92350800	1.42048300	1.30749100
H	2.08011600	0.77578700	2.26480000	H	2.08011600	0.77578700	2.26480000

C	4.57232100	1.52974800	0.07926200	C	4.57232100	1.52974800	0.07926200
H	4.38973900	1.17883400	-2.04958900	H	4.38973900	1.17883400	-2.04958900
H	4.39907200	1.73796200	2.22887600	H	4.39907200	1.73796200	2.22887600
H	5.57441000	1.94282900	0.01767400	H	5.57441000	1.94282900	0.01767400
H	-1.37245000	1.41421200	2.18905800	H	-1.37245000	1.41421200	2.18905800
C	-1.33895400	2.03606700	1.30172700	C	-1.33895400	2.03606700	1.30172700
C	-1.98226800	3.26869600	1.26873300	C	-1.98226800	3.26869600	1.26873300
C	-1.99416100	3.99648900	0.08078800	C	-1.99416100	3.99648900	0.08078800
H	-2.47683400	3.63062700	2.16331000	H	-2.47683400	3.63062700	2.16331000
C	-1.37235900	3.45641100	-1.04364100	C	-1.37235900	3.45641100	-1.04364100
H	-2.49103900	4.96012200	0.02304400	H	-2.49103900	4.96012200	0.02304400
H	-1.37741900	3.98387800	-1.99287200	H	-1.37741900	3.98387800	-1.99287200
H	-2.96241100	-1.56798300	-3.49396800	H	-2.96241100	-1.56798300	-3.49396800
C	-2.91087200	-1.47209300	-2.41385800	C	-2.91087200	-1.47209300	-2.41385800
C	-4.01899100	-1.75341800	-1.61216300	C	-4.01899100	-1.75341800	-1.61216300
C	-3.91217200	-1.59377200	-0.23340400	C	-3.91217200	-1.59377200	-0.23340400
H	-4.95186500	-2.07790800	-2.06308700	H	-4.95186500	-2.07790800	-2.06308700
C	-2.70197900	-1.16857100	0.31126400	C	-2.70197900	-1.16857100	0.31126400
H	-4.75264400	-1.77981400	0.42624900	H	-4.75264400	-1.77981400	0.42624900
H	-2.60177500	-0.97468700	1.37826200	H	-2.60177500	-0.97468700	1.37826200
H	-0.67344900	1.64784200	-3.01358800	H	-0.67344900	1.64784200	-3.01358800
C	-1.68481500	-0.68108100	3.92374000	C	-1.68481500	-0.68108100	3.92374000
O	-2.59912200	-0.02887600	3.27339500	O	-2.59912200	-0.02887600	3.27339500
H	-1.17521600	-0.17447600	4.76628000	H	-1.17521600	-0.17447600	4.76628000
H	-1.82702200	-1.76726100	4.08909500	H	-1.82702200	-1.76726100	4.08909500
H	0.79357000	-1.26138800	2.13433200	H	0.79357000	-1.26138800	2.13433200
H	-0.73171000	-0.68778100	2.96784200	H	-0.73171000	-0.68778100	2.96784200
O	0.92879400	-1.99714000	-0.26294600	O	0.92879400	-1.99714000	-0.26294600
C	1.68362500	-2.70328000	0.54174100	C	1.68362500	-2.70328000	0.54174100
O	1.94718700	-2.39306500	1.71111900	O	1.94718700	-2.39306500	1.71111900
C	2.20745500	-3.99272200	-0.05857700	C	2.20745500	-3.99272200	-0.05857700
H	2.61044900	-3.82591200	-1.06218200	H	2.61044900	-3.82591200	-1.06218200
H	2.97421000	-4.42059600	0.58858700	H	2.97421000	-4.42059600	0.58858700
H	1.38197600	-4.70770500	-0.15200300	H	1.38197600	-4.70770500	-0.15200300

7				7			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
Fe	0.00015000	-0.35284400	-0.52241500	Fe	0.00021000	-0.35235000	-0.52345900
N	1.96492700	-0.35256700	-0.23861700	N	1.96629100	-0.35180400	-0.23965900
N	-1.96463300	-0.35552400	-0.23878100	N	-1.96588100	-0.35549500	-0.23988100
N	-0.00132700	1.61641800	-0.49299300	N	-0.00162800	1.61626400	-0.49197900
C	2.36542900	-0.51497200	1.04683100	C	2.36618500	-0.51454500	1.04601300

C	3.71110600	-0.47514600	1.39319000	C	3.71180500	-0.47479300	1.39257000
H	4.00952800	-0.59821100	2.42954700	H	4.01022300	-0.59807900	2.42891300
C	4.66438500	-0.28233600	0.39020900	C	4.66519100	-0.28195800	0.38959400
H	5.72045600	-0.25022400	0.63963400	H	5.72122800	-0.24992900	0.63919800
C	4.24197400	-0.13094200	-0.93000100	C	4.24311900	-0.13068300	-0.93070800
H	4.95099200	0.01707800	-1.73725100	H	4.95238800	0.01711300	-1.73777000
C	2.87973500	-0.16666300	-1.20906200	C	2.88080100	-0.16634400	-1.21001200
H	2.48942800	-0.05383700	-2.21424400	H	2.48978000	-0.05438400	-2.21501200
C	-2.36500700	-0.51873500	1.04659600	C	-2.36559500	-0.51919100	1.04571900
C	-3.71078900	-0.48120800	1.39280800	C	-3.71133500	-0.48226600	1.39212500
H	-4.00912200	-0.60489200	2.42911700	H	-4.00961300	-0.60630300	2.42841900
C	-4.66427400	-0.28990200	0.38973600	C	-4.66499800	-0.29129500	0.38905800
H	-5.72042900	-0.25962200	0.63903200	H	-5.72113200	-0.26150900	0.63852500
C	-4.24196000	-0.13763000	-0.93040500	C	-4.24307300	-0.13897800	-0.93117200
H	-4.95113200	0.00928100	-1.73772100	H	-4.95254900	0.00742600	-1.73830600
C	-2.87963300	-0.17103100	-1.20930800	C	-2.88065500	-0.17179900	-1.21031400
H	-2.48939000	-0.05743500	-2.21442600	H	-2.48974500	-0.05891400	-2.21525400
C	-0.00206000	2.21938800	0.71289200	C	-0.00258400	2.21873900	0.71432200
C	-0.00339900	3.60766400	0.83105200	C	-0.00432200	3.60697400	0.83278800
H	-0.00398600	4.06680400	1.81498300	H	-0.00508900	4.06569700	1.81691500
C	-0.00396400	4.38843100	-0.32269100	C	-0.00502900	4.38817800	-0.32063300
H	-0.00500500	5.47165100	-0.25136700	H	-0.00638200	5.47137200	-0.24892300
C	-0.00317200	3.75576600	-1.56720800	C	-0.00398300	3.75596900	-1.56536000
H	-0.00356500	4.32352200	-2.49124600	H	-0.00447900	4.32395700	-2.48925000
C	-0.00186900	2.36919100	-1.61575100	C	-0.00231000	2.36941100	-1.61451900
H	-0.00123200	1.81902800	-2.54923600	H	-0.00147400	1.82037400	-2.54866300
C	1.25436200	-0.81001600	2.03113900	C	1.25507700	-0.81056400	2.03041400
H	1.52357600	-0.50930000	3.04976100	H	1.52454400	-0.51040300	3.04912400
C	-1.25356100	-0.81202400	2.03099800	C	-1.25402500	-0.81306000	2.03022900
H	-1.06837700	-1.89087800	2.04796800	H	-1.06868700	-1.89189400	2.04663100
H	-1.52335200	-0.51175300	3.04960000	H	-1.52421100	-0.51346500	3.04891500
C	-0.00130000	1.32133000	1.92683100	C	-0.00156700	1.32042400	1.92792200
H	0.87474200	1.54232500	2.54539500	H	0.87454100	1.54135100	2.54641600
H	-0.87763100	1.54090600	2.54548800	H	-0.87792600	1.53958700	2.54668400
N	-0.00011000	-0.13992800	1.57129800	N	-0.00010400	-0.14060900	1.57199000
O	0.00018200	-0.39693700	-2.14403500	O	0.00031100	-0.39437400	-2.14377200
H	1.07091700	-1.88916600	2.04808000	H	1.07187100	-1.88975700	2.04680400
C	0.00440000	-3.47513700	-0.66420300	C	0.00521100	-3.47412900	-0.66316100
N	0.00174400	-2.34045000	-0.43970500	N	0.00218000	-2.33907900	-0.44025600
C	0.00672600	-4.89991900	-0.96165500	C	0.00819100	-4.89921100	-0.95907700
H	-0.07786800	-5.04257100	-2.04459800	H	-0.07532100	-5.04313000	-2.04195800
H	0.93926300	-5.35592800	-0.61371500	H	0.94050900	-5.35460900	-0.60972900
H	-0.84015900	-5.38963600	-0.47014100	H	-0.83906400	-5.38861600	-0.46786500

7

Charge=2 Multiplicity =5

Fe	-0.16620100	0.28897000	-0.56749900
N	-2.12692800	-0.23599700	-0.27211300
N	1.72986100	0.99563700	-0.18954100
N	0.61306700	-1.66833500	-0.60085000
C	-2.52565100	-0.25486700	1.02488100
C	-3.80839900	-0.65672000	1.37748800
H	-4.10847000	-0.67366700	2.42049100
C	-4.70102600	-1.03046100	0.36828800
H	-5.70838400	-1.34596500	0.62222900
C	-4.28426200	-0.99720200	-0.96280000
H	-4.95049700	-1.27953200	-1.77064300
C	-2.98352900	-0.59664100	-1.24741800
H	-2.59761200	-0.55117400	-2.26021300
C	2.06034300	1.05976000	1.12225900
C	3.35017100	1.38802300	1.52490700
H	3.59998000	1.42816500	2.58046400
C	4.31022400	1.67364500	0.55036200
H	5.32243500	1.93506700	0.84342900
C	3.95545600	1.61811300	-0.79814000
H	4.67384100	1.83601100	-1.58087800
C	2.65273600	1.26655400	-1.13259200
H	2.31628300	1.19311700	-2.16134100
C	0.82554100	-2.22157500	0.60999900
C	1.50725500	-3.42740900	0.74970500
H	1.67312100	-3.85318700	1.73452300
C	1.95958900	-4.08115600	-0.39779300
H	2.49033400	-5.02458700	-0.31392700
C	1.72194500	-3.50989400	-1.64958800
H	2.05503300	-3.99129700	-2.56255900
C	1.05168000	-2.29446300	-1.71145500
H	0.85141500	-1.78889600	-2.65021000
C	-1.50372500	0.25507400	2.01732500
H	-1.66878900	-0.15684200	3.01916400
C	0.91774900	0.85436500	2.09241000
H	0.44089000	1.82422200	2.26753700
H	1.27395500	0.48854900	3.06134000
C	0.18974600	-1.51491200	1.78455100
H	-0.75602500	-2.02087400	2.00711400
H	0.81038600	-1.60349500	2.68210600
N	-0.12342100	-0.06253700	1.52145100
O	-0.17990200	0.43875800	-2.17113300

H	-1.59137300	1.34319600	2.08746700
C	-1.15980600	3.50805600	-0.52182300
N	-0.84116900	2.43286200	-0.22575400
C	-1.55955100	4.85808400	-0.89389200
H	-1.56682400	4.95085100	-1.98513200
H	-2.56277900	5.07140900	-0.51104900
H	-0.85528900	5.58598600	-0.47827400

8				8			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
N	-1.62978200	-0.79839500	-0.47509800	N	-1.63115900	-0.79625100	-0.47361200
N	2.07708400	0.02379200	0.54750800	N	2.07686300	0.02448000	0.54945600
N	-0.13762500	1.51776700	-0.30645300	N	-0.13752200	1.51834400	-0.30770800
C	-1.58133500	-1.37798900	-1.70084600	C	-1.58253500	-1.37497600	-1.69997200
C	2.87547000	-0.36969000	-0.47473200	C	2.87488500	-0.36848400	-0.47351900
C	0.21297900	1.80212100	-1.57754700	C	0.21305600	1.80322100	-1.57879000
C	-0.19046800	-1.66175100	-2.22664200	C	-0.19198500	-1.65924700	-2.22736500
H	-0.17016900	-1.68287200	-3.32204400	H	-0.17344100	-1.68006700	-3.32278900
C	2.17100100	-1.13086900	-1.57599100	C	2.17111100	-1.12917700	-1.57604200
H	2.14440700	-2.19389000	-1.31611900	H	2.14417100	-2.19232700	-1.31679500
H	2.69812800	-1.04294400	-2.53259900	H	2.69964400	-1.04075500	-2.53181500
C	0.68592900	0.65047900	-2.43327900	C	0.68664400	0.65218000	-2.43482200
H	1.66844300	0.88001900	-2.85809500	H	1.66948900	0.88196100	-2.85873100
N	0.76087500	-0.64746000	-1.67755400	N	0.76111700	-0.64587700	-1.67971400
H	0.13408900	-2.64689900	-1.87688400	H	0.13242400	-2.64472600	-1.87846700
C	2.61114900	0.64594600	1.61493700	C	2.61159500	0.64520600	1.61720200
C	4.24491600	-0.13104300	-0.45489900	C	4.24445400	-0.13040700	-0.45365700
C	3.97548300	0.90272700	1.70271900	C	3.97607800	0.90137900	1.70501900
H	1.91374300	0.92509200	2.39658100	H	1.91470700	0.92411100	2.39943500
C	4.80442900	0.51251400	0.65157500	C	4.80456100	0.51182600	0.65329400
H	4.86416600	-0.44704000	-1.28848600	H	4.86343800	-0.44591200	-1.28763700
H	4.37205600	1.40322200	2.57932900	H	4.37307600	1.40080800	2.58203500
H	5.87186600	0.70683000	0.68817300	H	5.87210700	0.70555600	0.68982900
H	-0.96233400	2.18784600	1.47529900	H	-0.96191200	2.18650900	1.47473500
C	-0.63596900	2.49240500	0.48694200	C	-0.63637500	2.49197700	0.48648700
C	-0.76470200	3.79914600	0.03469600	C	-0.76576000	3.79883600	0.03457000
C	-0.37568000	4.11045600	-1.26838500	C	-0.37687100	4.11106700	-1.26829600
H	-1.16718600	4.55494400	0.70015200	H	-1.16864600	4.55402300	0.70046500
C	0.11138000	3.09385300	-2.08768800	C	0.11077800	3.09516900	-2.08813800
H	-0.45976200	5.12487200	-1.64577100	H	-0.46146400	5.12564000	-1.64514100
H	0.40540800	3.29569500	-3.11322800	H	0.40477700	3.29762000	-3.11357000
H	-2.68104800	-2.17537900	-3.36670900	H	-2.68237700	-2.17138400	-3.36621000
C	-2.74232100	-1.72034900	-2.38310100	C	-2.74361100	-1.71711600	-2.38223900
C	-3.97876100	-1.47193700	-1.78145200	C	-3.98008900	-1.46970600	-1.78022400

C	-4.01359900	-0.87010300	-0.52521900	C	-4.01499500	-0.86903000	-0.52346300
H	-4.89811500	-1.73622600	-2.29483300	H	-4.89939600	-1.73402000	-2.29367300
C	-2.81754200	-0.53419700	0.10412600	C	-2.81887100	-0.53321600	0.10587200
H	-4.95398600	-0.65025500	-0.03170900	H	-4.95537200	-0.65015100	-0.02951300
H	-2.79376600	-0.02607600	1.06597100	H	-2.79523700	-0.02613200	1.06830200
H	0.00444000	0.53000100	-3.28208200	H	0.00575300	0.53204200	-3.28414800
N	0.42145500	-2.23343500	0.80702600	N	0.42263500	-2.23642700	0.80080600
C	0.49792200	-3.26091500	1.33241100	C	0.49902000	-3.26483800	1.32452000
C	0.59062000	-4.54819100	2.00600000	C	0.59074600	-4.55277300	1.99688600
H	-0.12803200	-5.25186700	1.57365800	H	-0.12906400	-5.25523100	1.56448800
H	1.60134400	-4.95615700	1.90347300	H	1.60091000	-4.96187000	1.89334600
H	0.36532500	-4.41700700	3.06992300	H	0.36635300	-4.42215900	3.06109600
Fe	0.13167600	-0.33067900	0.30324100	Fe	0.13156100	-0.32999900	0.30335100
O	-0.32887500	0.00982400	1.82212200	O	-0.32749100	0.00724800	1.82011800
H	-1.95447400	0.57057100	4.00468300	H	-1.94976500	0.56459300	4.00610800
C	-2.83672200	1.21185700	3.96929700	C	-2.83173300	1.20649900	3.97468300
O	-3.00302600	1.59418300	2.59517100	O	-3.00211300	1.59222800	2.60204600
H	-2.67024400	2.08388600	4.61341100	H	-2.66286900	2.07689600	4.62039600
H	-3.70297200	0.65151900	4.34229400	H	-3.69717100	0.64574400	4.34895700
H	-3.77882000	2.17502000	2.54745600	H	-3.77804300	2.17317400	2.55823700

8				TS_{8,9}			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
N	-1.87345000	-0.47621600	-0.50345300	Fe	0.00253500	-0.33790900	0.23199300
N	2.04322400	-0.47734800	0.54791000	N	-1.87393500	-0.18605100	-0.47723500
N	0.19233500	1.70428000	-0.19545800	N	1.98425000	-0.55620000	0.36648600
C	-1.89878900	-0.97415500	-1.76554900	N	0.28879800	1.62169300	0.10126300
C	2.72027500	-0.82424400	-0.57249000	C	-1.99830300	-0.49575300	-1.79436800
C	0.65160600	1.92861600	-1.44289100	C	2.62456000	-0.78120300	-0.80496900
C	-0.56071900	-1.42601100	-2.30904200	C	0.57487000	2.10789100	-1.12487600
H	-0.53638400	-1.38826900	-3.40398600	C	-0.73000300	-0.97403900	-2.46147200
C	1.86091200	-1.28030100	-1.72974300	H	-0.74585600	-0.79391200	-3.54262100
H	1.67500200	-2.35318200	-1.61608000	C	1.72062300	-1.02471100	-1.99208200
H	2.36840800	-1.13845300	-2.69001800	H	1.49233300	-2.09452900	-2.04387600
C	0.59084500	0.75717300	-2.39798600	H	2.20650100	-0.75275400	-2.93569100
H	1.42933700	0.77772900	-3.10141400	C	0.50893700	1.13166200	-2.27140700
N	0.53221300	-0.58676500	-1.71429000	H	1.37030400	1.26221400	-2.93478300
H	-0.38340900	-2.46280900	-2.00933500	N	0.43013400	-0.29603400	-1.80984000
C	2.71544400	-0.14984200	1.66797500	O	-0.19830700	-0.37154100	1.96656700
C	4.11029800	-0.83811400	-0.60000900	H	-0.62172700	-2.05199100	-2.30940700
C	4.10492800	-0.15803200	1.71345500	C	2.69610600	-0.42298400	1.50041000
H	2.10627400	0.11803800	2.52458400	C	4.01139300	-0.86068200	-0.87129800
C	4.81207600	-0.50217500	0.56078900	C	4.08467700	-0.50765900	1.50762900

H	4.63644100	-1.11257100	-1.50885600	H	2.11013600	-0.25608600	2.39696400
H	4.61676600	0.10586800	2.63244400	C	4.75390100	-0.72273800	0.30340000
H	5.89777600	-0.50876800	0.56177800	H	4.50166000	-1.03373100	-1.82416900
H	-0.36386700	2.48026900	1.63918100	H	4.62458200	-0.40082400	2.44217300
C	0.06382500	2.72799000	0.67290400	H	5.83746000	-0.78310600	0.27542300
C	0.42349300	4.02447100	0.32198600	H	0.16126900	2.00304500	2.12193000
C	0.93830600	4.25932700	-0.95393400	C	0.34317100	2.45783100	1.15947300
H	0.30595600	4.83005700	1.03854900	C	0.63871400	3.80754300	1.02796100
C	1.04868700	3.19762200	-1.85406200	C	0.91217100	4.31748500	-0.24166300
H	1.24197700	5.25851900	-1.25106500	H	0.66359300	4.44024200	1.90848100
H	1.42433300	3.35715400	-2.86009700	C	0.88899400	3.44968800	-1.33056800
H	-3.09095400	-1.48445500	-3.48216100	H	1.15154800	5.36721300	-0.37982500
C	-3.09020400	-1.09150700	-2.47029100	H	1.11428200	3.80484900	-2.33151800
C	-4.28053800	-0.69638200	-1.85227900	H	-3.27885100	-0.65962100	-3.51135800
C	-4.23966500	-0.17489800	-0.55992900	C	-3.21833200	-0.41681200	-2.45508800
H	-5.22387700	-0.78405700	-2.38266200	C	-4.35407200	-0.02884300	-1.74124800
C	-3.01319600	-0.06828400	0.09041000	C	-4.22579800	0.26896900	-0.38692500
H	-5.14253800	0.15583700	-0.05824200	H	-5.31739800	0.03867900	-2.23711700
H	-2.91626500	0.37574000	1.07942500	C	-2.97171800	0.18150100	0.21150500
H	-0.32128100	0.86391700	-2.99530100	H	-5.07929700	0.56993500	0.21074700
N	-0.06094500	-2.58223400	0.59870900	H	-2.84831600	0.38972700	1.26616200
C	-0.20873600	-3.58800400	1.15667100	H	-0.38015100	1.35132400	-2.87179800
C	-0.39434800	-4.85155600	1.85687500	H	-1.01354300	0.27871900	2.71108600
H	-1.24142700	-5.39660400	1.42807400	C	-1.75912500	0.76877800	3.65169900
H	0.50781500	-5.46544600	1.76906800	O	-3.07442100	0.39996700	3.47178600
H	-0.59353100	-4.65882500	2.91627300	H	-1.67053300	1.85354500	3.55453500
Fe	0.00145000	-0.32505700	0.32034500	H	-1.28363100	0.37373400	4.55547100
O	-0.37234900	-0.05311100	1.86236400	H	-3.24166000	-0.45763000	3.89736900
H	-1.84553600	0.76071400	4.00272900	N	-0.15991800	-2.31450700	0.28218100
C	-2.57209700	1.57455500	3.97254000	C	-0.26788200	-3.43614500	0.54233400
O	-2.63637500	2.00916300	2.60553600	C	-0.40202900	-4.84566700	0.88425000
H	-2.23373100	2.37905500	4.63704600	H	-1.40146600	-5.20426700	0.61796000
H	-3.54151000	1.20255600	4.32687700	H	0.34588000	-5.43831000	0.34780300
H	-3.27173800	2.74154300	2.56467900	H	-0.25163700	-4.97522000	1.96124600

TS₈₋₉				TS₈₋₉			
Charge=2 Multiplicity =3				Charge=2 Multiplicity =5			
Fe	-0.00006300	-0.33086900	0.24298400	Fe	0.13233600	0.31772900	0.31777900
N	-1.88383900	-0.19509100	-0.45513100	N	1.97680700	-0.26906600	-0.59047900
N	1.97819300	-0.54939900	0.38344000	N	-1.87855200	0.99980700	0.26534300
N	0.29412400	1.62254500	0.04618500	N	-0.66988000	-1.66157700	0.45935700
C	-2.01773100	-0.55089100	-1.75957500	C	2.00307200	-0.31364600	-1.94303500
C	2.61157900	-0.81327800	-0.78392500	C	-2.48677200	1.01426800	-0.94134300

C	0.57820900	2.06433400	-1.19742000	C	-1.15950200	-2.21639100	-0.66660600
C	-0.75464800	-1.05422200	-2.42086500	C	0.76586700	0.20992500	-2.64480200
H	-0.77845700	-0.90712500	-3.50685300	H	0.69301400	-0.19267600	-3.66290800
C	1.70241700	-1.09366500	-1.96038800	C	-1.59122800	0.80302300	-2.14604800
H	1.47338000	-2.16436900	-1.97670000	H	-1.17932000	1.77638500	-2.43411500
H	2.18654500	-0.85303300	-2.91337600	H	-2.17280200	0.43838700	-3.00171300
C	0.49007600	1.05161200	-2.30952100	C	-0.80594300	-1.54186900	-1.97449200
H	1.34033300	1.15594300	-2.99161400	H	-1.61572700	-1.66853200	-2.70264900
N	0.41234900	-0.35925300	-1.79950500	N	-0.44804700	-0.09774100	-1.84087100
O	-0.23716300	-0.33879300	1.96895600	O	0.51785600	0.45880100	1.96549500
H	-0.64762200	-2.12720000	-2.23709200	H	0.84443800	1.29845800	-2.73054800
C	2.69614800	-0.38592900	1.50929300	C	-2.59182600	1.27219900	1.37554900
C	3.99787600	-0.89975700	-0.85434900	C	-3.84494700	1.29445700	-1.06419200
C	4.08445600	-0.47527400	1.51263400	C	-3.94735200	1.57639600	1.32512700
H	2.11633200	-0.19345500	2.40459500	H	-2.04285600	1.23630900	2.31044500
C	4.74672300	-0.72852400	0.31193800	C	-4.58488600	1.58254700	0.08414900
H	4.48307500	-1.10417900	-1.80361000	H	-4.31525500	1.29322600	-2.04260000
H	4.62953900	-0.34328600	2.44094100	H	-4.48828300	1.79513000	2.23934500
H	5.82990600	-0.79370400	0.28044900	H	-5.64478200	1.80570000	0.00898600
H	0.17938200	2.07917000	2.05387300	H	-0.44878800	-1.77591800	2.50643500
C	0.36418100	2.49424200	1.07449500	C	-0.86102300	-2.28226700	1.64152800
C	0.67437500	3.83513400	0.89583600	C	-1.54786400	-3.48473000	1.74386800
C	0.94654200	4.29862600	-0.39170500	C	-2.07150200	-4.05581800	0.58256100
H	0.71101400	4.49682200	1.75434900	H	-1.67535200	-3.95623100	2.71219300
C	0.90653200	3.39463100	-1.45012600	C	-1.87648900	-3.41130300	-0.63846800
H	1.19719500	5.34018400	-0.56669400	H	-2.62414900	-4.98933200	0.62620600
H	1.12942700	3.71279300	-2.46396000	H	-2.26695900	-3.83414500	-1.55906200
H	-3.31142500	-0.77337500	-3.46060500	H	3.11768200	-0.79853400	-3.71880100
C	-3.24248000	-0.49359300	-2.41401500	C	3.12411200	-0.76327000	-2.63380900
C	-4.37235500	-0.07874700	-1.70588500	C	4.25038900	-1.16344600	-1.91091600
C	-4.23405100	0.26681000	-0.36386200	C	4.22068800	-1.10370900	-0.51802200
H	-5.33917200	-0.02723000	-2.19687300	H	5.13483500	-1.51935900	-2.43045700
C	-2.97569400	0.19793900	0.22815500	C	3.06334600	-0.65228300	0.10840300
H	-5.08308400	0.59056100	0.22826400	H	5.07428400	-1.40661700	0.07860500
H	-2.84230700	0.44326800	1.27407600	H	2.99246100	-0.58337000	1.18996700
H	-0.40858900	1.25567200	-2.90106300	H	0.06424000	-2.06588300	-2.38594500
H	-0.95642400	0.36370200	2.68312000	H	1.23243200	0.42989900	3.12638800
C	-1.69032700	0.93348200	3.65071600	C	1.99189500	0.23695800	4.07197200
O	-3.01143900	0.58196600	3.49383800	O	3.27557100	0.09534600	3.58975300
H	-1.57866900	2.01030000	3.50687500	H	1.64697300	-0.71602500	4.48185600
H	-1.20800200	0.55624300	4.55779300	H	1.84317000	1.07956100	4.75569400
H	-3.19062400	-0.25601000	3.95245900	H	3.73424700	0.95194400	3.60462600
N	-0.16278000	-2.30809900	0.33502200	N	0.67455800	2.42724800	-0.24367800
C	-0.27440200	-3.42427300	0.61618200	C	0.97985300	3.54513600	-0.22279800

C	-0.41406000	-4.82629800	0.98561200	C	1.36151500	4.95097800	-0.20167600
H	-1.43057800	-5.17192300	0.77197200	H	2.41920500	5.05570100	-0.46400800
H	0.29818900	-5.43919700	0.42399700	H	0.75800100	5.51425700	-0.92075200
H	-0.21541800	-4.94244100	2.05631400	H	1.19853900	5.36389500	0.79917500

9				9			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
Fe	0.07902600	-0.34687300	0.31743500	Fe	0.07888000	-0.34691300	0.31746900
N	-1.78215700	-0.75098600	-0.30307300	N	-1.78232300	-0.75073600	-0.30315300
N	2.04883900	-0.14051000	0.46132400	N	2.04872000	-0.14085700	0.46141700
N	-0.02621200	1.51105700	-0.36399600	N	-0.02605800	1.51106300	-0.36390300
C	-1.82945600	-1.47162000	-1.45307500	C	-1.82973400	-1.47136900	-1.45313700
C	2.74714300	-0.56545000	-0.61779000	C	2.74698300	-0.56587600	-0.61769500
C	0.20395500	1.66487100	-1.68598600	C	0.20417200	1.66486300	-1.68588600
C	-0.48116400	-1.87066100	-2.01076900	C	-0.48148600	-1.87058000	-2.01084500
H	-0.51686100	-2.02129600	-3.09580700	H	-0.51720700	-2.02117400	-3.09588900
C	1.93150900	-1.30164200	-1.65836500	C	1.93127800	-1.30189400	-1.65835300
H	1.92088200	-2.36701600	-1.40517900	H	1.92050700	-2.36728500	-1.40524300
H	2.37027700	-1.21246100	-2.65803600	H	2.37010400	-1.21270400	-2.65799800
C	0.31366600	0.39946100	-2.49725400	C	0.31368300	0.39945700	-2.49721000
H	1.12241600	0.47783400	-3.23084000	H	1.12244400	0.47774800	-3.23079200
N	0.51556200	-0.81863600	-1.63755900	N	0.51539500	-0.81871200	-1.63757900
O	-0.23195800	0.09077600	2.01526400	O	-0.23223300	0.09084900	2.01528700
H	-0.16222500	-2.81307400	-1.55618500	H	-0.16268200	-2.81305600	-1.55629600
C	2.69250800	0.43342200	1.49363700	C	2.69245900	0.43293200	1.49376700
C	4.12587300	-0.40367900	-0.69833300	C	4.12574300	-0.40432800	-0.69819000
C	4.07259800	0.61009700	1.48488600	C	4.07257600	0.60938400	1.48506000
H	2.06283400	0.73158800	2.32434800	H	2.06281000	0.73116500	2.32447400
C	4.79928500	0.19312400	0.37008600	C	4.79922600	0.19232500	0.37026600
H	4.66482000	-0.74482700	-1.57665100	H	4.66465800	-0.74553200	-1.57650600
H	4.56090900	1.07060900	2.33678800	H	4.56094100	1.06978500	2.33699100
H	5.87581700	0.32733700	0.33012900	H	5.87578000	0.32636200	0.33034400
H	-0.29937100	2.44931400	1.46432200	H	-0.29910000	2.44932400	1.46444600
C	-0.15624100	2.61322600	0.40520100	C	-0.15593300	2.61323700	0.40531500
C	-0.09525700	3.89707500	-0.12007800	C	-0.09468700	3.89708700	-0.11992700
C	0.13336000	4.05839200	-1.48650800	C	0.13399000	4.05839600	-1.48634700
H	-0.21451100	4.74906100	0.54020000	H	-0.21379300	4.74907700	0.54037400
C	0.29176200	2.92256800	-2.27768500	C	0.29220000	2.92256300	-2.27754900
H	0.19639000	5.04844800	-1.92717200	H	0.19720900	5.04845300	-1.92698100
H	0.48188500	3.00738000	-3.34321400	H	0.48234000	3.00736700	-3.34307500
H	-3.04108000	-2.40952600	-2.96067400	H	-3.04156500	-2.40908700	-2.96069200
C	-3.03585800	-1.84360400	-2.03440100	C	-3.03621900	-1.84314900	-2.03443100
C	-4.23005600	-1.48371900	-1.40603200	C	-4.23034500	-1.48303100	-1.40604300
C	-4.17510000	-0.75516700	-0.21960400	C	-4.17525100	-0.75444500	-0.21963300

H	-5.18414200	-1.76606600	-1.84012600	H	-5.18448800	-1.76521600	-1.84011600
C	-2.93369900	-0.40296800	0.30245200	C	-2.93376600	-0.40249800	0.30237900
H	-5.07803600	-0.45529900	0.30098300	H	-5.07812500	-0.45438400	0.30095100
H	-2.85211600	0.16525100	1.22231000	H	-2.85184100	0.16575500	1.22218400
H	-0.61204800	0.26799300	-3.06731400	H	-0.61204800	0.26815700	-3.06727900
H	-0.97215000	0.70684100	2.18637500	H	-0.97224500	0.70715400	2.18631700
C	-2.74919600	3.00635200	2.91302600	C	-2.74782900	3.00681700	2.91239300
O	-2.48612500	1.64995600	2.99530200	O	-2.48486900	1.65047100	2.99484800
H	-3.07623800	3.31426500	1.92734300	H	-3.07496500	3.31461800	1.92671400
H	-3.12303500	3.50238900	3.80207900	H	-3.12088600	3.50336700	3.80148400
H	-2.42662300	1.38602600	3.92847900	H	-2.42513900	1.38663800	3.92804400
N	0.30216800	-2.20789200	0.96031400	N	0.30168600	-2.20799600	0.96032100
C	0.38741500	-3.18388800	1.57464700	C	0.38675500	-3.18402600	1.57462300
C	0.49210000	-4.40455100	2.36177900	C	0.49121800	-4.40472200	2.36173500
H	-0.25927800	-5.13052500	2.03509600	H	-0.26027900	-5.13056300	2.03503000
H	1.48864400	-4.84317600	2.24861600	H	1.48768900	-4.84351800	2.24858100
H	0.32453500	-4.16930000	3.41822900	H	0.32367700	-4.16945700	3.41818600

9				10			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
Fe	0.10381000	0.23481400	0.26183300	N	1.71699200	0.87442300	-0.13886300
N	2.00379600	0.08119000	-0.41544900	N	-2.09002300	-0.23285800	0.14097500
N	-1.78160500	0.89435300	0.51033000	N	0.52624200	-1.55618200	0.08287500
N	-0.66666900	-1.74068200	-0.14865200	C	1.94557900	1.12591000	-1.45159500
C	2.14665700	0.48913400	-1.70590000	C	-2.64562000	-0.02065000	-1.07987100
C	-2.40643200	1.25657000	-0.63428100	C	0.53497800	-2.05683400	-1.17281500
C	-1.06319500	-1.89918100	-1.42595100	C	0.71112300	1.13892500	-2.32653600
C	0.91922700	1.10741900	-2.33487300	H	0.95253300	0.89854000	-3.36797000
H	0.92772700	1.00775900	-3.42604500	C	-1.72298600	0.62756800	-2.08850500
C	-1.52060100	1.37124300	-1.85495900	H	-1.77991000	1.71547600	-1.99828900
H	-1.16562100	2.40448000	-1.92224000	H	-2.00030400	0.36872700	-3.11721900
H	-2.07525700	1.16056000	-2.77504900	C	-0.11911400	-1.20833400	-2.23000100
C	-0.53203900	-0.86405200	-2.38725400	H	-1.09959000	-1.63496100	-2.46549600
H	-1.17806300	-0.75448900	-3.26447100	N	-0.32236800	0.20988600	-1.77328600
N	-0.31142100	0.48321500	-1.74486300	H	0.28349100	2.14678800	-2.31985600
O	0.28887800	-0.04645900	2.00037100	C	-2.85642400	-0.78013800	1.10179700
H	0.90141800	2.17350100	-2.09413100	C	-3.96583300	-0.35326600	-1.36277800
C	-2.45826400	0.86833300	1.67269400	C	-4.18808300	-1.12902100	0.89813700
C	-3.75533300	1.59452300	-0.64298400	H	-2.38168500	-0.93625400	2.06311200
C	-3.80433200	1.21115700	1.73728300	C	-4.75537800	-0.91236300	-0.35607700
H	-1.87972100	0.55697100	2.53615700	H	-4.36993900	-0.17768200	-2.35493200
C	-4.46310800	1.57256600	0.56144300	H	-4.76083800	-1.56655000	1.70862800
H	-4.24341500	1.87712200	-1.57043400	H	-5.78921300	-1.17891000	-0.55193200

H	-4.32330400	1.18533500	2.68920700	H	1.16884300	-1.84876900	2.03925900
H	-5.51677800	1.83399400	0.57796400	C	1.10844000	-2.29235900	1.05538300
H	-0.66524000	-2.47109400	1.78275800	C	1.65957500	-3.54720600	0.82789100
C	-1.00043500	-2.66604000	0.76932300	C	1.64018100	-4.06960800	-0.46436800
C	-1.73601700	-3.79937000	0.43638400	H	2.10635600	-4.09222400	1.65228400
C	-2.15760800	-3.96161700	-0.88386100	C	1.07969700	-3.30114900	-1.48130800
H	-1.97997200	-4.53056600	1.19941200	H	2.06531800	-5.04495400	-0.67915500
C	-1.81970000	-2.99386100	-1.83291100	H	1.06375200	-3.65933900	-2.50614400
H	-2.74418000	-4.82812300	-1.17346800	H	3.36712100	1.59776300	-2.99600000
H	-2.13169200	-3.09447600	-2.86778600	C	3.21773300	1.40989900	-1.93729200
H	3.45048400	0.72902600	-3.39766900	C	4.29086700	1.45008600	-1.04545800
C	3.36716500	0.40433000	-2.36532500	C	4.05522800	1.18881900	0.30328900
C	4.47655400	-0.09595200	-1.68011600	H	5.29197100	1.67278200	-1.40110700
C	4.32761300	-0.50123600	-0.35496000	C	2.75862100	0.89556400	0.71458500
H	5.43899500	-0.16928000	-2.17710000	H	4.86178900	1.19846300	1.02843000
C	3.07660500	-0.40149500	0.24445500	H	2.53495100	0.65034200	1.74761100
H	5.16331000	-0.89532800	0.21288600	H	0.45874200	-1.22632200	-3.16014900
H	2.92383600	-0.71384100	1.27148300	N	-0.70371900	2.18287000	0.31248300
H	0.44185300	-1.21097400	-2.74978400	C	-1.01238400	3.29424000	0.44438800
H	1.07717600	-0.52106100	2.33840600	C	-1.40596900	4.69031800	0.59775900
C	2.02993600	-2.92635100	3.37678000	H	-0.54451400	5.29640500	0.89685000
O	2.34859900	-1.58267500	3.28812800	H	-1.79484200	5.07650000	-0.35042600
H	2.15162900	-3.45157100	2.43722400	H	-2.18779100	4.77993800	1.35917800
H	2.21371300	-3.42716700	4.32103400	H	0.04541000	1.49691600	2.52264700
H	2.44208300	-1.20943900	4.18035800	O	-0.13590700	0.56340900	2.32872800
N	0.61718800	2.60904700	0.39385500	Fe	-0.16258600	0.32050700	0.21589900
C	0.87184600	3.60772500	0.92639400	C	0.03414600	-0.21320300	3.53842100
C	1.18984400	4.86422400	1.59379700	O	1.37568700	-0.44629500	3.81062700
H	2.23291000	5.13661500	1.40434000	H	-0.45666800	-1.16312600	3.32610700
H	0.54036500	5.66246800	1.22061400	H	-0.48105400	0.30315300	4.35414800
H	1.03953200	4.75920400	2.67307500	H	1.67894200	0.08703400	4.56264000

10	Charge=2 Multiplicity =3			10	Charge=2 Multiplicity =5		
N	-0.09553500	-0.06948200	-0.09461700	N	-0.10626800	-0.02178800	-0.10862800
N	-0.05235800	-0.04583900	3.94178800	N	-0.15198100	0.00704100	4.13417300
N	1.93286100	0.11789100	1.76768700	N	2.15189100	0.24290800	1.67608100
C	-0.21259000	-1.37563500	-0.43404900	C	-0.07531200	-1.34368400	-0.38112800
C	-0.32240400	-1.32287300	4.30689100	C	-0.39949300	-1.29136500	4.42038900
C	2.46748700	-1.12135200	1.83725300	C	2.58374400	-1.03526200	1.74243200
C	-0.51059100	-2.35289900	0.69191700	C	-0.30216800	-2.29133100	0.78380300
H	-0.19760400	-3.36577600	0.40641600	H	0.13435600	-3.27416000	0.56353600
C	-0.66721500	-2.28138600	3.18129300	C	-0.62425400	-2.20267400	3.22987400
H	-1.73372900	-2.19056300	2.94807500	H	-1.67802700	-2.14540900	2.93496000

H	-0.49464800	-3.31963400	3.49468500	H	-0.42209700	-3.24759400	3.50163600
C	1.53136700	-2.28348300	2.09732600	C	1.63133000	-2.06297000	2.31688800
H	1.71250400	-2.65428800	3.11259500	H	1.78541600	-2.08970100	3.40157700
N	0.09849300	-1.92387800	1.96849400	N	0.19472200	-1.75819300	2.07644200
H	-1.59675300	-2.38870900	0.83481300	H	-1.38302300	-2.44528100	0.88156600
C	0.21472400	0.86031900	4.90199600	C	0.00765000	0.87498700	5.15191300
C	-0.31884600	-1.71840100	5.64150100	C	-0.48396800	-1.75266700	5.73170000
C	0.22774200	0.53746700	6.25507700	C	-0.07104000	0.49199000	6.48661300
H	0.41059200	1.87014400	4.56092000	H	0.19770000	1.90575500	4.87263300
C	-0.04281100	-0.77625600	6.63341900	C	-0.32101200	-0.84787200	6.78174500
H	-0.53039700	-2.75159700	5.89900100	H	-0.67388600	-2.80347200	5.92734200
H	0.45020500	1.30336300	6.99010700	H	0.06644100	1.22744200	7.27182600
H	-0.03516300	-1.06588000	7.67961100	H	-0.38214100	-1.18616000	7.81158600
H	2.28760300	2.12494600	1.37601800	H	2.61434100	2.18554500	1.10736400
C	2.75712300	1.15884000	1.51043300	C	3.00467200	1.17918200	1.21029900
C	4.12945200	1.01459800	1.36462200	C	4.31201700	0.89449100	0.83290400
C	4.68598700	-0.26041500	1.46839600	C	4.75920500	-0.42330400	0.91746500
H	4.74378700	1.88510600	1.16211800	H	4.95631400	1.68872400	0.47165300
C	3.83739900	-1.34013400	1.69398600	C	3.87567800	-1.40248200	1.36800700
H	5.75519200	-0.41257700	1.35896100	H	5.77141200	-0.68716300	0.62671600
H	4.22893400	-2.35104900	1.75637900	H	4.18476100	-2.44127100	1.43205500
H	-0.22471100	-2.84321200	-2.00441600	H	0.10452100	-2.88756600	-1.87168100
C	-0.13569500	-1.78889800	-1.76133500	C	0.07554300	-1.81888400	-1.68260100
C	0.05147200	-0.83803400	-2.76508700	C	0.18255100	-0.90601500	-2.73202200
C	0.16612000	0.50479700	-2.40886700	C	0.14966800	0.45926000	-2.44767000
H	0.11163200	-1.14329200	-3.80513400	H	0.29732100	-1.25622700	-3.75327600
C	0.09464100	0.84943700	-1.06323000	C	0.01358800	0.85704300	-1.12242700
H	0.31754400	1.27672900	-3.15550000	H	0.23809800	1.20232300	-3.23275500
H	0.20328600	1.87984700	-0.73687800	H	0.01792800	1.90805700	-0.84799800
H	1.78070600	-3.11271400	1.42374200	H	1.88189400	-3.06360500	1.94192000
N	-1.95923100	0.51538200	1.94048400	N	-2.23381100	0.72494200	1.92685800
C	-3.11293600	0.64134200	1.94137800	C	-3.39199900	0.75861400	1.86067200
C	-4.56243600	0.79591600	1.94384100	C	-4.84665300	0.80474900	1.77750700
H	-4.89324100	1.26276400	1.01020000	H	-5.15507700	1.51007900	0.99898800
H	-5.04345600	-0.18352200	2.03734300	H	-5.23986100	-0.18702900	1.53167600
H	-4.87348100	1.42186100	2.78676400	H	-5.26620600	1.12565400	2.73648600
H	-1.15801400	2.85403700	2.02558700	H	-1.11752000	2.92110200	2.24784300
O	-0.23985000	2.69095800	2.29655400	O	-0.20219200	2.62966200	2.39523700
Fe	-0.04343200	0.30422600	1.90519100	Fe	-0.00473200	0.47373300	2.00733900
C	0.52118600	3.85930000	2.01335600	C	0.71502800	3.73288200	2.19759600
O	0.82856300	3.83937400	0.64040600	O	1.01891400	3.90190700	0.85212600
H	1.41970400	3.78183500	2.63496700	H	1.61831200	3.43023500	2.72735300
H	-0.04488500	4.75576300	2.29295800	H	0.28908300	4.63053800	2.65524900
H	0.99236400	4.74274200	0.32164000	H	0.55528000	4.67149500	0.48523600

TS ₁₀₋₁₁				TS ₁₀₋₁₁			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
N	0.03888000	0.07281500	0.06341900	N	2.04447800	-0.27310000	-0.29417200
N	0.04731600	0.08311800	4.03410100	N	-1.93873800	0.78650200	-0.08937000
N	2.03274100	-0.05424200	2.16111600	N	-0.49118500	-1.48185900	0.66833300
C	-0.44844600	-1.13640700	-0.31738900	C	2.26387200	-0.45492400	-1.61554600
C	-0.28013100	-1.17219500	4.42584200	C	-2.38525400	0.60781900	-1.35136700
C	2.37510500	-1.36034600	2.15547900	C	-0.74652500	-2.32511600	-0.35756700
C	-0.92228200	-2.01526200	0.82047300	C	1.10688100	-0.11458900	-2.53727600
H	-0.87218700	-3.07861100	0.55726500	H	1.20571100	-0.65219300	-3.49013800
C	-0.75596800	-2.08234100	3.31401900	C	-1.32755100	0.35224400	-2.41076600
H	-1.83456700	-1.94620100	3.18464000	H	-0.95588500	1.32075800	-2.76439800
H	-0.59129700	-3.13824300	3.55742600	H	-1.77230000	-0.15150000	-3.27945000
C	1.25897300	-2.33485800	1.88296000	C	-0.42800000	-1.85776100	-1.76224000
H	1.33835400	-3.21228400	2.53346500	H	-1.23518200	-2.15743600	-2.44213300
N	-0.09818500	-1.70281100	2.02698800	N	-0.17792700	-0.39807400	-1.86457600
H	-1.96512900	-1.78542400	1.05538800	H	1.13760600	0.95541900	-2.76944700
C	0.41241900	0.97862200	4.96876000	C	-2.82307800	1.08758200	0.87945000
C	-0.24318500	-1.56069400	5.76114400	C	-3.73659500	0.72155300	-1.67122100
C	0.45733200	0.66795000	6.32438800	C	-4.18411900	1.23277600	0.63346800
H	0.67453100	1.96278700	4.59669800	H	-2.41293400	1.20697000	1.87763900
C	0.12751900	-0.62492000	6.72866800	C	-4.65024700	1.04280600	-0.66721000
H	-0.50318900	-2.57699200	6.04040000	H	-4.06699100	0.56374000	-2.69334900
H	0.75344700	1.42449700	7.04304000	H	-4.85932400	1.47976400	1.44556100
H	0.16124500	-0.90382400	7.77717700	H	-5.70704500	1.13778600	-0.89667200
H	2.69272900	1.88824600	2.41062400	H	-0.57427100	-1.18649900	2.71062200
C	3.00868800	0.85410900	2.36773000	C	-0.75386300	-1.90780400	1.92414400
C	4.34161100	0.50716000	2.54428800	C	-1.24430300	-3.17400800	2.20829900
C	4.69202100	-0.84300900	2.52887400	C	-1.49684000	-4.04790800	1.15059300
H	5.08467300	1.28154800	2.70103100	H	-1.43214600	-3.46182300	3.23699700
C	3.68819400	-1.78921900	2.33889200	C	-1.25008300	-3.60886900	-0.14649800
H	5.72268500	-1.15273000	2.67009400	H	-1.88554700	-5.04512900	1.33151800
H	3.91795100	-2.85034500	2.33081700	H	-1.44455900	-4.25498200	-0.99726000
H	-0.90569600	-2.49860100	-1.91731500	H	3.62967800	-1.04350600	-3.17016400
C	-0.52009400	-1.51887300	-1.65273200	C	3.49163000	-0.89734900	-2.10320100
C	-0.08985800	-0.62902200	-2.63876800	C	4.53140200	-1.14677300	-1.20716300
C	0.41291700	0.61111700	-2.24969500	C	4.30530400	-0.95473800	0.15527000
H	-0.13853700	-0.90470200	-3.68749600	H	5.49619100	-1.49098600	-1.56659800
C	0.46518300	0.91736000	-0.89335300	C	3.04877100	-0.52226400	0.56588200
H	0.76756000	1.33076300	-2.97961700	H	5.08152700	-1.14197900	0.88933900
H	0.85932700	1.86724700	-0.55123500	H	2.82756300	-0.36439700	1.61623100
H	1.36009700	-2.70104900	0.85586400	H	0.46654400	-2.39170700	-2.10300000

N	-1.83121100	0.61868500	2.07308500	N	0.55318700	2.16668500	-0.24154500
C	-2.96776800	0.84772100	2.13150700	C	0.80942900	3.25886900	-0.53749400
Fe	0.07233700	0.30180100	2.05621400	Fe	0.08737800	0.37017100	0.23798400
H	-1.26512500	3.06784700	1.03041100	H	1.60899000	2.56283600	2.32648300
C	-0.48954800	3.31793800	1.75618400	C	0.89307000	1.96870100	2.89763600
O	0.38945100	2.31869700	2.08732800	O	0.41218200	0.83456900	2.29507500
H	-0.86167000	3.93229900	2.58415400	H	0.15742700	2.58499200	3.42733400
O	0.55867900	4.13680600	0.99114600	O	1.71475400	1.20064000	3.94055000
H	1.15849900	3.23791400	1.42619200	H	1.13390400	0.37061700	3.35773800
H	0.75695900	5.01157300	1.38891200	H	1.42809300	1.34730100	4.86715000
C	-4.39735500	1.12962400	2.20587300	C	1.12993400	4.63077400	-0.91404800
H	-4.94597300	0.22398700	2.48532800	H	0.59417400	4.90484500	-1.82891100
H	-4.59210500	1.90059700	2.95865900	H	0.83396300	5.32091000	-0.11707300
H	-4.76660100	1.47799300	1.23572900	H	2.20577300	4.73288300	-1.09015400

TS₁₀₋₁₁				11			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
N	2.12529800	-0.56090000	-0.28509900	N	-1.87798700	-0.09573200	-0.43506900
N	-1.77709800	1.13598700	-0.13418500	N	1.99639000	-0.53399100	0.34329600
N	-0.87261700	-1.51731000	0.72999200	N	0.26494300	1.61280400	0.31485300
C	2.26336400	-0.79966100	-1.60826700	C	-2.01551200	-0.23054500	-1.77980400
C	-2.23914000	0.89548600	-1.37865400	C	2.61834700	-0.66594800	-0.85437500
C	-1.23858100	-2.22548400	-0.35688000	C	0.57708700	2.23378200	-0.84145600
C	1.12858100	-0.32245600	-2.49332600	C	-0.75720100	-0.65295300	-2.50403500
H	1.13423200	-0.86562400	-3.44843400	H	-0.77047500	-0.34365700	-3.55569800
C	-1.22652600	0.40060200	-2.39530900	C	1.68780600	-0.83139300	-2.03442400
H	-0.73991500	1.27917100	-2.83464100	H	1.43317900	-1.89050300	-2.14251500
H	-1.73557600	-0.11818200	-3.21849400	H	2.15920200	-0.51390100	-2.97152800
C	-0.57095900	-1.87094800	-1.67126400	C	0.56430000	1.37924100	-2.08470200
H	-1.21095500	-2.16523900	-2.51294100	H	1.47224100	1.54600300	-2.67344200
N	-0.16992800	-0.44312700	-1.78990500	N	0.41811100	-0.08737500	-1.77493400
H	1.28536900	0.73685800	-2.72551600	H	-0.67003700	-1.74313200	-2.48415400
C	-2.61400200	1.65733400	0.78189300	C	2.75061500	-0.43748600	1.45371300
C	-3.55884800	1.16802300	-1.73573000	C	4.00406500	-0.70290700	-0.96751500
C	-3.93837800	1.97148800	0.49867300	C	4.14106900	-0.48224700	1.42037100
H	-2.19801800	1.81855000	1.77234500	H	2.21133200	-0.31720000	2.38650200
C	-4.42002900	1.71758800	-0.78596700	C	4.78076900	-0.61525900	0.18922800
H	-3.90467900	0.95754900	-2.74307000	H	4.46799300	-0.80120800	-1.94397900
H	-4.57505800	2.39555500	1.26754800	H	4.70495700	-0.40526000	2.34368300
H	-5.45095600	1.93959000	-1.04425700	H	5.86406300	-0.64468500	0.12688800
H	-1.08052700	-1.24612200	2.76604000	H	-0.00984100	1.80458700	2.35463300
C	-1.38576100	-1.86190400	1.92616200	C	0.22679700	2.34668700	1.44748900
C	-2.26341400	-2.92612300	2.09560800	C	0.48640100	3.71063200	1.46650000
C	-2.64332600	-3.65770500	0.96995000	C	0.81109300	4.35082800	0.27003600

H	-2.64482600	-3.16846400	3.08166900	H	0.44109400	4.25498400	2.40347900
C	-2.12768500	-3.29719700	-0.27391800	C	0.85895900	3.59723100	-0.89994000
H	-3.33356800	-4.49119600	1.05740000	H	1.02577700	5.41464000	0.24873600
H	-2.40711100	-3.84401800	-1.16931400	H	1.11021300	4.05968300	-1.84969400
H	3.47636900	-1.59984500	-3.19659400	H	-3.29479800	-0.12665500	-3.50443200
C	3.40084000	-1.41205900	-2.12998200	C	-3.22765800	-0.01800800	-2.42641700
C	4.43372700	-1.77770400	-1.26572100	C	-4.34679700	0.33567100	-1.67008200
C	4.29235900	-1.52854400	0.09900100	C	-4.20514700	0.47678200	-0.29169400
H	5.32890400	-2.25540700	-1.65191300	H	-5.30460400	0.50531500	-2.15192500
C	3.12163500	-0.92346800	0.54365600	C	-2.95730900	0.26038700	0.28785400
H	5.06707800	-1.80211500	0.80704700	H	-5.04397900	0.75985900	0.33492100
H	2.96488500	-0.71653400	1.59759200	H	-2.82101700	0.36983700	1.35904400
H	0.33807700	-2.47846500	-1.74840700	H	-0.27448200	1.68751700	-2.71754700
N	1.02236200	2.33463900	-0.17519400	N	-0.16986900	-2.27269600	0.05794600
C	1.38484700	3.39378700	-0.47977200	C	-0.25758800	-3.42936000	0.08045500
Fe	0.21364300	0.33439500	0.31632200	Fe	0.01371000	-0.35130800	0.17497500
H	2.13013700	2.09892100	2.48617200	H	-1.66877400	-1.91819000	2.47119600
C	1.30839800	1.61968200	3.02195500	C	-0.95300200	-1.19021200	2.87115100
O	0.61786000	0.64610600	2.34480200	O	-0.26255900	-0.48980100	2.13296700
H	0.70276900	2.33014000	3.59578900	H	-0.83351900	-1.12487600	3.95588600
O	1.94851200	0.63273800	4.00449200	O	-3.14948200	0.03549900	3.62741300
H	1.21295100	-0.02471100	3.37601600	H	-3.11626000	0.76944000	4.26211300
H	1.69906900	0.77546300	4.94240900	C	-0.36268900	-4.88405300	0.09863800
C	1.84057600	4.72475600	-0.86316400	H	0.12776900	-5.30752900	-0.78412700
H	1.44390200	4.98738700	-1.84918300	H	0.12285500	-5.28552800	0.99418800
H	1.49520300	5.46556600	-0.13489100	H	-1.41446500	-5.18816700	0.09698500
H	2.93435100	4.74817700	-0.90403200	H	-3.94610200	-0.45925900	3.87982000

11			11				
Charge=2 Multiplicity =3			Charge=2 Multiplicity =5				
N	-0.01965900	0.04052500	0.12147800	N	2.07534100	-0.24610200	-0.50871300
N	-0.07141100	-0.09921600	4.18193000	N	-1.94826300	0.98394900	0.15229900
N	1.94212000	-0.00818100	2.19816900	N	-0.64830000	-1.63152400	0.53946500
C	-0.35870700	-1.21240300	-0.26607800	C	2.12772000	-0.28932800	-1.86011400
C	-0.37549400	-1.38279800	4.48318400	C	-2.47734300	0.90015000	-1.08694400
C	2.35826400	-1.29282200	2.15317500	C	-1.05402000	-2.22284500	-0.60195800
C	-0.81938400	-2.15465100	0.83190800	C	0.89596800	0.20722900	-2.59279900
H	-0.71957900	-3.19857800	0.50581300	H	0.87309000	-0.18925500	-3.61684900
C	-0.79881600	-2.26391700	3.32073400	C	-1.49707500	0.69549200	-2.22753500
H	-1.87066100	-2.11868200	3.14503800	H	-1.11673400	1.68020000	-2.52298100
H	-0.65868000	-3.32329400	3.57373800	H	-2.01160600	0.28136000	-3.10455100
C	1.31217000	-2.38641100	2.04370700	C	-0.61336600	-1.59575200	-1.91176700
H	1.47088200	-3.11449500	2.84826200	H	-1.34976200	-1.80648900	-2.69725400

N	-0.08356300	-1.88597200	2.08464700	N	-0.33340100	-0.13500300	-1.83568700
H	-1.88398000	-1.97994900	1.02334100	H	0.94596000	1.29898200	-2.67196000
C	0.25675000	0.74564200	5.17810800	C	-2.76204300	1.24793700	1.19155900
C	-0.35362900	-1.84866200	5.79527100	C	-3.84074200	1.07498800	-1.31554000
C	0.28627000	0.35311400	6.51206400	C	-4.12949800	1.45162900	1.04188900
H	0.50454100	1.76007500	4.88272200	H	-2.29145900	1.28911900	2.16940900
C	-0.02321100	-0.96930100	6.82705500	C	-4.67897000	1.35964300	-0.23696900
H	-0.59448300	-2.88633400	6.00463800	H	-4.23889500	0.99466900	-2.32231000
H	0.55442200	1.06988500	7.28059900	H	-4.74574700	1.66797100	1.90779200
H	-0.00231000	-1.31369100	7.85633600	H	-5.74385700	1.50235700	-0.39330100
H	2.49051100	1.98068500	2.34804500	H	-0.61597700	-1.69270200	2.60429900
C	2.87281000	0.96875800	2.29451700	C	-0.94843400	-2.21821700	1.71506500
C	4.23468300	0.70849900	2.33940600	C	-1.65028300	-3.41413300	1.80329100
C	4.66644500	-0.61732200	2.28781900	C	-2.07638800	-4.02304300	0.62222800
H	4.93855100	1.52983800	2.41815500	H	-1.86448000	-3.85069800	2.77281600
C	3.71224400	-1.62575600	2.19604800	C	-1.77718800	-3.41569000	-0.59602000
H	5.72377600	-0.86065400	2.32256100	H	-2.63602100	-4.95305500	0.64866100
H	4.01022800	-2.66942500	2.15874200	H	-2.09597800	-3.86431400	-1.53200000
H	-0.59516200	-2.61309500	-1.87925800	H	3.26778400	-0.76376900	-3.62279500
C	-0.32581600	-1.59828200	-1.60325800	C	3.26045400	-0.73286800	-2.53764700
C	0.05370600	-0.66970000	-2.57317600	C	4.37693600	-1.13552500	-1.80305400
C	0.39885400	0.61868800	-2.16972500	C	4.31935300	-1.09405400	-0.41103300
H	0.08478100	-0.95143800	-3.62111400	H	5.27074600	-1.48423800	-2.31129500
C	0.35481400	0.93454600	-0.81502300	C	3.15023500	-0.64742700	0.19842800
H	0.70693700	1.37141400	-2.88723700	H	5.16050800	-1.40853000	0.19721000
H	0.62457500	1.92853800	-0.46859900	H	3.06621900	-0.61249900	1.28202800
H	1.47474600	-2.93416600	1.10793700	H	0.31219700	-2.09762600	-2.21660400
N	-1.89414600	0.71064600	2.16647800	N	0.74777600	2.47569700	0.09457100
C	-3.02590500	0.96284900	2.18781500	C	0.99938100	3.60482000	0.01298600
Fe	-0.00784500	0.35156300	2.16760200	Fe	0.14536500	0.37517500	0.29807200
H	-1.13278300	3.56690400	1.35619400	H	2.03489900	1.73609100	2.87295400
C	-0.25478200	3.59536800	2.01629800	C	1.17604300	1.13781300	3.20267600
O	0.29024500	2.57154600	2.40917400	O	0.40951800	0.61323200	2.40116800
H	0.08410800	4.58084200	2.36026500	H	0.98702500	1.07043000	4.28068200
O	0.84425500	4.29002800	-0.18437300	O	3.09647000	-0.47546900	3.66288600
H	1.72455800	4.69836700	-0.14800800	H	2.91467800	-1.29411900	4.15242000
C	-4.45009100	1.27309800	2.21948700	C	1.31398600	5.02420300	-0.09304700
H	-5.01664800	0.40240700	2.56595000	H	0.85798100	5.44248300	-0.99619600
H	-4.63861800	2.10767900	2.90278900	H	0.92780900	5.56068800	0.77960500
H	-4.79986300	1.54597700	1.21853800	H	2.39854600	5.16359100	-0.14642900
H	0.35512000	4.83848700	-0.81965100	H	3.92526500	-0.14655700	4.04864300

12

Charge=2 Multiplicity =1

12

Charge=2 Multiplicity =3

Fe	0.18759400	0.30659700	0.33516800	Fe	0.18844000	0.30553800	0.33409400
N	2.08652100	-0.24244900	0.59453200	N	2.08654100	-0.24611200	0.59534100
N	-1.50602100	0.97748500	-0.45295100	N	-1.50596300	0.97661200	-0.45237600
N	-0.26475000	-1.47126700	-0.37213200	N	-0.26888400	-1.47221500	-0.37095700
C	2.94509600	0.14146100	-0.38191800	C	2.94499700	0.13545400	-0.38243300
C	4.28850900	-0.21375000	-0.34351000	C	4.28834000	-0.22001800	-0.34341000
H	4.95628800	0.09701200	-1.14082700	H	4.95604900	0.08872400	-1.14158000
C	4.75907500	-0.96807600	0.73416700	C	4.75907000	-0.97192200	0.73590800
H	5.80489600	-1.25483900	0.78467000	H	5.80486400	-1.25871400	0.78680600
C	3.86942800	-1.34914000	1.73792900	C	3.86963700	-1.35054400	1.74075300
H	4.19633100	-1.93427600	2.59055500	H	4.19662400	-1.93379700	2.59462600
C	2.53478500	-0.97123300	1.63342400	C	2.53505200	-0.97244700	1.63563900
H	1.79383600	-1.23586500	2.37898200	H	1.79443600	-1.23534300	2.38219300
C	-1.37698200	1.57878900	-1.66253200	C	-1.37702600	1.57219300	-1.66500700
C	-2.48527400	2.04386400	-2.35960800	C	-2.48537100	2.03661200	-2.36248500
H	-2.35918900	2.51428300	-3.32968200	H	-2.35967300	2.50240200	-3.33484900
C	-3.75304100	1.89808200	-1.79053400	C	-3.75266600	1.89649400	-1.79092200
H	-4.63207600	2.25731800	-2.31671500	H	-4.63158400	2.25540400	-2.31752100
C	-3.87170900	1.27648900	-0.54930300	C	-3.87102700	1.28119200	-0.54655400
H	-4.83899500	1.13469300	-0.07971800	H	-4.83792400	1.14407800	-0.07480000
C	-2.72666800	0.81568800	0.09574800	C	-2.72606000	0.82064700	0.09887400
H	-2.77396000	0.29040900	1.04790100	H	-2.77317600	0.29997700	1.05359600
C	0.06992800	-1.72364200	-1.65470700	C	0.06364500	-1.72819700	-1.65352900
C	-0.20697500	-2.95100300	-2.25094900	C	-0.22061100	-2.95491900	-2.24748800
H	0.07599800	-3.12648300	-3.28441500	H	0.06061200	-3.13345800	-3.28090800
C	-0.85040900	-3.93767600	-1.50640700	C	-0.86866000	-3.93695100	-1.50078800
H	-1.07344100	-4.90222100	-1.95182900	H	-1.09736400	-4.90095000	-1.94450900
C	-1.21404400	-3.65832700	-0.18911500	C	-1.22945900	-3.65356600	-0.18363400
H	-1.73439700	-4.38830900	0.42110400	H	-1.75320700	-4.37966400	0.42830100
C	-0.91178000	-2.41443600	0.34943100	C	-0.92030400	-2.41044200	0.35295200
H	-1.21999500	-2.13261400	1.35052300	H	-1.22622200	-2.12527300	1.35365000
C	2.33514700	1.01582700	-1.45461500	C	2.33616900	1.00776200	-1.45799300
H	2.87740000	0.93544200	-2.40336000	H	2.87962800	0.92456800	-2.40580000
C	0.04443800	1.75226400	-2.15100500	C	0.04390600	1.74242200	-2.15725200
H	0.44370600	2.69719400	-1.76855500	H	0.44446100	2.68876400	-1.77969300
H	0.09250100	1.79899000	-3.24462300	H	0.08899000	1.78486000	-3.25115100
C	0.75436300	-0.61485900	-2.41720900	C	0.75597300	-0.62521500	-2.41707300
H	1.74854300	-0.94842400	-2.73196000	H	1.75114600	-0.96358200	-2.72348000
H	0.19716600	-0.39880700	-3.33476200	H	0.20571700	-0.41150300	-3.33935400
N	0.89514200	0.64751900	-1.61122300	N	0.89618700	0.63981900	-1.61575500
O	-0.32465900	-0.05180500	1.83616500	O	-0.32180700	-0.04409600	1.83404300
H	-2.14730300	-0.73428200	3.20493800	H	-2.13150500	-0.72705100	3.20318400
O	-2.82229700	-1.17205500	2.66311300	O	-2.81669000	-1.16142700	2.67142400
C	-3.87127900	-1.64247100	3.52378500	C	-3.86015800	-1.61774400	3.54618000

H	-3.49911000	-2.37342400	4.25149200	H	-3.48706400	-2.35020100	4.27191900
H	-4.60846300	-2.12948300	2.88240700	H	-4.61009200	-2.09907200	2.91538200
H	-4.35793400	-0.81753600	4.05806300	H	-4.33165000	-0.78594600	4.08340600
H	2.38391400	2.06256900	-1.13876400	H	2.38501900	2.05524700	-1.14478000
N	0.64387700	2.15271100	0.92460300	N	0.65085500	2.15692400	0.91152400
C	0.80453900	3.15118300	1.48573400	C	0.81382800	3.15613600	1.47083000
C	1.00213700	4.40350200	2.20143000	C	1.01390300	4.40881200	2.18508800
H	2.03551900	4.74587800	2.08545300	H	2.05799700	4.72769400	2.10300300
H	0.32275200	5.16927600	1.81328600	H	0.36538200	5.18659800	1.76904700
H	0.79513200	4.24965300	3.26600500	H	0.76685500	4.26669000	3.24276300

12				TS₁₂₋₁₃			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
Fe	0.28635400	0.26619400	0.31390200	Fe	0.03907000	0.24766500	0.07733900
N	2.21978500	-0.33942300	0.62877300	N	1.98191200	-0.12877800	-0.11978500
N	-1.38084900	1.03555300	-0.62042700	N	-1.92243800	0.36468300	-0.22412800
N	-0.60351800	-1.62892800	0.04728400	N	-0.23443700	-1.51785800	0.91897900
C	3.00893700	-0.35394100	-0.47482000	C	2.36221900	-0.56392200	-1.34614100
C	4.32536500	-0.79494600	-0.41320400	C	3.67924200	-0.91922000	-1.61274500
H	4.93967100	-0.80764700	-1.30796800	H	3.95810300	-1.27337400	-2.60015400
C	4.84041700	-1.21499400	0.81657300	C	4.62953300	-0.80725500	-0.59481100
H	5.86663100	-1.56249200	0.88675900	H	5.66450100	-1.07631500	-0.78162900
C	4.02372300	-1.18695700	1.94742600	C	4.23000700	-0.35158500	0.66080900
H	4.39048700	-1.50545600	2.91705100	H	4.93715800	-0.25157500	1.47696000
C	2.71245600	-0.74394600	1.81571200	C	2.89303900	-0.02645200	0.86562100
H	2.02657600	-0.69806800	2.65455300	H	2.52041900	0.32726000	1.81964100
C	-1.27063500	1.13310600	-1.96783700	C	-2.33655800	0.01358900	-1.46536500
C	-2.35007200	1.51542500	-2.75504900	C	-3.68595700	-0.01242700	-1.79825600
H	-2.24392900	1.58155900	-3.83329100	H	-3.99488200	-0.30467300	-2.79690600
C	-3.56532000	1.81629600	-2.13385400	C	-4.62761200	0.34745400	-0.83116200
H	-4.42038700	2.12120700	-2.72947300	H	-5.68665300	0.33666000	-1.06944100
C	-3.66843100	1.70701200	-0.74788700	C	-4.19002300	0.71418100	0.44120100
H	-4.59939300	1.91870800	-0.23339900	H	-4.89075400	0.99763200	1.21893600
C	-2.55661300	1.30103900	-0.01542900	C	-2.82572600	0.70562800	0.71300100
H	-2.60130700	1.14424000	1.06038500	H	-2.41965100	0.97007400	1.68243800
C	-0.40624700	-2.17813400	-1.16935700	C	-0.35977800	-2.56912900	0.08496400
C	-1.06562800	-3.33825800	-1.56207000	C	-0.58639900	-3.85813800	0.56261500
H	-0.89472500	-3.75986200	-2.54778900	H	-0.68467700	-4.68582700	-0.13322000
C	-1.94096200	-3.95024800	-0.66238600	C	-0.68078100	-4.06443600	1.93741800
H	-2.46322000	-4.85966500	-0.94350900	H	-0.85638500	-5.06071400	2.33120000
C	-2.14391900	-3.37305100	0.59111100	C	-0.54550100	-2.97206100	2.79574700
H	-2.82673700	-3.81223400	1.31013200	H	-0.61083800	-3.08738200	3.87214100
C	-1.46728900	-2.20069900	0.91167700	C	-0.32507300	-1.71411300	2.25165500

H	-1.64107500	-1.67416700	1.84560500	H	-0.21576700	-0.82322200	2.85927600
C	2.36464100	0.19927600	-1.72533200	C	1.26084300	-0.56703400	-2.38046600
H	2.81443600	-0.21621900	-2.63409200	H	1.44514200	-1.29856100	-3.17491800
C	0.10850800	0.88315700	-2.53611400	C	-1.21944600	-0.27205100	-2.44145100
H	0.65426700	1.83195200	-2.54837500	H	-0.90693000	0.66653700	-2.91038400
H	0.05593900	0.52505800	-3.56995000	H	-1.53585200	-0.94996300	-3.24171900
C	0.63672400	-1.51472400	-2.03760000	C	-0.22008300	-2.28708900	-1.39221200
H	1.58086100	-2.05394700	-1.90417200	H	0.64308600	-2.83441400	-1.78479300
H	0.37690900	-1.59244100	-3.09852900	H	-1.09550700	-2.66488200	-1.93027000
N	0.88982300	-0.07061400	-1.68018100	N	-0.04452300	-0.82089200	-1.69312800
O	-0.13587300	0.43322000	1.86166700	H	1.20552800	0.42039200	-2.84916200
H	-1.91541100	0.35790200	3.32260800	N	0.29965100	1.98014700	-0.79902400
O	-2.74373600	0.01410800	2.95260300	C	0.47188100	3.10314900	-1.01613900
C	-3.73878400	-0.00305800	3.98795000	C	0.69913800	4.51806600	-1.25785500
H	-3.44359700	-0.65164700	4.82140800	H	1.56418700	4.66006300	-1.91334900
H	-4.65113600	-0.40137600	3.53963200	H	-0.18274500	4.97310100	-1.71975700
H	-3.94375200	1.00428900	4.37011500	H	0.89220600	4.99551300	-0.29137400
H	2.50734200	1.28331500	-1.74900500	H	0.12575200	3.04804300	3.89009600
N	1.11197300	2.39756500	0.19204200	C	0.05498500	3.72776500	3.03251100
C	1.35406100	3.47525300	0.54546900	O	0.70146700	3.23057800	1.89105800
C	1.65837600	4.82938500	0.98757900	H	0.57335100	4.66563500	3.29137300
H	2.70548700	5.06764700	0.77469600	H	-0.99432700	3.99095900	2.83290500
H	1.01528300	5.54656400	0.46740700	H	0.54882100	2.06843300	1.80870600
H	1.48609800	4.91210100	2.06580700	O	0.09253900	0.98700700	1.64251000

TS₁₂₋₁₃				TS₁₂₋₁₃			
Charge=2 Multiplicity =3				Charge=2 Multiplicity =5			
Fe	0.05772300	0.24181000	0.07255700	Fe	-0.07257900	-0.00272000	-0.02384400
N	1.88762700	-0.48702500	-0.18850200	N	0.05886700	-0.03624100	2.08420900
N	-1.85653800	0.73075700	-0.16092500	N	0.56686100	0.06342200	-2.03165800
N	-0.51131000	-1.44581600	0.92843100	N	-0.02721400	-2.00451000	0.05879900
C	2.13346800	-0.99162900	-1.42271800	C	1.31594000	0.03849900	2.58238300
C	3.34948900	-1.58942300	-1.73193100	C	1.57015500	-0.12633900	3.93852200
H	3.51998000	-1.99420600	-2.72452100	H	2.58230000	-0.06866200	4.31829000
C	4.34154500	-1.65244500	-0.75025300	C	0.49193800	-0.35907600	4.79984400
H	5.29987000	-2.11225900	-0.97078400	H	0.66319100	-0.48824200	5.86127200
C	4.08280500	-1.12137600	0.51254800	C	-0.80413400	-0.42610600	4.28027200
H	4.82702200	-1.14963800	1.30088200	H	-1.65441600	-0.60396800	4.92479200
C	2.83909900	-0.55016200	0.76156000	C	-0.98753600	-0.26745200	2.91079700
H	2.57826800	-0.12476100	1.72321800	H	-1.96052600	-0.32520800	2.44021700
C	-2.37074800	0.47053200	-1.38718400	C	1.88790600	0.32226500	-2.20350900
C	-3.71046600	0.70362000	-1.67529800	C	2.46733900	0.33782200	-3.46569500
H	-4.10207000	0.47999000	-2.66261400	H	3.52472700	0.53923500	-3.58162600

C	-4.53392000	1.23258400	-0.67841700	C	1.65669000	0.09093800	-4.57979500
H	-5.58283700	1.42487500	-0.88152800	H	2.08435900	0.09848000	-5.57463600
C	-3.99263000	1.50457400	0.57764700	C	0.29630500	-0.17214000	-4.39773800
H	-4.60010000	1.91413200	1.37731800	H	-0.35056200	-0.37080000	-5.24158900
C	-2.64669900	1.23504100	0.80432200	C	-0.21992000	-0.18253300	-3.10568100
H	-2.16639400	1.41547600	1.75904700	H	-1.26175800	-0.38737600	-2.89575400
C	-0.85851600	-2.45347300	0.10340200	C	1.19510400	-2.56353000	0.22149500
C	-1.29347200	-3.68288200	0.59358100	C	1.33514900	-3.93133700	0.43014300
H	-1.56728000	-4.47609900	-0.09544900	H	2.31799700	-4.36531700	0.56431800
C	-1.36808200	-3.87490400	1.97158700	C	0.19202900	-4.73446800	0.45364100
H	-1.70402000	-4.82506300	2.37507900	H	0.28160300	-5.80197300	0.61215300
C	-1.00437000	-2.82824600	2.82032700	C	-1.06381500	-4.14814500	0.26940600
H	-1.04655600	-2.93422900	3.89883400	H	-1.96544000	-4.74560100	0.27822000
C	-0.58186200	-1.62842100	2.26443100	C	-1.14239900	-2.77504700	0.08147500
H	-0.28841700	-0.77537500	2.86473100	H	-2.07174400	-2.23742800	-0.04942200
C	1.01621300	-0.78780000	-2.41921800	C	2.36794200	0.39484400	1.55774100
H	1.03072600	-1.54221800	-3.21339200	H	3.36201500	0.04332400	1.84874100
C	-1.36106700	-0.01756200	-2.39934900	C	2.62621500	0.62671500	-0.91999100
H	-0.88891700	0.84649600	-2.87785000	H	2.50787400	1.68602600	-0.67300800
H	-1.82662700	-0.61735000	-3.18900700	H	3.69325400	0.39546900	-0.99418800
C	-0.73922800	-2.19161400	-1.37886400	C	2.38307700	-1.64419800	0.07481000
H	-0.02563500	-2.89693700	-1.81699700	H	3.15892400	-1.87691900	0.80985300
H	-1.69976700	-2.37991900	-1.86928200	H	2.80710400	-1.78352500	-0.92602400
N	-0.29066600	-0.78658100	-1.68854000	N	1.97579800	-0.17271000	0.20084400
H	1.13428300	0.19121900	-2.89403700	H	2.39920000	1.48462700	1.45134200
N	0.61261000	1.89609700	-0.81628600	N	-0.06020300	2.03901200	0.06239200
C	1.00429600	2.96512700	-1.02160800	C	-0.49968500	3.11256100	0.10796300
C	1.51185700	4.30683700	-1.25270900	C	-1.08599600	4.43284600	0.17687000
H	2.30078900	4.29240300	-2.01136900	H	-0.78473700	4.94740000	1.09596100
H	0.70493300	4.96871800	-1.58274700	H	-0.79058700	5.03830600	-0.68712100
H	1.92240900	4.67427800	-0.30621400	H	-2.17272200	4.28850000	0.17337300
H	1.14493800	2.89820200	3.88155500	H	-4.50020500	0.98038000	-1.26480900
C	1.22293500	3.57621800	3.02179300	C	-4.09678400	1.98396900	-1.09631700
O	1.59383600	2.92252300	1.84335700	O	-3.06456500	2.00570700	-0.08388200
H	2.02871400	4.30049800	3.23493800	H	-4.91029200	2.62259300	-0.71364100
H	0.29807000	4.16149600	2.90514700	H	-3.75176500	2.43135100	-2.03770000
H	0.99332100	1.83690300	1.74282100	H	-2.40808100	0.80225300	-0.04075200
O	0.29098500	0.95706500	1.62472000	O	-1.78599700	-0.07337500	-0.20701700

13

Charge=2 Multiplicity =1

Fe 0.06968200 -0.32017100 0.28346800

13

Charge=2 Multiplicity =3

Fe 0.07113700 -0.31898500 0.28647800

N	-1.75808100	-0.67398400	-0.45728900	N	-1.75556800	-0.68796200	-0.44924000
N	2.03437000	-0.14657300	0.54057200	N	2.03492900	-0.13600700	0.54215000
N	0.01567300	1.52994100	-0.41668600	N	0.00964900	1.52524000	-0.42838700
C	-1.74968500	-1.39812100	-1.60595300	C	-1.74452300	-1.42118900	-1.59214100
C	-2.92391300	-1.73225700	-2.27014500	C	-2.91764600	-1.76709300	-2.25222900
H	-2.88245100	-2.30363800	-3.19213900	H	-2.87408800	-2.34551000	-3.16973000
C	-4.14632900	-1.32568000	-1.73100100	C	-4.14168200	-1.36323800	-1.71472800
H	-5.07661200	-1.57775700	-2.23044900	H	-5.07112800	-1.62447400	-2.21101700
C	-4.14914200	-0.58622200	-0.55029700	C	-4.14724500	-0.61477300	-0.53972300
H	-5.07485200	-0.24480200	-0.10014800	H	-5.07434700	-0.27530600	-0.09096700
C	-2.93637100	-0.27476900	0.05788100	C	-2.93552500	-0.29162700	0.06445000
H	-2.90225000	0.30957200	0.96987000	H	-2.90368300	0.30016100	0.97173100
C	2.78757000	-0.60459100	-0.48702900	C	2.78973200	-0.59820800	-0.48239200
C	4.17082500	-0.46506700	-0.49144800	C	4.17246000	-0.45350200	-0.48788000
H	4.75370100	-0.83279900	-1.33006700	H	4.75666800	-0.82470400	-1.32404100
C	4.79107400	0.14468000	0.60167900	C	4.79049000	0.16590800	0.60105900
H	5.87008300	0.26254200	0.62122600	H	5.86905100	0.28794800	0.61969700
C	4.00804300	0.59523700	1.66382400	C	4.00587300	0.62063900	1.66025900
H	4.45377700	1.06601300	2.53326800	H	4.44990900	1.09890800	2.52647500
C	2.62689900	0.43874000	1.59660400	C	2.62532100	0.45858700	1.59419000
H	1.95531700	0.76060300	2.38443400	H	1.95253300	0.78337500	2.37979800
C	0.32571400	1.67231100	-1.72303800	C	0.31985800	1.65834200	-1.73573900
C	0.42136500	2.92480100	-2.32529100	C	0.41297600	2.90634500	-2.34752000
H	0.67634700	3.00100900	-3.37788200	H	0.66824100	2.97506600	-3.40055700
C	0.18702900	4.06571400	-1.56173900	C	0.17549800	4.05254600	-1.59289000
H	0.25479300	5.05157600	-2.01095400	H	0.24127300	5.03508300	-2.04962300
C	-0.12655500	3.91579300	-0.21076200	C	-0.13884900	3.91224400	-0.24108600
H	-0.30832700	4.77460900	0.42596600	H	-0.32332000	4.77548800	0.38884000
C	-0.19379700	2.63779100	0.32658500	C	-0.20320700	2.63827200	0.30619900
H	-0.41063000	2.47914200	1.37392200	H	-0.42058700	2.48740700	1.35458700
C	-0.38034500	-1.83926500	-2.07074900	C	-0.37342500	-1.85943400	-2.05468800
H	-0.34869300	-1.99465900	-3.15520500	H	-0.34205300	-2.02347000	-3.13788000
C	2.01759500	-1.34701600	-1.55644100	C	2.02277700	-1.35133900	-1.54653200
H	1.95371200	-2.40299900	-1.27400200	H	1.96433500	-2.40577200	-1.25723600
H	2.51955700	-1.30157100	-2.52893200	H	2.52419700	-1.30988100	-2.51947800
C	0.52861800	0.40342700	-2.51285100	C	0.52399500	0.38375900	-2.51581200
H	-0.31520600	0.27547400	-3.19900800	H	-0.32243400	0.24747000	-3.19714400
H	1.42540500	0.48041300	-3.13598900	H	1.41785000	0.45820300	-3.14344200
N	0.62104500	-0.81577800	-1.63589400	N	0.62350500	-0.82772100	-1.62907300
O	-0.30754100	0.12100200	1.96617900	O	-0.30853600	0.13345400	1.96581800
O	-2.60008500	1.70482300	2.72473100	O	-2.60593000	1.73442400	2.70172700
C	-2.97930900	2.14655600	3.96865200	C	-2.99887400	2.20430100	3.93090500
H	-3.88216400	1.61921600	4.31821600	H	-3.88879400	1.66505100	4.29533300
H	-3.31052600	3.19866200	3.82782900	H	-3.35660100	3.24278000	3.75759900

H	-2.17494700	2.13017900	4.71480800	H	-2.19605500	2.23113400	4.67842600
H	-0.11947800	-2.78802800	-1.59300900	H	-0.10768700	-2.80303700	-1.56947200
N	0.21609000	-2.18562500	0.94132000	N	0.22588600	-2.17866300	0.95947000
C	0.23924500	-3.15636000	1.56928100	C	0.25453700	-3.14424200	1.59510000
C	0.26580200	-4.36977500	2.37377900	C	0.28787000	-4.35085500	2.40951500
H	-0.50803200	-5.06545100	2.03392300	H	-0.48163300	-5.05389500	2.07502000
H	1.24423100	-4.85435700	2.29549400	H	1.26920700	-4.83022900	2.33570400
H	0.07851200	-4.11254300	3.42176900	H	0.09846700	-4.08611300	3.45525700
H	-1.03168900	0.75602200	2.13620900	H	-1.03443400	0.76804800	2.12898400

13				TS₁₃₋₁₄			
	Charge=2 Multiplicity =5				Charge=2 Multiplicity =1		
Fe	0.10841400	0.20493200	0.11986500	N	-2.05113700	-0.34840200	0.38174900
N	1.82122800	-0.61806500	-0.57444400	N	1.85852800	-0.40861700	-0.32172900
N	-1.62952900	1.22376000	0.22869000	N	-0.12185700	1.56455200	-0.11241200
N	-0.94880200	-1.58537100	0.68563300	C	-2.66000900	-0.78157200	-0.74867600
C	1.81096800	-0.81487600	-1.92167000	C	-4.04121100	-0.74149700	-0.90069400
C	2.86892700	-1.43486200	-2.57534100	H	-4.49778700	-1.09019800	-1.82160000
H	2.83039000	-1.58497400	-3.64961600	C	-4.82202800	-0.24950100	0.14736500
C	3.97369800	-1.85703500	-1.83205300	H	-5.90283000	-0.21020800	0.05384800
H	4.81059100	-2.34303800	-2.32407200	C	-4.19136700	0.19702000	1.30781200
C	3.97982200	-1.65241500	-0.45373200	H	-4.75960300	0.59272800	2.14261800
H	4.81500800	-1.96870600	0.16144800	C	-2.80350100	0.14036800	1.38635400
C	2.88554700	-1.03387100	0.14187100	H	-2.25925900	0.48651500	2.25687500
H	2.85872500	-0.85973500	1.21036000	C	2.01210100	-0.96239100	-1.55306800
C	-2.37123600	1.18385200	-0.90307700	C	3.25314100	-1.05011800	-2.17011900
C	-3.65879200	1.70714700	-0.93939700	H	3.33802500	-1.48850900	-3.15957700
H	-4.24324800	1.66227400	-1.85296800	C	4.37824200	-0.56185300	-1.50093800
C	-4.17886500	2.29736800	0.21559700	H	5.35948500	-0.62349800	-1.96122300
H	-5.18181300	2.71318600	0.20931500	C	4.21299000	0.02589600	-0.24954400
C	-3.39975400	2.34457200	1.37200600	H	5.05258100	0.44377300	0.29528600
H	-3.77237400	2.79632300	2.28481900	C	2.93872900	0.09689500	0.30860900
C	-2.12516500	1.78832900	1.34398100	H	2.77769900	0.59983100	1.25811100
H	-1.46346700	1.76782600	2.20376000	C	-0.37679700	1.85870200	-1.40558700
C	-1.56654400	-2.19282900	-0.34453100	C	-0.52727700	3.17021100	-1.84667000
C	-2.49177900	-3.21381700	-0.14899200	H	-0.73704600	3.37087200	-2.89294600
H	-2.98190100	-3.68451300	-0.99561300	C	-0.39423600	4.21297700	-0.93128000
C	-2.76593600	-3.62435400	1.15764700	H	-0.50333800	5.24369400	-1.25389300
H	-3.48022600	-4.42146000	1.33981100	C	-0.11151700	3.90731200	0.39913200
C	-2.11647300	-2.99761300	2.22212400	H	0.01625900	4.68357200	1.14539200
H	-2.30668300	-3.29067100	3.24888500	C	0.01190600	2.57488300	0.77275000
C	-1.21951800	-1.97057200	1.94559000	H	0.24381600	2.30166000	1.79189500
H	-0.70235200	-1.42087200	2.72486400	C	-1.71738800	-1.34723700	-1.78019900

C	0.60584100	-0.26747900	-2.65166100	H	-2.12368000	-1.27684600	-2.79502500
H	0.42512900	-0.80096100	-3.59163600	C	0.73659800	-1.47178900	-2.17868300
C	-1.66551500	0.63916400	-2.12517700	H	0.55684900	-2.50724600	-1.87544900
H	-1.18215100	1.47517500	-2.64067100	H	0.78303100	-1.45417200	-3.27327200
H	-2.37116500	0.18856300	-2.83070000	C	-0.43577100	0.69708600	-2.36808600
C	-1.09675500	-1.76111200	-1.71301700	H	-1.33168200	0.76110200	-2.99345200
H	-0.26119200	-2.40884500	-1.99987200	H	0.42171700	0.75538500	-3.04630900
H	-1.87634900	-1.89315900	-2.47030800	N	-0.40198300	-0.64131700	-1.67095800
N	-0.58883300	-0.33998800	-1.74702000	H	-1.54501900	-2.40778100	-1.57056500
O	0.53123800	0.65839600	1.78111500	N	0.02846200	-2.28829600	0.70906600
O	3.06663900	0.28097300	3.09152500	C	0.11257600	-3.38911300	1.06122800
C	3.47584800	0.80750700	4.29159300	C	0.21929600	-4.77397200	1.50166400
H	4.57302400	0.89412800	4.33803900	H	-0.62333700	-5.02557900	2.15423700
H	3.21827700	0.04038200	5.05487700	H	0.21061200	-5.44488500	0.63618200
H	2.97098100	1.74325800	4.56422100	H	1.15465400	-4.91854700	2.05261900
H	0.78115600	0.78474700	-2.89023600	Fe	-0.04219800	-0.36071600	0.30637700
N	0.94282300	2.25839900	-0.84056300	O	0.04130400	-0.07009500	2.15057700
C	1.40222600	3.32350300	-0.85611800	H	-0.06807000	-0.90531100	2.63957400
C	1.97684300	4.66306900	-0.87944500	H	1.00082600	0.49979700	2.97391700
H	3.03851100	4.61128800	-1.14080100	C	1.90774300	1.05069400	3.71795300
H	1.45817300	5.28097600	-1.61939100	O	2.37088400	1.89593000	2.85175500
H	1.87452800	5.12840700	0.10616300	H	2.53744300	0.18021100	3.98722200
H	1.44812400	0.57403000	2.11844400	H	1.30089000	1.44212000	4.55513000

TS₁₃₋₁₄				TS₁₃₋₁₄			
Charge=2 Multiplicity =3				Charge=2 Multiplicity =5			
N	2.13131000	-0.14363700	0.36854800	N	0.03603400	-0.04381500	-0.03260300
N	-1.65498700	0.84421800	-0.33868300	N	-0.00866900	-0.03626500	4.14286400
N	-0.35562100	-1.53324900	-0.08956500	N	2.20404200	0.05194900	2.30947400
C	2.82691300	0.13592400	-0.76183400	C	-0.31058000	-1.31169800	-0.35637400
C	4.17213000	-0.19243200	-0.88663400	C	-0.35435000	-1.74036100	-1.67869700
H	4.70368600	0.03398300	-1.80560600	H	-0.62714100	-2.76437800	-1.91384200
C	4.82069800	-0.81569100	0.18215600	C	-0.03989600	-0.83133300	-2.69247700
H	5.87105200	-1.07923400	0.10616500	H	-0.06740300	-1.14279700	-3.73217900
C	4.09757600	-1.10467600	1.33874600	C	0.31961200	0.47326100	-2.35294500
H	4.56097000	-1.59655900	2.18704500	H	0.57799000	1.20328400	-3.11226900
C	2.75079300	-0.76052700	1.39292800	C	0.35112500	0.82884400	-1.00854800
H	2.13707100	-0.97249600	2.26095900	H	0.63280300	1.82501600	-0.68378200
C	-1.70279700	1.24471300	-1.63395400	C	-0.16534100	-1.34227000	4.45550300
C	-2.90753300	1.54629900	-2.25709500	C	-0.07952000	-1.79583800	5.76710700
H	-2.91865500	1.85634800	-3.29734900	H	-0.20322800	-2.85058600	5.99205800
C	-4.09348500	1.44317200	-1.52526800	C	0.16643700	-0.86966800	6.78433300
H	-5.04563800	1.67693500	-1.99143700	H	0.23525500	-1.19885200	7.81666200

C	-4.03495100	1.01995800	-0.19943400	C	0.33727500	0.47429600	6.45510900
H	-4.93188300	0.90619200	0.39961100	H	0.54641700	1.22013600	7.21420100
C	-2.79742900	0.71758600	0.36360200	C	0.25317100	0.85442200	5.11839700
H	-2.72135700	0.33453300	1.37852400	H	0.42970100	1.88166100	4.81149800
C	-0.19585900	-1.94380400	-1.36729900	C	2.57159000	-1.24827500	2.32907300
C	-0.58146900	-3.21437300	-1.78459800	C	3.85910700	-1.64545400	2.67798000
H	-0.44053300	-3.50970900	-2.81998100	H	4.12248300	-2.69865700	2.68922900
C	-1.14963200	-4.09114300	-0.86211800	C	4.80142300	-0.66982000	3.00686900
H	-1.45629000	-5.08672200	-1.16741000	H	5.81286200	-0.95544300	3.27915800
C	-1.33087700	-3.65773500	0.44988800	C	4.41867900	0.67050600	2.99383400
H	-1.79154000	-4.29059300	1.20031500	H	5.11204200	1.46096000	3.25928900
C	-0.92827100	-2.37439200	0.79853100	C	3.10948500	0.99007400	2.64959400
H	-1.11021600	-1.99319500	1.79354400	H	2.76333200	2.01593400	2.68692300
C	2.03317600	0.84471000	-1.83759300	C	-0.67686200	-2.18853600	0.82049500
H	2.45039800	0.66098800	-2.83438700	H	-0.52777500	-3.25095400	0.59374300
C	-0.36090800	1.38537300	-2.31915000	C	-0.51047300	-2.24775500	3.29366100
H	0.03631600	2.38873300	-2.13330500	H	-1.59559100	-2.22645200	3.14615100
H	-0.45129000	1.26988300	-3.40516200	H	-0.23424300	-3.28777000	3.50069600
C	0.44438100	-0.97146500	-2.32999100	C	1.54085000	-2.25202100	1.86642600
H	1.43204500	-1.34934600	-2.61424800	H	1.70844500	-2.44235900	0.80072200
H	-0.14143500	-0.91305700	-3.25345600	H	1.66877000	-3.21072100	2.38061000
N	0.60966400	0.40277500	-1.74820100	N	0.12088700	-1.77626500	2.01848500
H	2.06432100	1.92490100	-1.66523500	H	-1.73567300	-2.04903300	1.05941800
N	0.65939100	2.22498000	0.62004000	N	-2.09957500	0.54740600	2.02446800
C	0.85169600	3.33106600	0.90583500	C	-3.23283200	0.78705600	2.08720200
C	1.09295200	4.72101500	1.26901700	C	-4.65644600	1.08705100	2.16607000
H	2.04820600	4.81014900	1.79690800	H	-4.97945100	1.60606200	1.25762800
H	1.12337100	5.34442900	0.36919600	H	-5.22965600	0.15991100	2.26932100
H	0.28855000	5.07877900	1.92055700	H	-4.85433200	1.72625900	3.03284900
Fe	0.18262100	0.33634100	0.29577600	Fe	0.11617700	0.33134800	2.04541800
O	-0.13216700	0.21803500	2.17175700	O	0.16563900	2.19386900	1.98619500
H	0.34632600	0.92508700	2.64142000	H	-0.71198300	2.55612700	1.76327000
H	-0.93969800	-0.20392800	3.13697100	H	0.80764600	3.42589300	2.47684400
C	-1.90756200	-0.58323400	3.97115600	C	1.31096600	4.36253100	3.12436200
O	-2.69782300	-1.05461800	3.06486900	O	1.89811500	3.64789200	4.04645600
H	-2.16942900	0.37745400	4.45368300	H	0.43164700	4.95970200	3.42701500
H	-1.37811200	-1.29342100	4.63319700	H	1.95538200	4.85690900	2.37472800

14				14			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
N	-1.81841700	-0.52778000	-0.46164100	N	-2.07332500	-0.32141000	0.12686600
N	2.00744300	-0.25138600	0.59566000	N	1.97817100	-0.59715500	0.25654000
N	0.16115700	1.52581800	-0.39996200	N	0.12120100	1.12350600	-1.02373800

C	-1.84395700	-1.23633200	-1.62016100	C	-2.46488800	-1.34652200	-0.66432300
C	-3.01734900	-1.44901700	-2.33503500	C	-3.79596100	-1.51195200	-1.03888300
H	-2.99396200	-2.01249800	-3.26263800	H	-4.07785400	-2.33912200	-1.68306300
C	-4.21572300	-0.92942100	-1.84238300	C	-4.75300100	-0.60836400	-0.57538500
H	-5.14524400	-1.08497800	-2.38095000	H	-5.79573500	-0.72131800	-0.85539700
C	-4.19092100	-0.19970900	-0.65616600	C	-4.34587900	0.44222400	0.24592800
H	-5.09521500	0.23159200	-0.24074600	H	-5.05467400	1.16969300	0.62636500
C	-2.97598900	-0.01598800	-0.00155000	C	-2.99751300	0.55200200	0.56877700
H	-2.92495300	0.56287200	0.91343100	H	-2.63059300	1.35549600	1.19931100
C	2.72700600	-0.79870600	-0.41491400	C	2.27896800	-1.64374000	-0.54573300
C	4.11629800	-0.74340500	-0.44705500	C	3.59708700	-1.97011100	-0.85511900
H	4.65993700	-1.18495000	-1.27646100	H	3.80679900	-2.81069800	-1.50936700
C	4.79375800	-0.11748200	0.60100500	C	4.63404800	-1.21011300	-0.31290000
H	5.87796600	-0.06479600	0.59997500	H	5.66787900	-1.44997900	-0.54119900
C	4.05394800	0.44285900	1.64094400	C	4.31913100	-0.13776200	0.52090500
H	4.53893300	0.94353400	2.47195500	H	5.09260700	0.48093100	0.96280900
C	2.66529000	0.36322700	1.59613700	C	2.97994200	0.13753300	0.77539000
H	2.04590800	0.80195900	2.37055300	H	2.68339800	0.96543100	1.41143700
C	0.51943100	1.63639700	-1.69650900	C	0.13880600	0.64232200	-2.28732100
C	0.74025700	2.87037100	-2.30518100	C	0.28488300	1.48158300	-3.39204600
H	1.03202700	2.91544000	-3.35005300	H	0.29667400	1.05531000	-4.39086500
C	0.57898600	4.03452500	-1.55822500	C	0.41141200	2.85385600	-3.20381600
H	0.74317000	5.00716000	-2.01120200	H	0.52509100	3.51959800	-4.05363200
C	0.20773300	3.92297400	-0.21795900	C	0.38846500	3.35057400	-1.90080100
H	0.07496500	4.80037000	0.40557300	H	0.48204100	4.41140200	-1.69640800
C	0.01687800	2.65778000	0.32106000	C	0.24500700	2.45905100	-0.84757000
H	-0.25059200	2.53251800	1.36285300	H	0.22779800	2.82345900	0.17073300
C	-0.50593000	-1.79534800	-2.04940800	C	-1.38111600	-2.32947200	-1.07228900
H	-0.46216900	-1.95554400	-3.13321800	H	-1.68191600	-2.87740700	-1.97533000
C	1.90295700	-1.52154700	-1.45672400	C	1.10542300	-2.47655100	-1.03210300
H	1.73429300	-2.55098400	-1.12444500	H	0.86193300	-3.21673800	-0.26162200
H	2.42099000	-1.57233600	-2.42121000	H	1.38275400	-3.03653300	-1.93522100
C	0.62244300	0.34687500	-2.47268000	C	-0.02785500	-0.85022100	-2.49944000
H	-0.21049700	0.29596200	-3.18165200	H	-0.94512100	-1.01776300	-3.07637500
H	1.53908900	0.32863200	-3.07139400	H	0.79215100	-1.21649400	-3.12887800
N	0.56597000	-0.86553900	-1.58200700	N	-0.08894900	-1.63398300	-1.24293600
H	-0.34102800	-2.76391500	-1.56859700	H	-1.26134600	-3.07092000	-0.27452600
N	-0.02717600	-2.12950300	0.98228100	N	-0.17102100	-1.45615600	1.90238000
C	-0.07446300	-3.17432900	1.48632800	C	-0.24557000	-2.20231300	2.78770200
C	-0.13481700	-4.49246900	2.10790300	C	-0.34023300	-3.14476100	3.89613500
H	-1.09684400	-4.62807100	2.61291600	H	-1.26171000	-2.97048400	4.46130900
H	-0.02601600	-5.27195000	1.34641600	H	-0.34919700	-4.17189100	3.51654800
H	0.67121800	-4.60258700	2.84074200	H	0.51727700	-3.02544800	4.56648700
Fe	0.03971400	-0.33273400	0.27659900	Fe	-0.03589600	-0.17704800	0.47195000

O	-0.38405400	0.27576500	2.20110100	O	0.00193700	1.27746800	2.12970100
H	-0.29236400	-0.44869800	2.84048200	H	-0.06343400	0.89325300	3.01691000
H	-1.18938300	0.77808800	2.48363700	H	0.06075700	2.25662200	2.25324300
C	-3.01230800	2.27903100	3.93520300	C	0.20215600	4.95587200	2.98748500
O	-2.61602100	1.69127800	2.94304400	O	0.18194700	4.01311400	2.21624100
H	-4.00524500	2.75511800	3.95152700	H	0.29626400	5.98926500	2.61741500
H	-2.40096800	2.35981800	4.84966400	H	0.12795500	4.82048600	4.07976300

14				15			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
N	-1.57139800	-1.30814700	0.42517300	Fe	0.01633200	-0.44541700	-0.57717500
N	2.23591400	0.45099400	-0.19160200	N	1.97017500	-0.33826000	-0.26743900
N	-0.81582400	1.28446000	-0.83348900	N	-1.94740900	-0.64031000	-0.32385000
C	-1.66929200	-2.15594100	-0.62060200	N	-0.14134600	1.49653300	-0.37667700
C	-2.84845100	-2.84475500	-0.89679600	C	2.37346100	-0.61246100	0.99961500
H	-2.90084200	-3.51538800	-1.74887100	C	-2.34479100	-0.91935300	0.94541600
C	-3.95151400	-2.66448000	-0.06120200	C	-0.19665300	1.98615400	0.87923200
H	-4.87925300	-3.19331400	-0.25724900	C	1.27678000	-1.07777500	1.93256800
C	-3.84509200	-1.79445500	1.02383900	H	1.52043900	-0.87013600	2.98036400
H	-4.67860000	-1.62601000	1.69704700	C	-1.22296800	-1.21117000	1.91959500
C	-2.63893000	-1.13212000	1.22517100	H	-0.96809500	-2.27449300	1.86688400
H	-2.50818500	-0.43467100	2.04736600	H	-1.52166700	-1.00120500	2.95244300
C	2.73209600	-0.29508500	-1.20367800	C	-0.08248400	0.99055700	2.00986700
C	3.96737400	-0.01392700	-1.78262600	H	-0.93253800	1.10264900	2.69078800
H	4.33685000	-0.62414800	-2.60095200	N	-0.00985000	-0.43145400	1.52747100
C	4.71725000	1.05797500	-1.29573700	O	0.03257600	-0.38823700	-2.19380800
H	5.68280000	1.29388100	-1.73257400	H	1.15328600	-2.16038600	1.83193200
C	4.20487000	1.82403600	-0.24885900	H	-0.77738000	-2.79312500	-0.84945600
H	4.75320900	2.66833600	0.15455900	O	0.10145800	-2.47867700	-0.57446200
C	2.95904700	1.48792300	0.27024200	C	1.08311300	-3.19340500	-1.40007000
H	2.51395400	2.05684100	1.08111600	H	2.06243700	-2.98036100	-0.97752800
C	-0.92950400	0.86508600	-2.11103600	H	0.87252900	-4.26176300	-1.32981900
C	-1.79165300	1.48140100	-3.01751100	C	-2.87055400	-0.43275600	-1.28590100
H	-1.86450500	1.11238800	-4.03604800	C	-3.69246400	-0.99054700	1.27887600
C	-2.54475800	2.57827100	-2.60281000	C	-4.23304000	-0.50413800	-1.01816100
H	-3.21978600	3.07401200	-3.29374700	H	-2.48281200	-0.21270300	-2.27458900
C	-2.41229400	3.02608200	-1.28888800	C	-4.65098500	-0.78314400	0.28326000
H	-2.97233600	3.88018900	-0.92397200	H	-3.98845900	-1.20989200	2.29990100
C	-1.54524000	2.34805900	-0.43970400	H	-4.94660300	-0.33829200	-1.81797600
H	-1.42282700	2.66828700	0.58958800	H	-5.70825400	-0.83681900	0.52402100
C	-0.40012600	-2.38533300	-1.41975400	H	-0.16581700	1.88023000	-2.40824200
H	-0.64105800	-2.77867100	-2.41627900	C	-0.21582500	2.34224600	-1.42958200
C	1.88783700	-1.48052000	-1.63288800	C	-0.34849600	3.71242400	-1.25727000

H	2.10871900	-2.32592200	-0.97176300	C	-0.41015000	4.22840700	0.03865400
H	2.15338900	-1.79208500	-2.65213200	H	-0.40350700	4.35773700	-2.12721300
C	0.00307700	-0.23770900	-2.57451200	C	-0.33363200	3.35175500	1.11878800
H	-0.45060100	-0.79238200	-3.40528700	H	-0.51585000	5.29582600	0.20572100
H	0.89738100	0.24855300	-2.98123000	H	-0.37691000	3.71951000	2.13949500
N	0.44362700	-1.16994200	-1.50197500	H	4.01200100	-0.74002000	2.38517800
H	0.18202800	-3.16051200	-0.90813700	C	3.71143700	-0.51995700	1.36565100
N	1.16905000	-1.61635200	1.83025000	C	4.65449500	-0.14722900	0.40420500
C	1.64189700	-2.42250400	2.51769600	C	4.22961100	0.13013900	-0.89518200
C	2.23544300	-3.43545600	3.38211800	H	5.70441500	-0.07197000	0.66994200
H	1.48295800	-3.82035300	4.07794700	C	2.87564900	0.02999400	-1.19569800
H	2.61865100	-4.26552200	2.77991600	H	4.93073300	0.42324500	-1.66904400
H	3.06188300	-3.00189900	3.95442500	H	2.48407100	0.23159100	-2.18650300
Fe	0.24411200	-0.10443000	0.47620100	H	0.81368000	1.21412200	2.59818800
O	0.03525500	0.94478700	2.31531900	H	1.02138000	-2.84158900	-2.43148800
H	0.37451400	0.52558900	3.12064600				
H	-0.35306900	1.81672000	2.57805300				
C	-1.30085100	4.15654800	3.74184000				
O	-1.15157900	3.34951000	2.84129300				
H	-1.88381200	5.07795900	3.58587300				
H	-0.86448100	4.00325500	4.74326900				

15				15			
Charge=2 Multiplicity =3				Charge=2 Multiplicity =5			
Fe	0.01192800	-0.44490900	-0.57790900	Fe	0.08577400	-0.00117600	0.40961100
N	1.96765200	-0.35183600	-0.26845600	N	-0.60114000	1.79476600	-0.21494400
N	-1.95308300	-0.62561700	-0.32208600	N	-0.91043800	-1.58434300	-0.35622600
N	-0.12548600	1.49926700	-0.37747500	N	2.02052400	-0.16822700	0.96896100
C	2.36814500	-0.62523000	0.99985800	C	-0.40884200	2.05353100	-1.53532500
C	-2.35211000	-0.90502400	0.94668100	C	-0.37357000	-2.09190100	-1.49873600
C	-0.17794400	1.98951200	0.87829500	C	2.93136900	0.02194400	-0.02184200
C	1.26849000	-1.08320100	1.93328000	C	0.12392200	0.89356200	-2.34909300
H	1.51477800	-0.87760200	2.98092100	H	0.69924900	1.23315000	-3.21771200
C	-1.23229900	-1.20160500	1.92212000	C	0.90924100	-1.43331300	-1.95540500
H	-0.98389100	-2.26660400	1.87159400	H	1.02954500	-1.48731500	-3.04359500
H	-1.53041500	-0.98806100	2.95439100	H	1.76634800	-1.95026400	-1.50792300
C	-0.07962600	0.99344500	2.01013000	C	2.35347700	0.48638300	-1.33969700
H	-0.93486900	1.11220900	2.68340300	H	2.96841000	0.17199600	-2.19077300
N	-0.01448300	-0.42944700	1.52983500	N	0.94912400	-0.01064200	-1.48592000
O	0.02575000	-0.38938800	-2.19278900	O	-0.52782700	0.00435300	1.89677400
H	1.13825800	-2.16502500	1.83255700	H	-0.72123600	0.30707200	-2.72750800
H	-0.80302900	-2.78790700	-0.83839200	H	-4.61522000	-0.09804500	1.65495200
O	0.08037400	-2.47966100	-0.57108500	O	-3.68813600	-0.12222600	1.94004800

C	1.04976200	-3.20538900	-1.40155700	C	-3.67843000	-0.00025100	3.37053900
H	2.03460300	-2.99125800	-0.99282500	H	-2.63084700	-0.02249900	3.67656800
H	0.83653000	-4.27229500	-1.31809400	H	-4.12457100	0.94707000	3.69761400
C	-2.87452500	-0.41492400	-1.28495100	C	-2.03743100	-2.11982100	0.16515700
C	-3.70034800	-0.97352000	1.27852600	C	-0.95441500	-3.17023500	-2.14997100
C	-4.23747700	-0.48349900	-1.01870600	C	-2.65445100	-3.21086700	-0.43892900
H	-2.48457600	-0.19570400	-2.27295400	H	-2.45390600	-1.62501700	1.04106500
C	-4.65729400	-0.76298300	0.28204400	C	-2.10672400	-3.74600200	-1.60396300
H	-3.99799600	-1.19333300	2.29898700	H	-0.51609800	-3.55870900	-3.06383200
H	-4.94987500	-0.31529900	-1.81904800	H	-3.55537100	-3.62467500	0.00072700
H	-5.71491700	-0.81479600	0.52167800	H	-2.57340000	-4.59523900	-2.09382100
H	-0.14345200	1.88212100	-2.40944200	H	1.64969600	-0.62821400	2.95248800
C	-0.19082800	2.34485800	-1.43108300	C	2.43193100	-0.50061800	2.21229900
C	-0.31134800	3.71625800	-1.25913100	C	3.77884200	-0.66356200	2.51069000
C	-0.36948200	4.23335200	0.03650800	C	4.72034200	-0.48325000	1.49622600
H	-0.35971100	4.36163400	-2.12941900	H	4.07796100	-0.92942400	3.51864800
C	-0.30180100	3.35652900	1.11707800	C	4.29075800	-0.13732500	0.21105000
H	-0.46565700	5.30176600	0.20297900	H	5.77933500	-0.61026700	1.69936700
H	-0.34266100	3.72490000	2.13766300	H	5.00428000	0.01244700	-0.59301400
H	4.00498800	-0.75758800	2.38690000	H	-0.59602600	3.47324700	-3.13991700
C	3.70627300	-0.53872600	1.36656900	C	-0.76299000	3.27819700	-2.08530100
C	4.65203000	-0.17336000	0.40492500	C	-1.34535900	4.24601800	-1.26037000
C	4.22981000	0.10300700	-0.89546700	C	-1.55740900	3.96266200	0.08958300
H	5.70209200	-0.10290900	0.67140500	H	-1.63030900	5.20963600	-1.67160500
C	2.87553600	0.00906800	-1.19694500	C	-1.17021900	2.72308600	0.58349200
H	4.93313500	0.39047600	-1.66943200	H	-2.01209400	4.68888500	0.75434800
H	2.48546600	0.21023700	-2.18844300	H	-1.30628900	2.43719400	1.62034400
H	0.81312500	1.21067400	2.60600900	H	2.31976800	1.58230500	-1.35057900
H	0.97696800	-2.86358500	-2.43560200	H	-4.20838700	-0.83010000	3.85417100

TS₁₅₋₁₆				TS₁₅₋₁₆			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
Fe	0.06801000	-0.48055200	-0.47438200	Fe	0.06726100	-0.48477600	-0.47692100
N	2.02540100	-0.32229800	-0.19526000	N	2.02368800	-0.31440800	-0.19826600
N	-1.88364200	-0.74977500	-0.20345800	N	-1.88538400	-0.74723000	-0.20898400
N	-0.20324600	1.45030000	-0.44903400	N	-0.20596100	1.44764700	-0.44771800
C	2.44406300	-0.54354200	1.07631500	C	2.44256900	-0.54523300	1.07176300
C	-2.27782500	-0.89603000	1.08733600	C	-2.27922500	-0.90071100	1.08112000
C	-0.27263200	2.02636200	0.76941200	C	-0.27259800	2.01905300	0.77327700
C	1.34768400	-0.96468700	2.02620600	C	1.34740300	-0.97439800	2.01985900
H	1.58330300	-0.71195900	3.06602200	H	1.58280800	-0.72602400	3.06076700
C	-1.14650300	-1.04871100	2.07888000	C	-1.14717600	-1.06408600	2.07014100
H	-0.88899900	-2.11016400	2.17214900	H	-0.88906800	-2.12635200	2.15291200

H	-1.43335400	-0.70631400	3.07880900	H	-1.43280500	-0.73175800	3.07391600
C	0.04232800	1.13722500	1.94978200	C	0.03806600	1.12504300	1.95134900
H	-0.67015900	1.30439500	2.76373700	H	-0.67761300	1.28862000	2.76322500
N	0.06653900	-0.32485900	1.58126200	N	0.06480000	-0.33562500	1.57807000
O	0.09770200	-0.54996400	-2.21788700	O	0.09491800	-0.55783000	-2.21076400
H	1.21837300	-2.05033300	1.96906500	H	1.22052000	-2.06002400	1.95810600
H	-0.54925500	-2.99778700	-0.50152800	H	-0.54411200	-2.99651600	-0.50423600
O	0.30471600	-2.54357000	-0.60937500	O	0.30974000	-2.54150800	-0.61190500
C	0.79767400	-2.82931100	-1.92196200	C	0.81361200	-2.84610600	-1.91335600
H	1.88485600	-2.85066700	-1.92012700	H	1.90054100	-2.84890000	-1.91005700
H	0.30526100	-3.67800600	-2.39300800	H	0.32735400	-3.70083600	-2.37864000
H	0.44615600	-1.66161300	-2.49614000	H	0.43937700	-1.63457200	-2.49480200
C	-2.81059000	-0.67627200	-1.18160900	C	-2.81316700	-0.66190700	-1.18513700
C	-3.62261100	-0.97195000	1.43024000	C	-3.62398400	-0.97217800	1.42518500
C	-4.17099700	-0.76081300	-0.90627200	C	-4.17370100	-0.74083200	-0.90900500
H	-2.42520200	-0.54664800	-2.18703100	H	-2.42852800	-0.52736200	-2.19018800
C	-4.58408600	-0.90640600	0.41836600	C	-4.58628300	-0.89416800	0.41493500
H	-3.91426200	-1.08503500	2.46967900	H	-3.91487500	-1.09106000	2.46417300
H	-4.88760500	-0.70469800	-1.71848700	H	-4.89084500	-0.67489000	-1.72001000
H	-5.63985700	-0.96517600	0.66436600	H	-5.64210300	-0.94918000	0.66156900
H	-0.32831000	1.67194600	-2.49964800	H	-0.33277500	1.68038900	-2.49748800
C	-0.39904300	2.19963200	-1.55499600	C	-0.39997600	2.20323000	-1.55021600
C	-0.67155700	3.55936200	-1.47777300	C	-0.66756600	3.56357800	-1.46622400
C	-0.75648200	4.16048400	-0.22097300	C	-0.74919700	4.15945400	-0.20682000
H	-0.81849000	4.12934300	-2.38866300	H	-0.81331100	4.13822900	-2.37437100
C	-0.55482600	3.38149100	0.91804000	C	-0.54956900	3.37459700	0.92824400
H	-0.97536000	5.21965900	-0.12762800	H	-0.96415100	5.21897300	-0.10843000
H	-0.60900100	3.82016700	1.90969700	H	-0.60168300	3.80883700	1.92199300
H	4.09242400	-0.60012700	2.45540300	H	4.09111200	-0.61008200	2.45027800
C	3.78217500	-0.42292900	1.43048200	C	3.78042500	-0.42469400	1.42693600
C	4.71315000	-0.07411500	0.44823700	C	4.71076200	-0.06550000	0.44790100
C	4.27386400	0.15576900	-0.85538500	C	4.27111800	0.17560400	-0.85358700
H	5.76415100	0.02296600	0.70219200	H	5.76159500	0.03100700	0.70276100
C	2.91854100	0.02907400	-1.14164800	C	2.91612400	0.04824900	-1.14093300
H	4.96480000	0.43453000	-1.64357800	H	4.96151500	0.46308300	-1.63909900
H	2.51435000	0.19847700	-2.13338100	H	2.51184100	0.22577500	-2.13119800
H	1.02925700	1.40829200	2.33948500	H	1.02334900	1.39484400	2.34582500

TS₁₅₋₁₆				16			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
Fe	-0.08130700	0.00081000	0.43177100	Fe	0.07835900	-0.44195400	-0.53322300
N	0.77761800	1.88993500	0.31997900	N	2.02800500	-0.23196600	-0.25598000
N	-1.69385600	-0.38570200	-0.83298500	N	-1.86677600	-0.78201900	-0.28400200

N	1.26260400	-1.54174100	0.72036900	N	-0.27682600	1.46962500	-0.38033800
C	1.27672100	2.27269300	-0.88148500	C	2.46158200	-0.51079300	1.00026700
C	-1.40217500	-0.69832500	-2.12057600	C	-2.24741800	-1.02427100	0.99644000
C	2.20177200	-1.73145300	-0.24023900	C	-0.36053500	1.96570300	0.87189900
C	1.01312200	1.32891400	-2.03696700	C	1.38649000	-1.02841000	1.92817600
H	1.77526800	1.43731600	-2.81879400	H	1.61751600	-0.82328000	2.97934100
C	0.06415900	-0.91494200	-2.43388700	C	-1.10337800	-1.21791900	1.96637700
H	0.27349200	-0.73105600	-3.49504000	H	-0.80790500	-2.27289500	1.96876500
H	0.31476000	-1.96434800	-2.23635700	H	-1.39217800	-0.96645100	2.99233900
C	2.26000300	-0.68079000	-1.33037100	C	-0.00122800	1.01637700	1.98967900
H	2.67498300	-1.09536900	-2.25741600	H	-0.71373800	1.09781200	2.81657600
N	0.92159200	-0.07520500	-1.55763900	N	0.08094600	-0.41444300	1.52131300
O	-0.82853700	0.06165400	1.94755400	O	0.06490800	-0.34693700	-2.31033600
H	0.04961800	1.58870700	-2.49208400	H	1.29668200	-2.11315400	1.81488300
H	-4.08879800	-0.86819800	3.28332100	H	-0.54385500	-2.93210700	-0.78019700
O	-3.88055500	0.02509100	2.95995900	O	0.32062700	-2.50532100	-0.64301700
C	-2.76801500	0.51877200	3.60285300	C	1.26489900	-3.11515000	-1.47988600
H	-2.79763400	1.61164400	3.60400200	H	2.27557800	-2.78169400	-1.29429200
H	-2.56911200	0.08568700	4.58883900	H	1.03426100	-4.12444100	-1.79862900
H	-1.77914800	0.26882700	2.91922500	H	0.46559200	-1.11052200	-2.76564900
C	-2.98432600	-0.26239400	-0.45081500	C	-2.80111200	-0.66083700	-1.24958000
C	-2.40489800	-0.87447700	-3.06707400	C	-3.58748000	-1.15227000	1.34181000
C	-4.03278600	-0.43516200	-1.34611100	C	-4.15760500	-0.79298600	-0.97202400
H	-3.15970400	-0.02745500	0.59436200	H	-2.42250000	-0.45145700	-2.24413800
C	-3.73935400	-0.74164200	-2.67517400	C	-4.55748500	-1.03818100	0.34187600
H	-2.14799500	-1.11744500	-4.09335600	H	-3.86923700	-1.34199400	2.37274900
H	-5.05609600	-0.32591200	-1.00397300	H	-4.88168600	-0.69571500	-1.77366500
H	-4.53646800	-0.87550000	-3.40013000	H	-5.61000400	-1.13577000	0.58950300
H	0.43594500	-2.16653300	2.50984200	H	-0.42795700	1.80766400	-2.40934100
C	1.20333400	-2.38433000	1.77589600	C	-0.51127700	2.27738800	-1.43653700
C	2.07617900	-3.45594600	1.90829600	C	-0.83756800	3.61762800	-1.27087100
C	3.03541200	-3.66598600	0.91639400	C	-0.93618800	4.13604300	0.02089100
H	2.00109300	-4.11080600	2.76944500	H	-1.01480100	4.23688500	-2.14341600
C	3.09711000	-2.79308500	-0.17236000	C	-0.69521000	3.29602600	1.10773400
H	3.72810000	-4.49908000	0.98685400	H	-1.19607600	5.17772600	0.18162800
H	3.83592200	-2.93241400	-0.95533200	H	-0.75923900	3.66852600	2.12552600
H	2.33069700	3.77353000	-2.00480400	H	4.11798300	-0.58113600	2.36920700
C	1.93230600	3.48906100	-1.03596600	C	3.79540800	-0.35547600	1.35767900
C	2.06286600	4.33504400	0.06801900	C	4.70600700	0.09237500	0.39642000
C	1.53938500	3.93859300	1.29968400	C	4.25067900	0.38552800	-0.88912800
H	2.57030400	5.28948000	-0.03388100	H	5.75325000	0.21807100	0.65340100
C	0.90456900	2.70668000	1.38890200	C	2.90061000	0.21921900	-1.17932700
H	1.62372000	4.56851300	2.17842100	H	4.92506600	0.74385900	-1.65928400
H	0.48215900	2.33806200	2.31673500	H	2.48253900	0.43913400	-2.15516500

H	2.93762600	0.11898400	-1.00820700	H	0.97650800	1.30147000	2.39217000
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16				16			
Charge=2 Multiplicity =3				Charge=2 Multiplicity =5			
Fe	0.07290700	-0.44583600	-0.53135700	Fe	-0.08436500	0.01423300	0.47316900
N	2.02327200	-0.24957500	-0.25075000	N	0.56594900	1.97793000	0.16465200
N	-1.87479000	-0.76810100	-0.28155700	N	-1.57448400	-0.69212400	-0.82183800
N	-0.25904800	1.47058000	-0.38319900	N	1.44496900	-1.32731000	0.90865300
C	2.45343200	-0.52556400	1.00718200	C	1.05128100	2.29912000	-1.05929200
C	-2.25797000	-1.01034100	0.99826500	C	-1.19238000	-1.09361100	-2.05964800
C	-0.34074200	1.97020400	0.86759600	C	2.43664400	-1.47922400	-0.00287400
C	1.37415900	-1.03342200	1.93526500	C	0.93981500	1.22110700	-2.11769400
H	1.60458700	-0.82544400	2.98601700	H	1.70494300	1.34998300	-2.89371400
C	-1.11579800	-1.21238900	1.96843500	C	0.30042200	-1.15114000	-2.30808300
H	-0.82592200	-2.26892700	1.96968000	H	0.52683500	-1.04881400	-3.37695200
H	-1.40369000	-0.96076300	2.99465600	H	0.67013300	-2.13595100	-1.99750800
C	-0.00622700	1.01747700	1.99043500	C	2.40371800	-0.53066900	-1.18401600
H	-0.73229700	1.10439000	2.80487200	H	2.90355600	-0.96964400	-2.05666700
N	0.07218300	-0.41441300	1.52425200	N	1.01020400	-0.12779900	-1.50174600
O	0.06736000	-0.35631400	-2.30770900	O	-0.88298400	0.11748500	2.03591200
H	1.27917000	-2.11824200	1.82661400	H	-0.03462300	1.31105900	-2.61302200
H	-0.57000200	-2.93213200	-0.76216300	H	-4.49030700	-0.75469800	3.18814600
O	0.30005000	-2.51187900	-0.64039700	O	-4.25611900	0.01603300	2.64247200
C	1.21918700	-3.11509700	-1.50776600	C	-3.39868700	0.82708400	3.30395700
H	2.23882100	-2.80562900	-1.32990200	H	-3.35262900	1.82714400	2.88248200
H	0.96255200	-4.10721200	-1.85865000	H	-3.27090700	0.69018800	4.37598900
H	0.43609100	-1.13941000	-2.75821600	C	-2.88728800	-0.69889900	-0.49659600
C	-2.80821700	-0.63644100	-1.24676400	C	-2.12342200	-1.49105800	-3.01277400
C	-3.59905500	-1.12914200	1.34292800	C	-3.86648100	-1.09300300	-1.39960900
C	-4.16572100	-0.75898500	-0.96987200	H	-3.14029700	-0.38517000	0.51029600
H	-2.42834900	-0.42672200	-2.24071900	C	-3.47966100	-1.49159100	-2.67947200
C	-4.56792600	-1.00518000	0.34313000	H	-1.79300900	-1.80063900	-3.99930100
H	-3.88235300	-1.31907900	2.37340600	H	-4.90912300	-1.08142400	-1.10162800
H	-4.88878700	-0.65362900	-1.77140100	H	-4.22127100	-1.79848600	-3.41068900
H	-5.62121800	-1.09557000	0.59019200	H	0.63475900	-1.89146400	2.72603000
H	-0.39510800	1.80782300	-2.41368000	C	1.45101100	-2.07392000	2.03601500
C	-0.47573800	2.28022300	-1.44196100	C	2.44530400	-3.00927900	2.29080900
C	-0.78166400	3.62567400	-1.28024500	C	3.46116500	-3.18086300	1.34914300
C	-0.87766000	4.14794300	0.01016200	H	2.41940500	-3.58993300	3.20634100
H	-0.94526300	4.24606800	-2.15464900	C	3.45501700	-2.40670500	0.18648600
C	-0.65499200	3.30628400	1.09947800	H	4.24979600	-3.90842600	1.51516700
H	-1.12157100	5.19393800	0.16789400	H	4.23549100	-2.51784000	-0.55972000
H	-0.71779000	3.68173100	2.11627700	H	1.95539300	3.79695900	-2.30994000
H	4.10777600	-0.59919200	2.37850500	C	1.56580000	3.56364600	-1.32401000

C	3.78766400	-0.37649400	1.36553400	C	1.56889300	4.52206900	-0.30789700
C	4.70212400	0.06148100	0.40348700	C	1.06413500	4.18680700	0.94959900
C	4.25038100	0.35136700	-0.88399100	H	1.96553100	5.51508800	-0.49608500
H	5.74973300	0.18218400	0.66137000	C	0.57288500	2.90354000	1.14975100
C	2.89969300	0.19186900	-1.17526800	H	1.05478200	4.90293700	1.76395900
H	4.92790800	0.70209400	-1.65489000	H	0.17603400	2.57951600	2.10539600
H	2.48366600	0.40923200	-2.15254200	H	2.96201100	0.37581800	-0.92076900
H	0.96627300	1.29553700	2.41005200	H	-1.67566800	0.34025400	2.60191100

17				17			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
Fe	0.01979800	-0.47480900	-0.22609500	Fe	-0.11184300	0.48609500	-0.21153300
N	1.96815600	-0.22764700	-0.00848300	N	-2.01839400	0.01412600	-0.01183300
N	-1.93234400	-0.67650000	-0.05169300	N	1.79835300	0.90631000	0.04335100
N	-0.19608600	1.40525700	-0.81135300	N	0.40153500	-1.38964600	-0.91584500
C	2.32880100	0.01527100	1.27946500	C	-2.37314000	-0.29755500	1.26465300
C	-2.37700300	-0.49899000	1.22005600	C	2.25302900	0.65382300	1.30000700
C	-0.31207700	2.31124000	0.18008700	C	0.63053400	-2.27862300	0.07095300
C	1.20680500	-0.13085200	2.28545300	C	-1.28118600	-0.11394700	2.30082300
H	1.40877400	0.43329700	3.20318900	H	-1.46229300	-0.73858100	3.18388200
C	-1.28355400	-0.36748800	2.25930100	C	1.19717800	0.28316500	2.32483500
H	-0.98687000	-1.36956200	2.59069600	H	0.82459700	1.20281800	2.79163600
H	-1.63145200	0.17190000	3.14754100	H	1.62596700	-0.32661900	3.12864600
C	-0.21820600	1.78184900	1.59613700	C	0.25905900	-1.86960700	1.48837400
H	0.64384000	2.23503100	2.09687700	H	-0.66963500	-2.38545000	1.75601100
H	-1.10196300	2.08646900	2.16623300	H	1.02150800	-2.22221700	2.19153000
N	-0.08252700	0.28408600	1.64933300	N	0.04243600	-0.39892800	1.67270300
O	0.80036000	-4.56886500	-1.11554200	O	-1.33442100	4.48105100	-1.20136000
H	1.11293300	-1.18510000	2.57159800	H	-1.27386100	0.92821000	2.64168300
O	0.13691200	-2.33339000	-0.94458900	O	-0.43637800	2.36459600	-0.81507700
C	1.18319700	-3.29409500	-1.41512300	C	-1.55168800	3.15175100	-1.42100100
H	1.23125500	-3.19665100	-2.50050200	H	-1.52153700	2.97398700	-2.49720200
H	2.10085500	-2.95195000	-0.93322400	H	-2.45525300	2.74222900	-0.96523500
H	1.08377800	-4.82534300	-0.22230900	H	-1.69813800	4.76338100	-0.34558100
C	-3.73146200	-0.50830600	1.53275700	C	3.59590200	0.80125700	1.63322100
C	-4.66283500	-0.72143700	0.51361800	C	4.49862600	1.23269200	0.66015300
H	-4.05467300	-0.35745900	2.55797100	H	3.93052800	0.58634100	2.64328100
C	-2.83837900	-0.86703800	-1.03302200	C	2.68055200	1.30909700	-0.89678100
C	-4.20728600	-0.90567400	-0.79151300	C	4.03106400	1.49342000	-0.62824400
H	-5.72508100	-0.73739000	0.73648400	H	5.54916100	1.35708500	0.90354900
H	-2.44488700	-0.97948800	-2.03954000	H	2.28185700	1.47300200	-1.89401800
H	-4.89645500	-1.06792100	-1.61313000	H	4.69889900	1.82330500	-1.41657400
C	-0.49584600	3.66770400	-0.08262000	C	1.12634700	-3.55513200	-0.19130200
C	-0.55805100	4.10050600	-1.40537800	C	1.37611200	-3.92984000	-1.51014700

H	-0.58759400	4.37322000	0.73775300	H	1.30791700	-4.24672600	0.62599600
C	-0.43596500	3.16078400	-2.43139300	C	1.12921900	-3.01145200	-2.53221600
H	-0.69992500	5.15244700	-1.63241200	H	1.75821100	-4.92046900	-1.73612400
C	-0.25833100	1.82662200	-2.09313600	C	0.65255200	-1.75250600	-2.19170300
H	-0.47885600	3.45338800	-3.47479300	H	1.30858400	-3.26014000	-3.57251400
H	-0.16209700	1.06268300	-2.85966100	H	0.46160800	-1.00419200	-2.95577200
C	3.63720900	0.32545800	1.63238700	C	-3.65743700	-0.72351200	1.58523200
C	2.91423200	-0.15398600	-0.96672400	C	-2.94318600	-0.11055600	-0.98651600
C	4.61436000	0.38205200	0.63584000	C	-4.61418500	-0.82928000	0.57342200
H	3.88982200	0.51861600	2.67026600	H	-3.90648500	-0.96982500	2.61268200
C	4.24469200	0.13915600	-0.68674000	C	-4.24798000	-0.52046400	-0.73624800
H	2.58352500	-0.33134500	-1.98579800	H	-2.61488100	0.12080000	-1.99550200
H	5.64288400	0.61951000	0.88896900	H	-5.62287400	-1.15730500	0.80418400
H	4.96918800	0.18227300	-1.49274100	H	-4.95469900	-0.60142600	-1.55500600
H	-0.71211100	-2.79657500	-1.07529500	H	0.34937700	2.93872800	-0.88192600

17				TS₁₇₋₁₈			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =1			
Fe	-0.01132500	-0.04523100	0.49239900	Fe	-0.05700300	0.51255700	-0.13559300
N	1.90927100	-0.90115200	0.55134100	N	-2.01542300	0.27884300	0.01578400
N	0.04722100	2.00578600	-0.00803700	N	1.89001000	0.65128300	0.11413900
N	-1.72513300	-1.07251600	-0.21774900	N	0.17930700	-1.30545500	-0.90874700
C	2.54737000	-0.96857600	-0.64315700	C	-2.41345900	-0.04932400	1.27325500
C	0.04093100	2.26615800	-1.33990400	C	2.30660800	0.28432900	1.35229900
C	-1.59303000	-1.55496100	-1.47920800	C	0.26282200	-2.31238100	-0.01604100
C	1.90918800	-0.21752500	-1.79730600	C	-1.30461600	-0.03971000	2.30457500
H	2.20566600	-0.65672600	-2.75867600	H	-1.54892200	-0.67011000	3.16779300
C	-0.13637500	1.07535000	-2.26489800	C	1.19381800	0.04336100	2.35051000
H	0.29661900	1.28467200	-3.25163100	H	0.93605400	0.99792800	2.82406800
H	-1.20834400	0.90404300	-2.42030900	H	1.50860700	-0.63463700	3.15179900
C	-0.23063400	-1.39022900	-2.12448400	C	0.00834000	-1.94614500	1.43016800
H	-0.31529300	-1.42276300	-3.21877100	H	-0.95632300	-2.36564400	1.73543700
N	0.43450600	-0.15079400	-1.66200300	H	0.76332000	-2.40048200	2.08023500
H	2.29003100	0.81081200	-1.78911500	N	-0.02766200	-0.45948700	1.64901300
C	0.16949500	3.04229500	0.84974000	O	-0.07636800	4.34033700	-1.48048800
C	0.14959500	3.56427200	-1.83289000	H	-1.16639800	0.98102900	2.68002300
C	0.27353000	4.36215900	0.43213500	H	0.59305300	3.46564000	-1.05854100
H	0.19752300	2.79307400	1.90647800	O	-0.12769500	2.36176700	-0.74185300
C	0.26029000	4.62848600	-0.93790700	C	-1.09247700	3.28940300	-1.11463900
H	0.14802500	3.73904500	-2.90426600	H	-1.64591000	3.05808100	-2.02568300
H	0.37098600	5.15809700	1.16239100	H	-1.73169300	3.65873000	-0.30737800
H	0.34509900	5.64689900	-1.30446000	H	-0.11763200	5.15143600	-0.93082000
H	-2.97706300	-0.80908900	1.41844400	C	3.65513000	0.21732700	1.68516300
C	-2.90821800	-1.22681500	0.41840000	C	4.60886700	0.55103800	0.72124500

C	-3.99086800	-1.87415300	-0.16509400	H	3.95555300	-0.08555600	2.68332100
C	-3.85447900	-2.37352500	-1.46014200	C	2.81512500	0.96487400	-0.81357500
H	-4.91943300	-1.97661300	0.38593900	C	4.18011700	0.93466500	-0.54922700
C	-2.64000800	-2.20298100	-2.12719700	H	5.66708900	0.50786200	0.95908400
H	-4.68113300	-2.88039700	-1.94846800	H	2.43782600	1.23987400	-1.79375000
H	-2.50598800	-2.57174300	-3.13931000	H	4.88758400	1.19775200	-1.32810600
H	4.25116400	-1.67091300	-1.75227200	C	0.52115200	-3.62434700	-0.40860800
C	3.76759100	-1.62371400	-0.78154000	C	0.68841000	-3.90662300	-1.76288200
C	4.35992000	-2.20712900	0.33957300	H	0.58666400	-4.41230800	0.33564300
C	3.71131900	-2.12059600	1.57196800	C	0.59537100	-2.86415300	-2.68719600
H	5.31243600	-2.72046700	0.25070900	H	0.88884400	-4.92161600	-2.09127900
C	2.48896200	-1.46424000	1.63377100	C	0.34582900	-1.58093800	-2.21970100
H	4.13914200	-2.55602800	2.46836100	H	0.71845200	-3.03836400	-3.75051600
H	1.94446000	-1.37278500	2.56765000	H	0.27496000	-0.73961700	-2.90322200
H	0.40664400	-2.23368200	-1.83073300	C	-3.74007600	-0.33401200	1.57633800
O	-0.48607700	-0.42240500	2.56143400	C	-2.94217500	0.31629300	-0.96205100
C	-1.14576800	0.35019300	3.62817100	C	-4.69698600	-0.27358700	0.56056300
H	-0.74129900	-1.35324700	2.68713500	H	-4.02170700	-0.59906600	2.59061100
O	-2.48145500	0.55226100	3.34720900	C	-4.28891000	0.05473200	-0.73169900
H	-0.56401900	1.27062700	3.70849600	H	-2.58065300	0.55123400	-1.95880200
H	-1.06150700	-0.24116200	4.54117600	H	-5.73892000	-0.48986300	0.77472400
H	-2.63294000	1.43944300	2.98467200	H	-4.99621000	0.09929300	-1.55279600

TS₁₇₋₁₈				TS₁₇₋₁₈			
Charge=2 Multiplicity =3				Charge=2 Multiplicity =5			
Fe	-0.13085300	0.53228900	-0.11026000	Fe	-0.07287800	-0.01517200	0.49189400
N	-2.06199900	0.13608200	0.02259900	N	-1.93941400	-0.49556900	-0.41616100
N	1.78868300	0.82639800	0.21222400	N	1.48442900	-1.45161100	0.41218200
N	0.31890200	-1.30837300	-1.02408000	N	0.64564500	1.95330400	0.22252200
C	-2.45278500	-0.27018200	1.26103600	C	-1.88434500	-0.81078000	-1.73235800
C	2.22286000	0.37975800	1.41918400	C	2.16052800	-1.54330400	-0.75817800
C	0.49956500	-2.29555000	-0.12430800	C	0.78321900	2.35867100	-1.06257600
C	-1.35787700	-0.25948400	2.30877400	C	-0.49927000	-0.93257300	-2.33548100
H	-1.58213700	-0.95334400	3.12823600	H	-0.53638300	-0.78070300	-3.42272100
C	1.14244000	-0.07008400	2.38417500	C	1.85321400	-0.48307500	-1.79833500
H	0.83004100	0.79281400	2.98421100	H	2.07775100	-0.85184100	-2.80796800
H	1.52663200	-0.81882600	3.08664500	H	2.51258800	0.37556100	-1.62272900
C	0.03872300	-2.02579700	1.29812900	C	0.29304100	1.39357200	-2.12657600
H	-0.95962600	-2.46179800	1.41383000	H	0.79765700	1.58291900	-3.08341700
H	0.68803200	-2.54078500	2.01441100	N	0.45575000	-0.00934700	-1.68509600
N	-0.05516700	-0.57157400	1.64799600	H	-0.13477200	-1.95410400	-2.17099100
O	-0.45302100	4.37023000	-1.40416000	C	1.78479400	-2.31785900	1.40182600
H	-1.27940200	0.74269900	2.74692800	C	3.13414500	-2.51699800	-0.96684900

H	0.26942500	3.56574400	-0.93628900	C	2.74959200	-3.30798600	1.27137300
O	-0.33167700	2.36421500	-0.76132000	H	1.22724400	-2.20229700	2.32604300
C	-1.35796100	3.18009600	-1.21614600	C	3.43545200	-3.41128600	0.06049400
H	-1.75907600	2.93562500	-2.20137900	H	3.65225200	-2.57102300	-1.91926700
H	-2.13679500	3.42044300	-0.48582800	H	2.95444300	-3.98131700	2.09646800
H	-0.66865900	5.13520300	-0.82980700	H	4.19219100	-4.17639500	-0.08309600
C	3.56937000	0.41052200	1.76958800	H	0.90055000	2.40963900	2.22385000
C	4.49742900	0.92412700	0.86302500	C	1.02168400	2.78772500	1.21360300
H	3.88656500	0.04145700	2.73992000	C	1.53808200	4.05451100	0.97151700
C	2.69194400	1.31479600	-0.66245700	C	1.68102100	4.47286000	-0.35207200
C	4.04906100	1.38748800	-0.37444300	H	1.82727100	4.69224400	1.79968600
H	5.55209400	0.95750600	1.11780400	C	1.30313100	3.61017500	-1.38199200
H	2.29960800	1.64681000	-1.61837300	H	2.08732700	5.45330100	-0.58097700
H	4.73737600	1.78921400	-1.11009100	H	1.40920500	3.90637200	-2.42093200
C	1.00556700	-3.54210500	-0.48857000	H	-2.96002300	-1.30022200	-3.52944000
C	1.31718300	-3.78291000	-1.82608700	C	-3.03633300	-1.05871300	-2.47388100
H	1.14666000	-4.31412900	0.26188800	C	-4.28009000	-0.99616600	-1.84427400
C	1.12044700	-2.76444900	-2.75953100	C	-4.33643500	-0.67269500	-0.48843700
H	1.70847400	-4.74785200	-2.13302400	H	-5.18901700	-1.18956600	-2.40556100
C	0.63071000	-1.54230200	-2.31480800	C	-3.14597900	-0.42468400	0.18326400
H	1.34866800	-2.90789700	-3.81006100	H	-5.28200800	-0.60525100	0.03838300
H	0.47901100	-0.71858800	-3.00682300	H	-3.14026200	-0.15193700	1.23316400
C	-3.76436000	-0.64276500	1.53306400	H	-0.77680800	1.56799400	-2.29387800
C	-2.98062800	0.16031100	-0.96435700	H	-1.70599800	-1.55938500	3.15222400
C	-4.71365500	-0.59270500	0.50979300	C	-1.14288400	-0.67032100	3.44659800
H	-4.04000300	-0.96870500	2.53110400	O	-2.14658600	0.32565300	3.99286600
C	-4.31175300	-0.18808800	-0.76255300	O	-0.73476000	0.16201900	2.42183800
H	-2.62303600	0.45547500	-1.94620400	H	-0.39225200	-0.87730300	4.21687100
H	-5.74344100	-0.87698600	0.70193800	H	-1.97374300	0.61967800	4.91304300
H	-5.01126300	-0.15093800	-1.59066300	H	-1.60189200	0.92285400	3.13426100

18				18			
Charge=2 Multiplicity =1				Charge=2 Multiplicity =3			
Fe	0.07427500	-0.49992000	0.47269700	Fe	0.00101600	-0.61256100	0.40964100
N	-0.16797500	1.43165000	0.24492700	N	-0.00173500	1.51579200	0.47439900
N	-1.89212300	-0.73232100	0.28130200	N	-1.96485800	-0.62901900	0.17382900
N	2.04865000	-0.38953800	0.24289600	N	1.96689000	-0.62518200	0.17401600
C	-0.22777700	1.84962500	-1.03821500	C	-0.00278500	2.08567900	-0.74122100
C	-2.27052600	-1.04866000	-0.98418100	C	-2.36120400	-0.71819900	-1.12526500
C	2.46105900	-0.76758900	-0.99694900	C	2.36354900	-0.71438700	-1.12497500
C	0.06785700	0.80980700	-2.09176600	C	0.00014100	1.17267000	-1.95931700
H	1.05158600	1.01925900	-2.52513900	H	0.87662200	1.40484300	-2.57348600
C	-1.13086000	-1.36453500	-1.92592700	C	-1.24977900	-0.96351700	-2.12364000

H	-0.88443000	-2.42769500	-1.84287000	H	-1.05111800	-2.03847900	-2.18237700
C	1.35873800	-1.27900200	-1.89855300	C	1.25258300	-0.96192600	-2.12332700
H	1.21480900	-2.35142300	-1.73924800	H	1.05551600	-2.03720400	-2.18155600
N	0.08450100	-0.58725700	-1.52855600	N	0.00090600	-0.29787600	-1.65488700
O	0.23745000	-2.56904900	0.62706000	O	0.00307500	-2.90702900	0.22049100
H	-0.65201700	0.87389000	-2.91414300	H	-0.87428400	1.40343100	-2.57693800
O	0.00206400	-0.37734800	2.41778600	O	0.00159600	-0.89672400	2.39560600
C	0.47734300	-0.96843400	3.38754800	C	0.00249600	-1.74927100	3.28061900
H	1.18344300	-1.80258400	3.26973900	H	0.00321600	-2.82106400	3.04001900
H	0.19990500	-0.66403400	4.40337000	H	0.00261400	-1.44847100	4.33604600
H	1.60452000	-1.13782600	-2.95726400	H	1.53878000	-0.63172900	-3.12872100
H	1.05554000	-3.04284200	0.85112700	H	0.77974900	-3.49111300	0.20879100
H	-0.50334000	-3.10346900	0.95867800	H	-0.77298500	-3.49192000	0.20855400
H	-3.87367000	-1.38424300	-2.37790700	H	-3.98022000	-0.70592200	-2.53866900
C	-3.60799100	-1.13427600	-1.35553800	C	-3.70016100	-0.63846600	-1.49207800
C	-4.59505700	-0.89756600	-0.39688900	C	-4.67055800	-0.47188500	-0.50235200
C	-4.20817500	-0.56976400	0.90212300	C	-4.26488300	-0.37520000	0.82788600
H	-5.64543400	-0.96166100	-0.66322600	H	-5.72116900	-0.40994900	-0.76818400
C	-2.85168900	-0.48799900	1.19737400	C	-2.90798500	-0.44923300	1.12171000
H	-4.94141000	-0.37013600	1.67601200	H	-4.98261800	-0.23428700	1.62871500
H	-2.50642200	-0.21311400	2.18792500	H	-2.55127900	-0.35331800	2.14116600
C	2.96998300	0.08393900	1.10602800	C	2.90955500	-0.44325900	1.12194200
C	4.32249900	0.16818200	0.79338800	C	4.26636900	-0.36710400	0.82826400
H	2.60100300	0.41515900	2.07077000	H	2.55249100	-0.34739000	2.14127800
C	3.79510900	-0.70088800	-1.38392500	C	3.70242000	-0.63263100	-1.49164300
C	4.74538200	-0.23562500	-0.47243400	C	4.67239400	-0.46388300	-0.50186100
H	5.02299200	0.55340200	1.52643400	H	4.98375600	-0.22453400	1.62911200
H	4.08625100	-1.00507700	-2.38448500	H	3.98275000	-0.70019700	-2.53815500
H	5.79251800	-0.17704400	-0.75235800	H	5.72294000	-0.40036700	-0.76757600
H	-0.53709300	3.47214900	-2.41765400	H	-0.00674300	3.90311600	-1.90379800
C	-0.49203300	3.17529600	-1.37419100	C	-0.00591600	3.47154300	-0.90704200
C	-0.69110600	4.10705500	-0.35779000	C	-0.00789100	4.28731200	0.22180800
C	-0.62430500	3.67761900	0.96812200	C	-0.00673000	3.69333200	1.48590100
H	-0.89618900	5.14597100	-0.59602200	H	-0.01029500	5.36786800	0.11754000
C	-0.36899200	2.33745100	1.22680400	C	-0.00370600	2.30717400	1.56635600
H	-0.77427500	4.36558100	1.79304400	H	-0.00817200	4.29092000	2.39103100
H	-0.32897000	1.95795700	2.24044900	H	-0.00277400	1.79715500	2.52457400
H	-1.40472100	-1.17867600	-2.97027200	H	-1.53642500	-0.63328700	-3.12889900

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Charge=2 Multiplicity =5

Fe	0.09817600	0.02094900	-0.43734200
N	-0.11607300	2.11340800	-0.23105100

19

Charge=2 Multiplicity =5

Fe	-0.16131000	-0.01116500	0.46524100
N	-2.12575700	-0.07008700	0.92962000

N	1.32948100	-0.92929900	0.98246600	N	0.78126800	-1.66068300	-0.22037600
N	-1.54257000	-1.18416200	-1.01161800	N	0.70752200	1.69966400	-0.17556500
C	-0.69971000	2.52472100	0.92070100	C	-2.96553000	-0.29962000	-0.11411800
C	0.74242800	-1.20978600	2.17229300	C	-4.34328800	-0.29361000	0.05657800
C	-2.63650900	-1.06531100	-0.22031100	H	-4.99951600	-0.47306500	-0.78913300
C	-0.92844700	1.46170700	1.97795600	C	-4.86502200	-0.06244100	1.33333200
H	-1.74031700	1.75708500	2.65583300	H	-5.93965800	-0.05591300	1.48820100
C	-0.75476000	-0.97500600	2.26156000	C	-3.99488200	0.15916700	2.40194800
H	-1.05973200	-0.80143800	3.30178700	H	-4.36594800	0.33858300	3.40506400
H	-1.27102200	-1.88364700	1.92925000	C	-2.62616300	0.15140700	2.16508100
C	-2.56261700	-0.01997800	0.87767600	H	-1.89606500	0.31850500	2.94920800
H	-3.26274900	-0.26251900	1.68825500	C	0.66009600	-1.87715200	-1.55707300
N	-1.17686900	0.13359800	1.37415700	C	1.18154500	-3.01937000	-2.14913000
O	1.09074500	0.00991800	-2.28720700	H	1.06944500	-3.18251900	-3.21634700
H	-0.02037900	1.38178900	2.58798500	C	1.86176000	-3.94384500	-1.34972500
O	3.74520100	-0.38127600	-2.38707700	H	2.27715100	-4.84344300	-1.79362300
C	4.67137700	-0.35573100	-3.18092800	C	2.00668300	-3.69724000	0.01588200
H	4.52591200	-0.08773800	-4.24027500	H	2.53883100	-4.38792000	0.66067300
H	5.69512200	-0.60254700	-2.86068600	C	1.45140300	-2.54205900	0.55223600
C	2.64584200	-1.19099200	0.82820200	H	1.53816800	-2.28274000	1.60032400
C	1.46280400	-1.74584100	3.23572300	C	0.17247500	2.21304500	-1.31586000
C	3.42337800	-1.73405800	1.84394500	C	0.67739300	3.37094400	-1.88937900
H	3.07905100	-0.95260200	-0.13842800	H	0.24227500	3.76456200	-2.80255200
C	2.82192500	-2.01539500	3.07040900	C	1.75066700	4.01823900	-1.26750600
H	0.96661900	-1.95274600	4.17879200	H	2.15707700	4.92915400	-1.69645000
H	4.47711300	-1.92690100	1.67506700	C	2.30085700	3.47509400	-0.10704600
H	3.40038300	-2.43464300	3.88793000	H	3.14465500	3.94293200	0.38819000
H	-0.65619800	-2.15349400	-2.61348300	C	1.76098200	2.30495000	0.41673500
C	-1.56367900	-2.07865800	-2.02212500	H	2.18182500	1.79904600	1.28236500
C	-2.66908300	-2.87295100	-2.29873500	C	-2.28148500	-0.63162000	-1.42018400
C	-3.79800900	-2.74670400	-1.48826200	H	-2.88477700	-0.33688400	-2.28647900
H	-2.64065700	-3.57691100	-3.12324100	C	0.01922200	-0.75092300	-2.33856900
C	-3.77685100	-1.83581700	-0.43109900	H	-0.48726300	-1.11320100	-3.24016500
H	-4.67911400	-3.35464400	-1.66932100	H	0.80223000	-0.05612300	-2.66326500
H	-4.63636100	-1.72438000	0.22249800	C	-1.01950200	1.45845100	-1.86191600
H	-1.48116500	4.16319500	2.07393500	H	-1.94189100	1.86135100	-1.42736300
C	-1.00507400	3.86398000	1.14541700	H	-1.10146700	1.55952000	-2.95023100
C	-0.68597700	4.80956200	0.16969200	N	-0.93133300	0.01393700	-1.46877500
C	-0.07302300	4.38630700	-1.00986700	O	0.36804500	-0.03054100	1.98612200
H	-0.91468900	5.85888500	0.32863700	H	2.76083700	0.00097300	2.96761500
C	0.18974400	3.03184000	-1.17170900	O	3.23407000	0.04418100	2.12209800
H	0.19239800	5.08817100	-1.79283700	C	4.64351900	0.00696200	2.40082500
H	0.66117000	2.65130900	-2.07165400	H	4.95759500	0.85037000	3.02752300
H	-2.87671400	0.94797900	0.46791600	H	5.15544900	0.07226000	1.43861800

H	2.06713200	-0.10023900	-2.45202600	H	4.93342900	-0.93027100	2.89089300
H	0.65371100	0.06610200	-3.15165500	H	-2.13151900	-1.71608800	-1.48209800

TS₁₉₋₂₀				20			
Charge=2 Multiplicity =5				Charge=2 Multiplicity =5			
N	-0.61392300	1.81860300	-0.23035200	Fe	-0.01439000	-0.01469000	0.34360300
N	-1.07763000	-1.56823200	-0.31188200	N	1.70758000	-0.79135300	1.05876800
N	1.98939600	-0.23603600	0.82736500	N	0.01647300	1.98187300	-0.15834900
C	-0.50800900	2.03309100	-1.56772300	N	-1.33421100	-1.19827700	-0.65297100
C	-0.83609800	3.25844800	-2.13220700	C	2.74525600	-0.80471800	0.18497700
H	-0.73774200	3.41235500	-3.20214200	C	3.96998900	-1.36481300	0.52330500
C	-1.30046800	4.28201100	-1.30020400	H	4.78711700	-1.37159900	-0.19104200
H	-1.56519300	5.24713700	-1.72119300	C	4.12943800	-1.90828300	1.80197900
C	-1.41598800	4.05210200	0.07099000	H	5.07855400	-2.34994100	2.08994000
H	-1.77278100	4.82317900	0.74490600	C	3.06265400	-1.87563600	2.70101700
C	-1.05741000	2.80758900	0.57480500	H	3.15628000	-2.28244600	3.70190900
H	-1.12012700	2.57208300	1.63059200	C	1.85943000	-1.31007800	2.29461800
C	-0.61842400	-2.10557800	-1.47308800	H	0.99151800	-1.24154300	2.94112100
C	-1.27097100	-3.16216400	-2.09277000	C	0.39571200	2.23185800	-1.43548800
H	-0.88962000	-3.57151000	-3.02290200	C	0.54966600	3.52910300	-1.90697600
C	-2.42025700	-3.68834600	-1.49466300	H	0.86038200	3.70759800	-2.93152300
H	-2.94534900	-4.51690500	-1.95998800	C	0.29327300	4.59474100	-1.03847700
C	-2.88786300	-3.13106300	-0.30502400	H	0.40473200	5.61763400	-1.38485700
H	-3.78208500	-3.50660700	0.18021300	C	-0.09667400	4.33046200	0.27462500
C	-2.19439100	-2.06716500	0.26175000	H	-0.29624300	5.13312800	0.97608500
H	-2.53067800	-1.57257800	1.16753100	C	-0.21998800	3.00709500	0.68420000
C	2.84729800	-0.07870100	-0.21413800	H	-0.50278800	2.72986700	1.69374500
C	4.21383400	-0.26784500	-0.05920500	C	-0.83666600	-1.74461000	-1.79459100
H	4.88396900	-0.14341400	-0.90386400	C	-1.61057800	-2.55094300	-2.61860400
C	4.70669700	-0.61144100	1.20376400	H	-1.18798300	-2.96788400	-3.52723600
H	5.77210100	-0.76268100	1.34830500	C	-2.93229900	-2.81882100	-2.25332200
C	3.82020700	-0.75790600	2.27164800	H	-3.55552700	-3.44815900	-2.88118700
H	4.17060100	-1.02051000	3.26379700	C	-3.43759100	-2.26483300	-1.07784200
C	2.46211100	-0.56501800	2.04831400	H	-4.45859700	-2.44736500	-0.76120000
H	1.71744400	-0.66152200	2.83086000	C	-2.61334700	-1.45819600	-0.30152100
C	-0.08257200	0.82733200	-2.37379400	H	-2.97747900	-1.00058300	0.61078700
H	0.44218600	1.11138600	-3.29289100	C	2.47005600	-0.10074000	-1.12351600
C	0.66893300	-1.50329700	-1.98597600	H	3.05296700	-0.52031300	-1.95139100
H	0.74724400	-1.56978900	-3.07718000	C	0.57300700	0.99627400	-2.28635500
H	1.52390500	-2.04401700	-1.56347500	H	1.28880600	1.15477000	-3.10103200
C	2.19912600	0.38444100	-1.49816400	H	-0.38674900	0.72653100	-2.74166600
H	2.19248000	1.48034900	-1.52564700	C	0.62471000	-1.46460000	-2.04882400
H	2.74239300	0.03877900	-2.38495500	H	1.23346100	-2.24294900	-1.57377000

N	0.77302800	-0.07582200	-1.53733300	H	0.86489400	-1.46996900	-3.11831400
H	-0.97228600	0.25938500	-2.66851800	N	1.00362500	-0.15542600	-1.42813000
Fe	0.04332100	-0.01210400	0.37368200	O	-0.72396500	0.18981300	1.92906600
O	-0.42486400	0.04605100	2.01289200	O	-3.51265400	0.19123200	2.38280300
H	-1.51804200	0.25668200	2.25831100	C	-4.20255100	0.58764500	3.50213100
O	-2.72865600	0.24447400	2.47109100	H	-4.32543600	-0.33410400	4.11410200
C	-3.03408400	0.05557500	3.82235500	H	-5.22873000	0.89734300	3.24952800
H	-2.92708300	-0.99639600	4.12746700	H	-3.67487400	1.33245800	4.11092200
H	-2.46758400	0.71760100	4.48787900	H	2.74845200	0.95530900	-1.03074900
H	-4.10808800	0.29549900	3.92068700	H	-1.70092100	0.23262500	2.05396400

TS₂₀₋₁₈			
Charge=2 Multiplicity =5			
Fe	0.04118900	0.01339500	0.44160500
N	2.02570200	-0.22797400	0.85003700
N	-0.71580200	1.88184900	-0.04062000
N	-0.91063300	-1.61185500	-0.41496700
C	2.84756100	0.15535400	-0.16275200
C	4.22822400	0.02299500	-0.06805800
H	4.86299400	0.33225600	-0.89240500
C	4.78070500	-0.51282000	1.09753800
H	5.85683600	-0.62172400	1.19171700
C	3.93376700	-0.92021000	2.12976300
H	4.32387600	-1.35571800	3.04322000
C	2.56346700	-0.76779000	1.96684700
H	1.86655200	-1.09495500	2.73100900
C	-0.63614100	2.19819300	-1.35748000
C	-1.06141700	3.43131000	-1.83669800
H	-0.98076300	3.66356400	-2.89394800
C	-1.60135300	4.35607100	-0.93907500
H	-1.94356100	5.32379200	-1.29277500
C	-1.69497500	4.02131900	0.41227800
H	-2.11237500	4.71099900	1.13768100
C	-1.23830300	2.77584100	0.82523500
H	-1.28850600	2.46048500	1.86078900
C	-0.42177000	-1.96122800	-1.63443700
C	-0.98336700	-2.98851800	-2.38003800
H	-0.57705500	-3.24191500	-3.35420800
C	-2.07481500	-3.68669500	-1.85383500
H	-2.52915000	-4.49468600	-2.41908700
C	-2.57605900	-3.32284300	-0.60574400
H	-3.43010500	-3.82863300	-0.16886100
C	-1.97178600	-2.27786000	0.08728700

H	-2.36292700	-1.94341900	1.04444900	
C	2.15498200	0.75642400	-1.36567400	
H	2.73660400	0.60173300	-2.28225800	
C	-0.13019100	1.09235400	-2.25557600	
H	0.36815200	1.48883900	-3.14834600	
H	-0.98144900	0.49281900	-2.59824000	
C	0.80027000	-1.19200100	-2.08527800	
H	1.70517500	-1.69409600	-1.72383200	
H	0.87019500	-1.14608200	-3.17846000	
N	0.78242200	0.18469400	-1.50001100	
O	-0.60393100	-0.03836300	2.18010300	
O	-3.59658300	-0.78639800	2.32720500	
C	-2.97605200	-0.49875600	3.43775500	
H	-2.73110900	-1.33848400	4.11489400	
H	-3.26407600	0.43403500	3.95456500	
H	-1.86314500	-0.23900500	2.95160100	
H	2.05125100	1.83897600	-1.22607800	
H	0.02746300	0.22721100	2.87493700	