

Supporting information for:

Understanding asymmetric hydrogenation of alkenes catalyzed by first-row transition metal, Fe: a first-principles exploration

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Table S1: Calculated relative energy positions of different intermediate and transition states following 1-2 mode of catalytic hydrogenation of alkene at different levels of theories.

Relative energies within different level of theories → Species ↓	M06L/ 6-311G** (kcal/mol) Gas phase	M06L/ Def2-svp (kcal/mol) Gas phase	M06L/ Def2-tzvp (kcal/mol) Gas phase	B3LYP/ 6-311G** (kcal/mol) Gas phase	B3LYP(GD3)/ 6-311G** (kcal/mol) Gas phase	M06L/ 6-311+G** (kcal/mol) Gas phase	M06L/ 6-311G** (kcal/mol) in Acetonitrile solvent
I₀	0	0	0	0	0	0	0
I	-2.02	0.62	0.93	36.02	15.57	-1.01	6.63
TS₁	2.55	4.66	5.08	36.50	17.02	4.13	11.60
II	-13.90	-11.64	-9.15	2.90	-13.47	-14.40	-8.32
III	-14.54	-12.36	-8.77	2.67	-13.48	-14.50	-6.44
TS₂	0.78	5.46	8.93	44.60	14.76	4.38	15.14
IV	-20.11	-17.53	-14.03	10.50	-3.87	-22.46	-11.44
V	-18.42	-16.55	-14.56	-8.70	-18.99	-22.10	-14.88
TS₃	-10.34	-8.93	-6.84	6.30	4.99	-10.06	-4.12
VI	-18.17	-16.68	-16.28	-13.70	-19.83	-20.92	-17.47

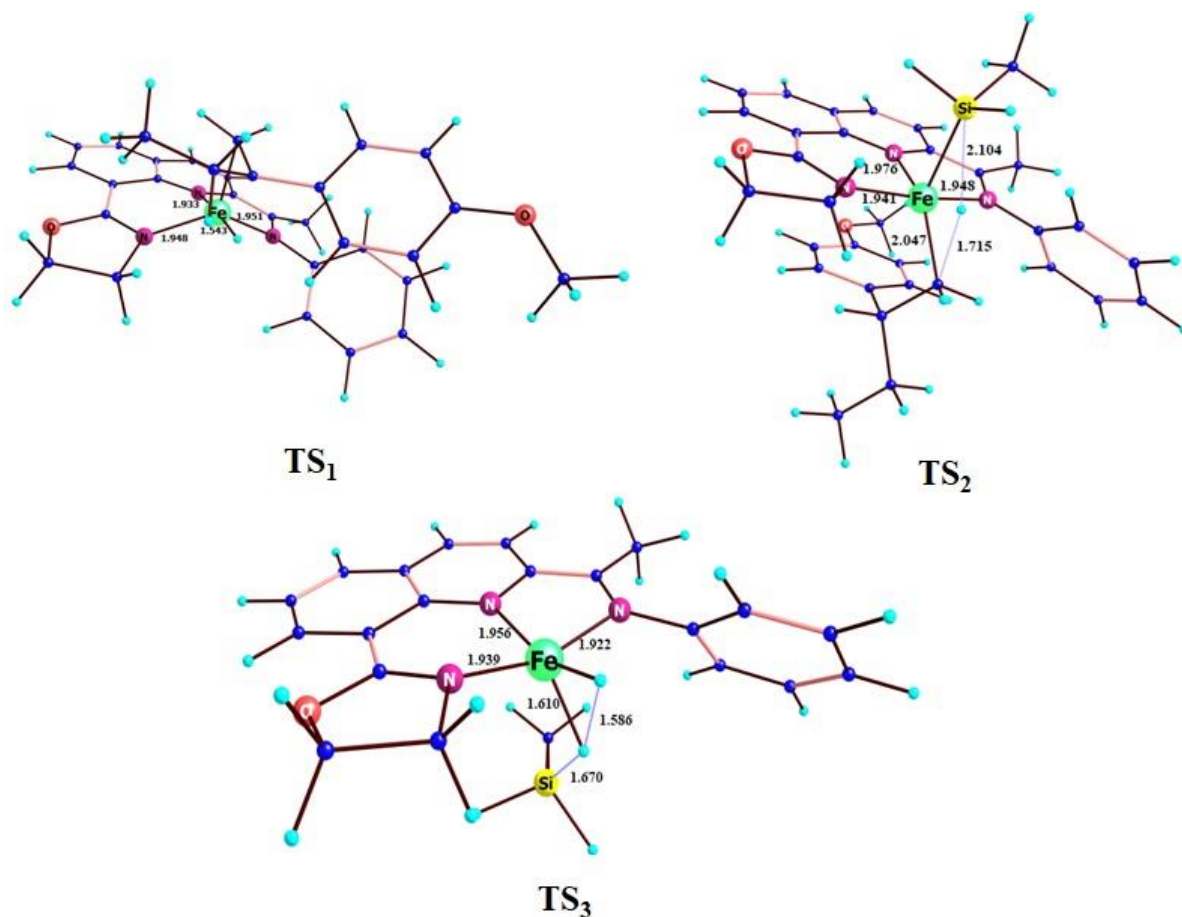


Figure S1: Optimized geometries of the transition state structures for the 1-2 mode of catalytic hydrogenation of alkene.

Table S2: Calculated relative energy positions of different intermediate and transition states following 2-1 mode of catalytic hydrogenation of alkene at different levels of theories.

Relative energies within different level of theories → Species ↓	M06L/6-311G** (kcal/mol) Gas phase	M06L/Def2-svp (kcal/mol) Gas phase	M06L/Def2-tzvp (kcal/mol) Gas phase	B3LYP/6-311G** (kcal/mol) Gas phase	B3LYP(GD3)/6-311G** (kcal/mol) Gas phase	M06L/6-311+G** (kcal/mol) Gas phase	M06L/6-311G** (kcal/mol) in Acetonitrile solvent
I₀	0	0	0	0	0	0	0
I''	-9.33	-7.13	-6.10	20.08	0.36	-8.04	0.31
TS₁''	-8.84	-7.04	-5.63	21.54	1.55	-7.16	1.17
II''	-14.89	-14.07	-11.69	14.17	-6.07	-14.85	-6.13
III''	-14.98	-12.85	-10.09	10.04	-14.50	-14.48	-5.26
TS₂''	24.38	27.30	30.16	80.04	34.92	26.10	36.18
IV''	-11.50	-9.00	-6.49	-0.67	-16.52	-14.35	-4.23
V	-18.42	-16.55	-14.56	-8.70	-18.99	-22.10	-14.88
TS₃	-10.34	-8.93	-6.84	6.30	4.99	-10.06	-4.12

VI	-18.17	-16.68	-16.28	-13.70	-19.83	-20.92	-17.47
TS₃^{''}	13.70	16.11	18.46	30.72	15.37	12.72	20.24
V^{''}	-5.16	-4.04	-2.30	4.16	-5.55	-7.61	3.28

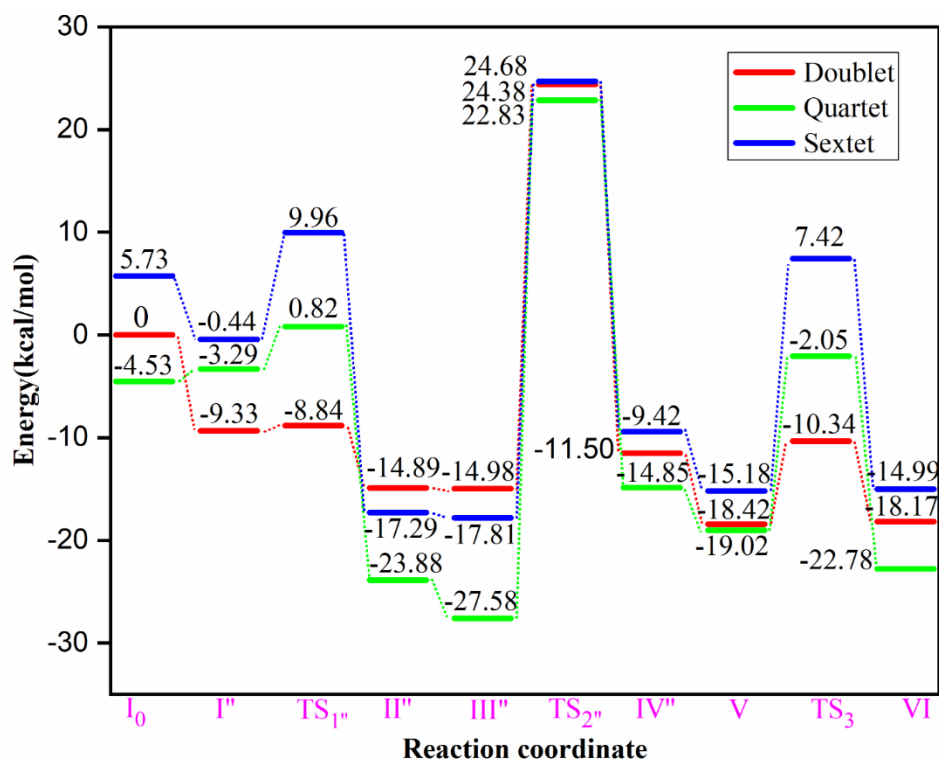


Figure S2: Energy profile diagram for the iron-catalysed hydrogenation of alkene via 2-1 mode in different spin states. The computations are performed within M06-L/6-311G**,LANL2DZ level of theory.

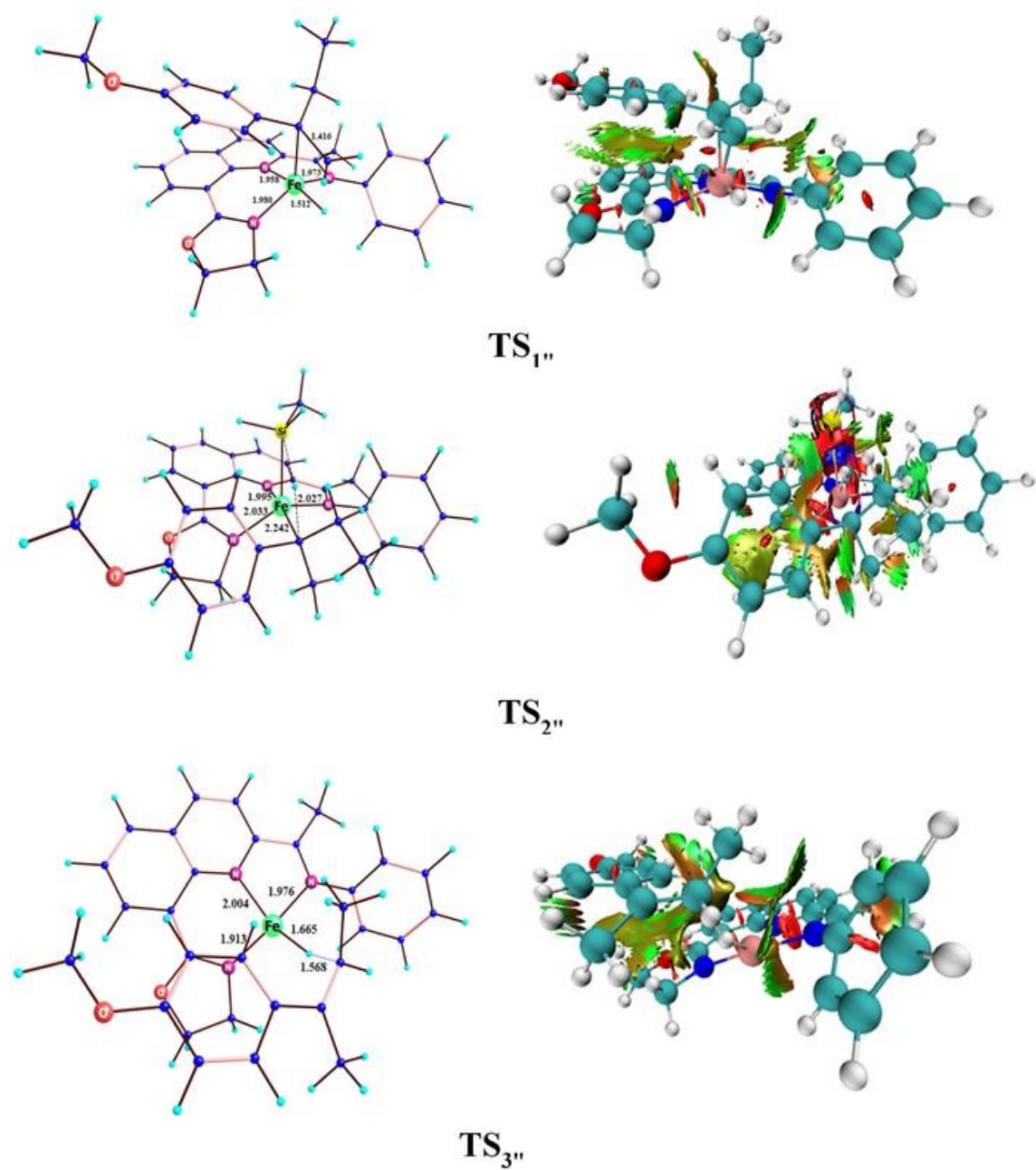


Figure S3: Optimized geometries of the transition states and the corresponding isosurface plots of the nonbonding interactions for 2-1 mode of interaction.

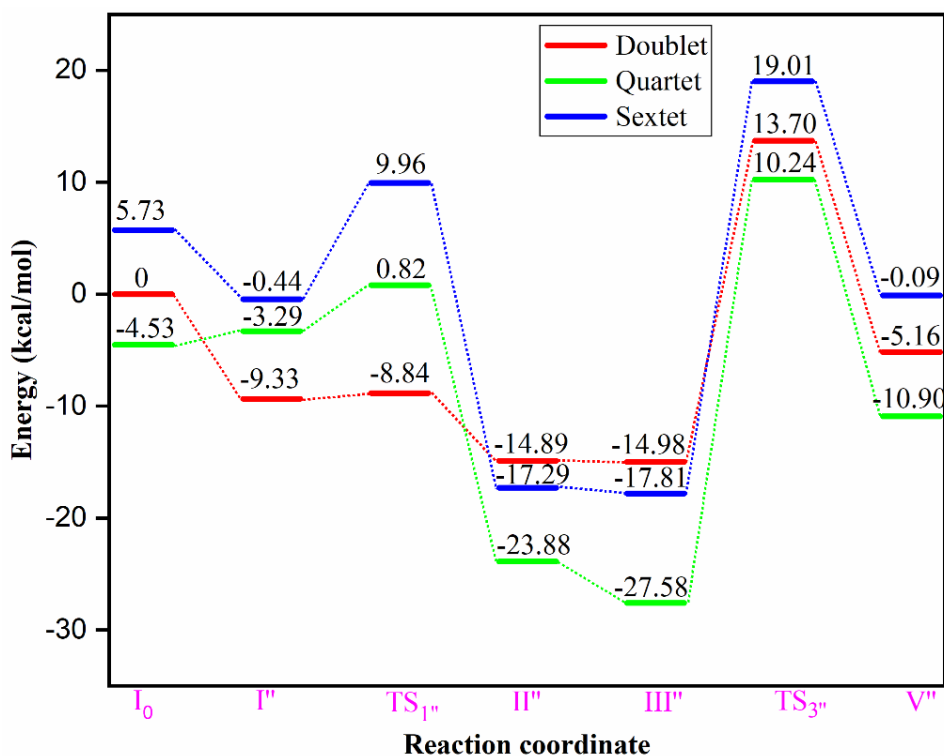


Figure S4: Energy profile diagram for the formation of isomeric alkene by-product in different spin states. The computations are performed within M06L/6-311G**,LANL2DZ level of theory.

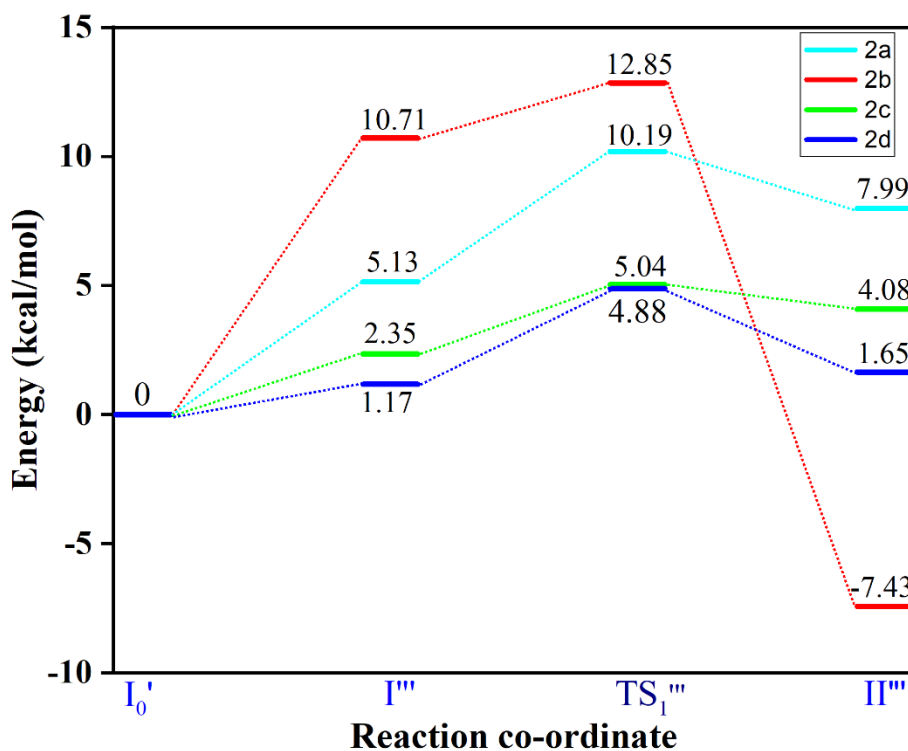


Figure S5: Energy profile diagram of four different possibilities for the formation of chiral alkane from alkene through different possible pathways. The computations are performed within M06L/6-311G**,LANL2DZ level of theory.

Table S3: Calculated relative energy positions of different intermediate and transition states corresponding to Figure S3 at different levels of theories.

Relative energies within different level of theories → Species ↓	M06L/6-311G** (kcal/mol) Gas phase	M06L/Def2-svp (kcal/mol) Gas phase	M06L/Def2-tzvp (kcal/mol) Gas phase	B3LYP/6-311G** (kcal/mol) Gas phase	B3LYP(GD3)/6-311G** (kcal/mol) Gas phase	M06L/6-311+G** (kcal/mol) Gas phase	M06L/6-311G** (kcal/mol) in Acetonitrile solvent
I₀'	0	0	0	0	0	0	0
I₁'''(2a)	5.13	6.39	11.84	35.71	10.97	7.48	14.46
I₁'''(2b)	10.71	14.17	12.65	38.19	7.51	13.41	19.80
I₁'''(2c)	2.35	3.49	4.11	24.13	-5.10	5.17	12.42
I₁'''(2d)	1.17	2.69	3.24	29.41	2.58	3.14	10.57
TS₁'''(2a)	10.19	11.03	12.07	40.23	33.65	13.75	19.42
TS₁'''(2b)	12.85	13.73	14.68	40.32	28.41	17.03	21.75
TS₁'''(2c)	5.04	5.56	6.71	43.47	24.89	7.61	14.88
TS₁'''(2d)	4.88	5.38	6.36	32.67	23.28	7.15	14.84
II''''(2a)	7.99	8.37	9.94	17.23	-0.40	9.80	14.84
II''''(2b)	-7.43	-7.23	-4.67	11.42	-8.33	-7.31	-2.54
II''''(2c)	4.08	3.78	6.60	6.51	-11.58	5.81	11.04
II''''(2d)	1.65	1.58	3.26	12.90	-7.13	2.23	10.68

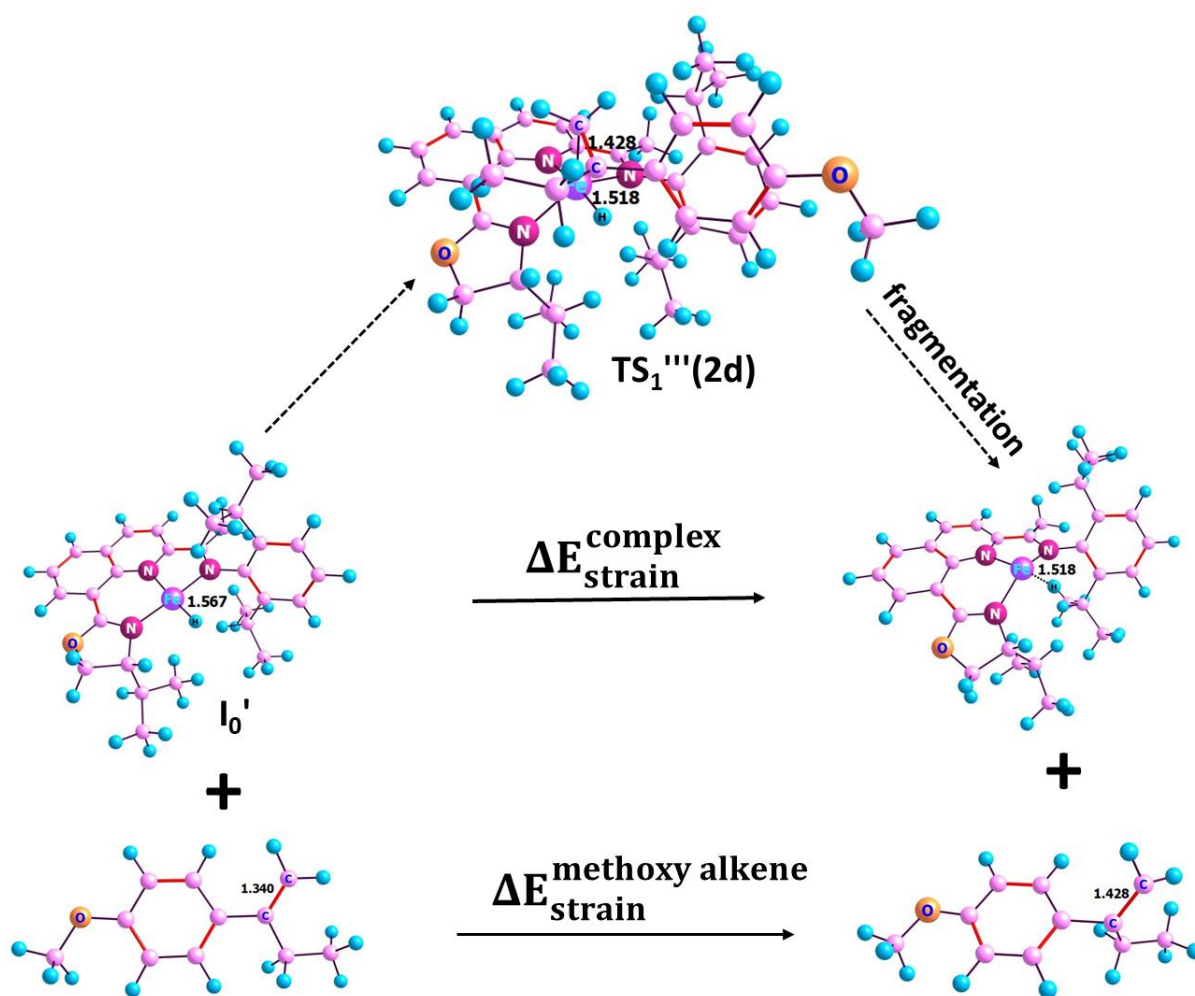


Figure S6: calculating of strain energy of $TS_1'''(2d)$ originating from methoxy benzene and iron hydride reaction.

Table S4: Calculated strain energies in the all possible hydride transfer transition states (TS_1''').

Different possibilities that alkene coordinate to active iron catalyst	$\Delta E_{\text{methoxybenzene (strain)}}$ (kcal/mol)	$\Delta E_{\text{Fe-complex (strain)}}$ (kcal/mol)	$\Delta E_{\text{Total(strain)}}$ (kcal/mol)
$TS_1'''(2a)$	21.32	17.37	38.69
$TS_1'''(2b)$	24.03	18.58	42.61
$TS_1'''(2c)$	22.25	12.59	36.84
$TS_1'''(2d)$	19.11	13.05	32.16

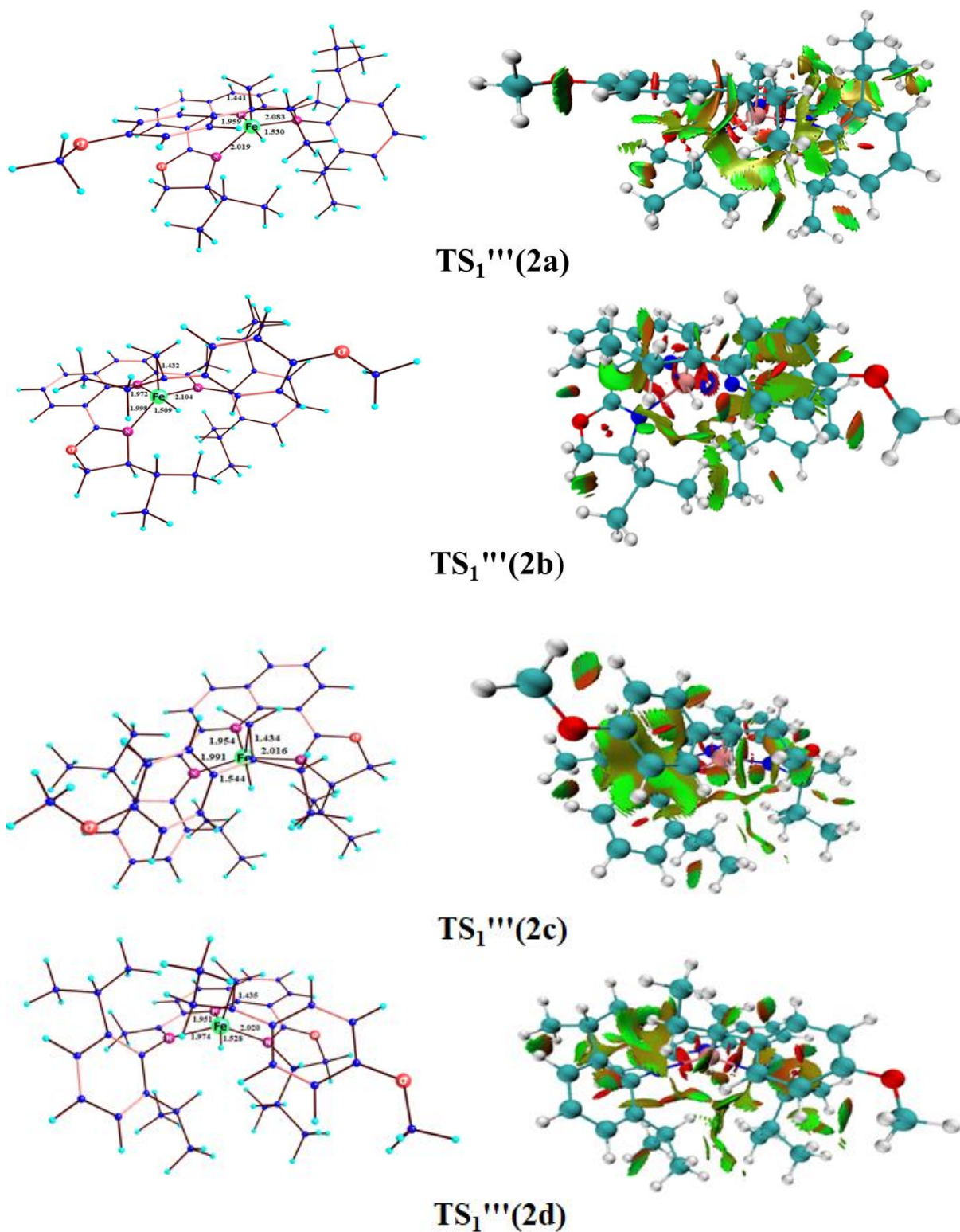


Figure S7: Optimized geometries of the transition state structures and the corresponding isosurface plots of the noncovalent interactions in four possible hydride transfer pathways.

Table S5: Calculated relative energy positions of different intermediate and transition states in absence of silane at different levels of theories.

Relative energies within different level of theories → Species ↓	M06L/6-311G** (kcal/mol) Gas phase	M06L/Def2-svp (kcal/mol) Gas phase	M06L/Def2-tzvp (kcal/mol) Gas phase	B3LYP/6-311G** (kcal/mol) Gas phase	B3LYP(GD3)/6-311G** (kcal/mol) Gas phase	M06L/6311+G** (kcal/mol) Gas phase	M06L/6-311G** (kcal/mol) in Acetonitrile solvent
I₀	0	0	0	0	0	0	0
I	-2.02	0.62	0.93	36.02	15.57	-1.01	6.63
TS₁	2.55	4.66	5.08	36.50	17.02	4.13	11.60
II	-13.90	-11.64	-9.15	2.90	-13.47	-14.40	-8.32
III	-14.54	-12.36	-8.77	2.67	-13.48	-14.50	-6.44
III'	-12.81	-10.25	-7.22	4.62	-11.96	-12.83	-5.44
IV'	-4.82	-3.07	-0.67	22.25	3.24	-2.57	3.51
TS₄	5.84	0.27	9.86	26.38	10.14	10.38	13.63
V'	-22.52	-22.40	-17.26	-12.74	-21.98	-24.11	-16.13

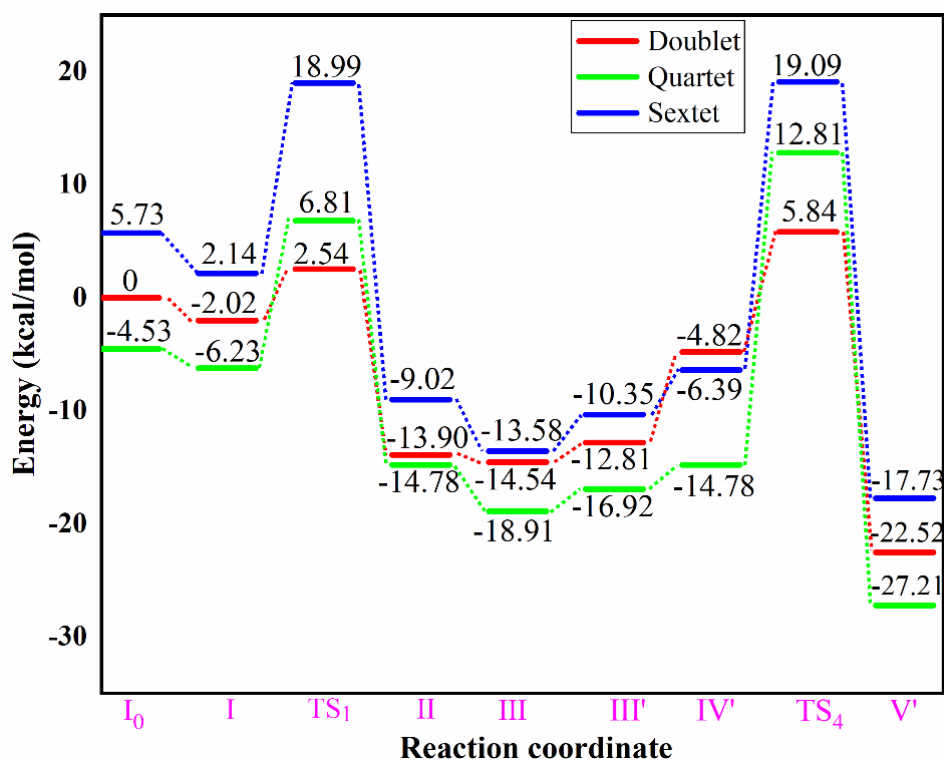


Figure S8: Energy profile diagram for catalytic hydrogenation of alkene via 1-2 mode in absence of silane in different spin states. The computations are performed within M06L/6-311G**, LANL2DZ level of theory.

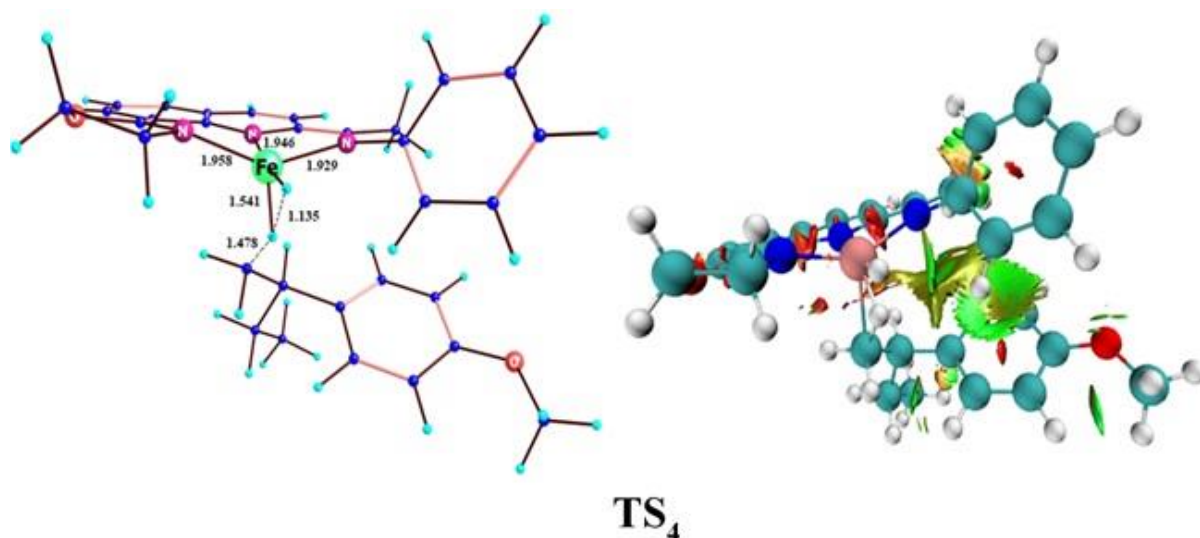


Figure S9: Optimized geometry of the transition state structure, TS₄ and the corresponding isosurface plots of the noncovalent interactions.

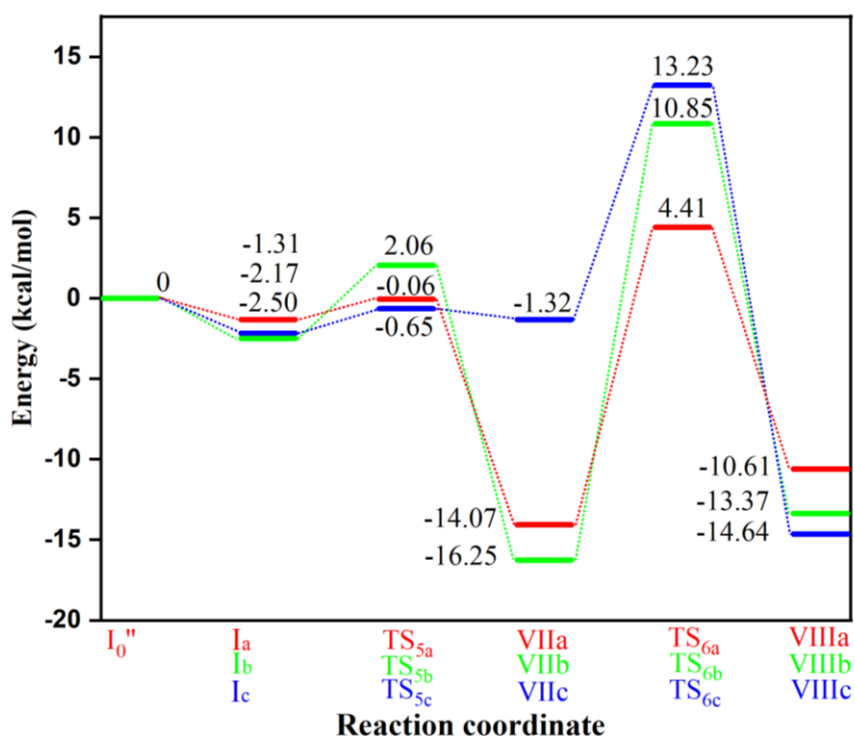
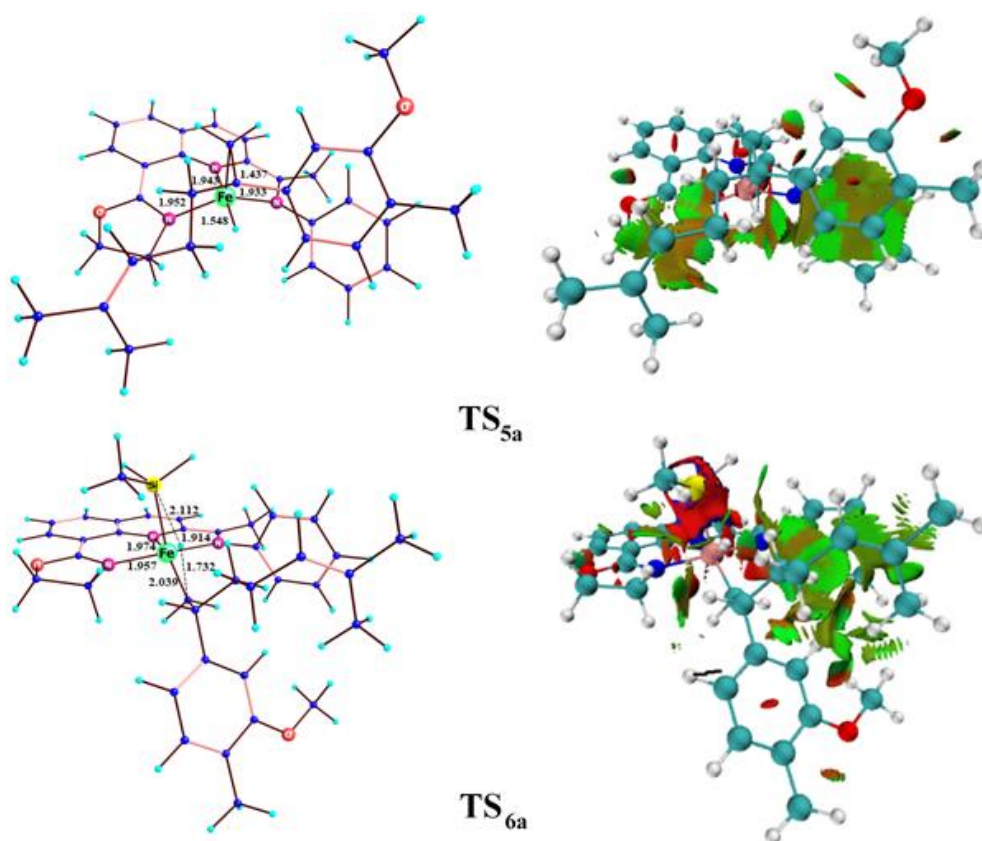


Figure S10: Energy profile diagram for the formation of Fe-catalysed isomeric alkane from alkene I'. The computations are performed within M06L/6-311G**, LANL2DZ level of theory.

Table S6: Calculated relative energy positions of different intermediate and transition states for the formation of Fe-catalysed isomeric alkane at different levels of theories.

Relative energies within different level of theories → Species ↓	M06L/ 6-311G** (kcal/mol) Gas phase	M06L/ Def2-svp (kcal/mol) Gas phase	M06L/ Def2-tzvp (kcal/mol) Gas phase	M06L/ 6-311+G** (kcal/mol) Gas phase	M06L/ 6-311G** (kcal/mol) in Acetonitrile solvent)
I₀''	0	0	0	0	0
I_a	-1.31	1.45	1.71	-1.31	8.02
TS_{5a}	-0.06	3.17	4.27	3.40	11.01
VII_a	-14.07	-9.62	-6.43	-11.86	-6.46
TS_{6a}	4.41	12.14	14.35	10.10	18.50
VIII_a	-10.61	-3.17	-0.95	-8.08	1.91
I_b	-2.17	0.75	1.34	-2.17	7.95
TS_{5b}	2.06	4.44	5.29	1.56	8.61
VII_b	-16.25	-14.37	-10.50	-1.33	5.39
TS_{6b}	10.85	13.10	15.76	14.80	23.56
VIII_b	-13.37	-10.91	-8.71	-16.61	-6.97
I_c	-2.50	0.56	1.23	-2.50	6.49
TS_{5c}	-0.65	1.89	2.91	3.38	12.58
VII_c	-1.32	1.65	4.14	11.93	-6.55
TS_{6c}	13.23	15.45	17.61	11.56	20.14
VIII_c	-14.64	-11.47	-8.84	-15.09	-8.90



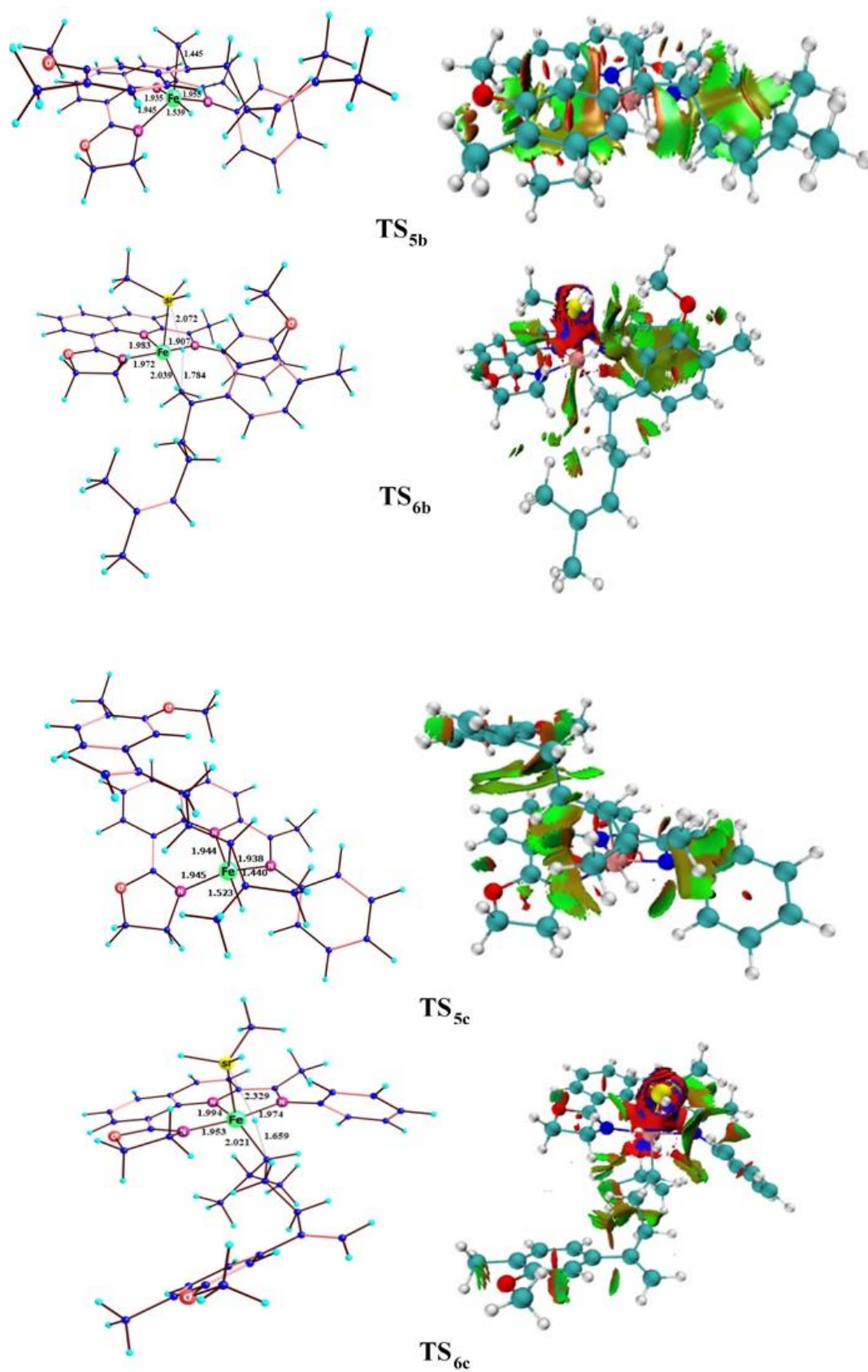


Figure S11: Optimized geometries of the transition state structures and the corresponding isosurface plots of the noncovalent interactions for the formation of Fe-catalysed isomeric alkane from alkene I'.

Cartesian coordinates of the optimized structures using M06L/6-311G,LANL2DZ**

level of theory.

Doublet

I₀

0 2

Fe	0.02208700	-0.01728300	-0.01117600
N	-0.00406400	-0.05418200	1.93561200
C	1.19471200	-0.10055900	2.77605800
C	-1.04610600	-0.10266500	2.71148000
C	0.64403100	0.03485800	4.19191900
H	1.72081000	-1.04530000	2.60357200
H	0.99669900	-0.72425200	4.89110100
N	-1.99915100	-0.07693500	-0.05518200
C	-2.87975100	-0.12587100	0.97553800
C	-3.83565900	-0.13834400	-1.63492300
C	-4.29492400	-0.17209200	0.73712000
C	-4.74113600	-0.17632500	-0.61238000
H	-4.17252400	-0.13613500	-2.66493100
H	-5.80776500	-0.20961600	-0.81054300
C	-2.44045700	-0.13278100	2.34015200
C	-5.19520300	-0.21385100	1.81054800
C	-4.74856000	-0.21369200	3.12175000
H	-5.45350600	-0.24551300	3.94453400
C	-3.38606500	-0.17380100	3.37635300
H	-3.02466100	-0.17524000	4.39675000
H	-6.25812600	-0.24737200	1.58847200
O	-0.78011300	-0.13737900	4.03535000
C	-2.45670100	-0.08448100	-1.35489500
C	-1.45234300	-0.01626300	-2.37297400
C	0.87132800	0.27632500	-2.85475500
C	2.00014300	-0.54791600	-2.81641000
C	0.84197900	1.34130100	-3.76202300
C	3.05713200	-0.32857200	-3.68682800
C	1.91136700	1.56626500	-4.62017500
C	3.02090500	0.72881900	-4.59325900
H	3.92254600	-0.98273200	-3.65097800
H	1.87808900	2.40529300	-5.30812400
H	3.85555800	0.90442200	-5.26357800
H	2.03067600	-1.34599700	-2.08341100
H	-0.01594100	2.00657000	-3.76897400
H	1.88093500	0.70044800	2.49585300
H	0.81310300	1.02323100	4.62973600
N	-0.18771400	0.05428700	-1.94824700
C	-1.84116600	-0.09224300	-3.81706000
H	-0.99019700	-0.36136500	-4.44155300
H	-2.62004500	-0.84353300	-3.96683600
H	-2.23586700	0.85662200	-4.19781700
H	1.58131200	-0.00753800	-0.05493400

I

02

Fe	0.19831600	-0.08247900	0.07915300
N	0.02188200	-0.07586600	2.02805100
C	1.11755500	-0.03819000	2.99716900
C	-1.08698400	0.19093400	2.66476200
C	0.46332100	0.48000800	4.27640300
H	1.54118600	-1.04186800	3.10537700
H	0.61960200	-0.15315100	5.15132600
N	-1.72749700	-0.59624500	-0.03734200
C	-2.71941800	-0.29718400	0.83248600
C	-3.36488200	-1.46294600	-1.60062200
C	-4.09792400	-0.47420000	0.47662400
C	-4.38273900	-1.05727900	-0.79195900
H	-3.57588400	-1.93140300	-2.55497500
H	-5.41912100	-1.18956400	-1.08599000
C	-2.42426500	0.18782500	2.14808300
C	-5.10433700	-0.07865900	1.36250500
C	-4.79732400	0.45467600	2.60853300
H	-5.58985600	0.76060300	3.28225600
C	-3.47506100	0.56598800	3.00167400
H	-3.22618900	0.93184000	3.98998700
H	-6.13944800	-0.20198200	1.05675900
O	-0.94802500	0.47952800	3.98012100
C	-2.02002200	-1.24509900	-1.21464800
C	-0.89077000	-1.65261200	-1.96521400
C	1.50432500	-1.67412300	-2.07517500
C	2.52973500	-2.25474500	-1.31879200
C	1.73052200	-1.42562600	-3.43324100
C	3.72959700	-2.61268900	-1.91538500
C	2.93804900	-1.77493700	-4.02439500
C	3.93948100	-2.37980300	-3.27273900
H	4.50729100	-3.07685400	-1.31679200
H	3.10205200	-1.54927400	-5.07424400
H	4.87951200	-2.66092800	-3.73755000
H	2.35538300	-2.41706300	-0.26076500
H	0.96744800	-0.92249600	-4.01674100
H	1.91634700	0.60962700	2.62856600
H	0.75335100	1.50494300	4.52672400
N	0.29860800	-1.32450900	-1.42692600
C	-1.05762300	-2.48757900	-3.19755500
H	-0.18703000	-3.12241800	-3.36429100
H	-1.93118400	-3.13542100	-3.10774000
H	-1.19268700	-1.88723900	-4.10410000
C	-0.33123900	1.77732000	-0.62675500
H	1.69241700	-0.18157600	0.28625200
C	1.06610400	1.83101200	-0.53180500
C	1.90470600	1.64814900	-1.74384300
C	3.23155500	1.21750300	-1.64390500
C	1.43879700	1.98564000	-3.02214000
C	4.05917700	1.11296200	-2.75273800
H	3.61604300	0.91839100	-0.67286300
C	2.24881300	1.88483500	-4.14171700
H	0.42536200	2.35771400	-3.13917300
C	3.56398300	1.43855700	-4.01627200

H	5.06970200	0.74298600	-2.62802400
H	1.88189300	2.14637900	-5.12868000
C	1.75752400	2.59145100	0.59053700
H	2.52207000	1.95339200	1.04997000
C	0.85983300	3.18627100	1.66106800
H	1.45573700	3.66068200	2.44563400
H	0.19867800	3.95227600	1.24710200
H	0.22131800	2.43904500	2.13670700
O	4.27281000	1.32806500	-5.17634800
C	5.59567800	0.84900500	-5.07320100
H	6.22297800	1.51283200	-4.46541600
H	5.62670400	-0.15932300	-4.64077100
H	5.98901400	0.81768300	-6.08829400
H	-0.96546900	2.24550200	0.12122200
H	-0.81954500	1.58283800	-1.57803100
H	2.32555900	3.40801400	0.12240000

TS₁

0 2

Fe	-0.01296500	0.03801000	0.00709700
N	-0.02517000	-0.00189400	1.95458600
C	1.11654900	0.06807300	2.86690400
C	-1.11233500	0.17724800	2.66388900
C	0.51252300	0.58139300	4.17101600
H	1.56244800	-0.92793300	2.96550600
H	0.78651300	0.00371700	5.05489000
N	-1.84072400	-0.59101900	-0.02130000
C	-2.80034200	-0.38164900	0.91269800
C	-3.49054100	-1.59602500	-1.48798200
C	-4.17977000	-0.65483800	0.62696800
C	-4.49007400	-1.25267500	-0.63059800
H	-3.71858200	-2.08772100	-2.42658900
H	-5.52877900	-1.45688800	-0.86965800
C	-2.46819900	0.09690500	2.22194100
C	-5.16014000	-0.34402800	1.57153100
C	-4.82474400	0.19307900	2.81110300
H	-5.60075800	0.43101700	3.53020400
C	-3.49719600	0.38930200	3.13853700
H	-3.22038700	0.75360900	4.11999000
H	-6.19855300	-0.54185700	1.32130800
O	-0.90788400	0.44740100	3.97799100
C	-2.14407600	-1.28699800	-1.17811400
C	-1.02492200	-1.63957100	-1.95823400
C	1.37010700	-1.59617900	-2.09230900
C	2.38044600	-2.18976900	-1.32599000
C	1.61471600	-1.34785700	-3.44836600
C	3.57967900	-2.57301200	-1.91110000
C	2.82121300	-1.71929600	-4.02672500
C	3.80298900	-2.34809800	-3.26643200
H	4.34314200	-3.05231000	-1.30591600
H	3.00170600	-1.49767500	-5.07489600
H	4.73989500	-2.65012500	-3.72426900

H	2.18978200	-2.35378300	-0.26958300
H	0.86336700	-0.83329100	-4.03816700
H	1.88660400	0.72866600	2.46036000
H	0.73185900	1.63793700	4.35742000
N	0.16480100	-1.25184900	-1.44552900
C	-1.17098100	-2.47154900	-3.19387000
H	-0.30355100	-3.11760100	-3.33912000
H	-2.05258600	-3.11051100	-3.12938200
H	-1.27370600	-1.87007100	-4.10414200
C	-0.27549300	1.81939800	-0.79981300
H	1.49401700	0.36587000	0.04253300
C	1.14184700	1.73063800	-0.57781500
C	2.04330200	1.59758600	-1.77490200
C	3.32251400	1.05706600	-1.64417700
C	1.68118600	2.10094900	-3.02748700
C	4.20814500	0.99414100	-2.71115600
H	3.62515900	0.64012400	-0.68593800
C	2.54596700	2.03881100	-4.10896700
H	0.70522200	2.55798300	-3.15756300
C	3.81258300	1.47444500	-3.96031500
H	5.17967000	0.53623500	-2.57077600
H	2.25921700	2.41944300	-5.08338400
C	1.77420100	2.64895400	0.47985000
H	2.61761300	2.12898100	0.95237300
C	0.84654200	3.22364000	1.53691600
H	1.41876500	3.72737400	2.32070400
H	0.16531700	3.96365000	1.11026700
H	0.22767800	2.45996000	2.01111800
O	4.57724500	1.41493600	-5.08675000
C	5.85266300	0.82406300	-4.96476300
H	6.49235700	1.37694600	-4.26582800
H	5.78432800	-0.21907700	-4.63119500
H	6.29924900	0.85523900	-5.95741800
H	-0.89484700	2.43494100	-0.15208000
H	-0.67632100	1.67646700	-1.80041700
H	2.23600500	3.48009700	-0.06838700

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II

0 2

Fe	0.08225200	-0.17337500	0.06444200
N	0.04318600	-0.09149300	1.98822000
C	1.19185200	-0.08593900	2.90340100
C	-1.04125600	-0.04158600	2.71822800
C	0.57773500	0.36886100	4.21510200
H	1.61436200	-1.09640400	2.95962400
H	0.92509400	-0.16904800	5.09694300
N	-1.87577200	-0.57538900	-0.04341800
C	-2.79724300	-0.45776400	0.95180400
C	-3.65008200	-1.06101700	-1.62921800
C	-4.19563900	-0.62993300	0.68458900

C	-4.58906000	-0.94309100	-0.64592300
H	-3.94502900	-1.28213200	-2.64846500
H	-5.64464600	-1.07682500	-0.86026200
C	-2.41060600	-0.16075300	2.30125900
C	-5.14097100	-0.48394100	1.70924700
C	-4.74838600	-0.17812300	3.00339800
H	-5.48609900	-0.06199300	3.78934200
C	-3.40282400	-0.02363400	3.28991900
H	-3.08550100	0.20519300	4.29923300
H	-6.19130900	-0.61010700	1.46314300
O	-0.82669900	0.09543500	4.05157300
C	-2.28851400	-0.86695900	-1.32544400
C	-1.25167500	-0.92455800	-2.30319000
C	1.06792400	-0.55770400	-2.74080800
C	2.21895700	-1.29288400	-2.44345700
C	1.07756100	0.30120600	-3.84425800
C	3.34643200	-1.18721800	-3.24460100
C	2.21337000	0.41147500	-4.63741000
C	3.35059700	-0.33407600	-4.34537200
H	4.23168600	-1.76669000	-3.00309400
H	2.21121700	1.09145300	-5.48347100
H	4.23681300	-0.24414300	-4.96420300
H	2.21590700	-1.93190000	-1.56517100
H	0.19826200	0.90290200	-4.05447100
H	1.97731400	0.58301100	2.54610100
H	0.69596200	1.44578600	4.38269800
N	-0.03284300	-0.62058700	-1.86183000
C	-1.54702000	-1.33966000	-3.71036200
H	-0.64734800	-1.69307000	-4.21362000
H	-2.28676500	-2.14217000	-3.73313200
H	-1.94928600	-0.51479800	-4.30925000
C	1.74197700	0.94642400	-0.09394400
H	0.99115500	2.24874600	1.47001700
C	1.62584900	2.32488500	0.57054000
C	2.95901500	2.86971900	1.03575100
C	3.12926400	3.36730400	2.32426300
C	4.07032900	2.90290600	0.18151800
C	4.34888300	3.88052500	2.76838300
H	2.28087900	3.36397000	3.00664900
C	5.28663700	3.41194900	0.59752200
H	3.97474200	2.51074800	-0.82792100
C	5.43582000	3.90466900	1.89799000
H	4.43629200	4.25528000	3.78131200
H	6.14580500	3.43843200	-0.06426200
C	0.92816400	3.33566400	-0.35331700
H	0.89854600	4.30976000	0.15090300
C	-0.47719600	2.92709500	-0.76272700
H	-0.99482500	3.73493700	-1.28769400
H	-0.46919400	2.05515100	-1.42366900
H	-1.08579600	2.66387200	0.11200800
O	6.67405600	4.38005300	2.21501600

C	6.84965700	4.88929800	3.51720300
H	6.18607400	5.74065400	3.71436200
H	6.67397800	4.12195400	4.28180500
H	7.88463000	5.22236700	3.57824600
H	2.08122000	1.06888900	-1.12998000
H	2.51364600	0.33873300	0.40723300
H	1.54913400	3.48095900	-1.24841500

III

0 2

Fe	0.23714900	-0.08945100	-0.13644400
N	0.09425200	-0.02200900	1.79446200
C	1.15753000	0.26738200	2.76203900
C	-1.02591900	-0.13023500	2.46835000
C	0.52640500	-0.12302300	4.08439200
H	2.05968600	-0.30026600	2.53271700
H	0.76773400	-1.15366000	4.37390700
N	-1.75638400	-0.03386900	-0.36630700
C	-2.69702000	-0.27088400	0.58395000
C	-3.46292100	-0.15621400	-2.08744600
C	-4.07041200	-0.48401900	0.22683500
C	-4.41924700	-0.41337200	-1.14906900
H	-3.72199600	-0.11421700	-3.13943500
H	-5.45436000	-0.57529000	-1.43379500
C	-2.35624400	-0.32643000	1.97836800
C	-5.03115500	-0.75344300	1.20978300
C	-4.68085800	-0.80691100	2.55262400
H	-5.43017900	-1.01561300	3.30805700
C	-3.36681500	-0.59045000	2.92510200
H	-3.08562100	-0.62818000	3.96981600
H	-6.05784800	-0.91867100	0.89661700
O	-0.88558700	-0.05249600	3.81912900
C	-2.12083500	0.01661700	-1.69299000
C	-1.05598700	0.20599100	-2.62376000
C	1.31828300	0.34429800	-2.89930700
C	1.57097400	-0.50977100	-3.97919200
C	2.29376600	1.28058500	-2.53825800
C	2.76323300	-0.41509500	-4.68757400
C	3.47606100	1.37865800	-3.25550600
C	3.71834700	0.53176800	-4.33469200
H	2.94838200	-1.09214400	-5.51556700
H	4.21931200	2.11416000	-2.96492200
H	4.64839700	0.60267400	-4.88815700
H	0.83620600	-1.26542900	-4.24105700
H	2.10857200	1.91593200	-1.67707400
H	1.41592500	1.33282200	2.71464300
H	0.74780800	0.54261900	4.91847000
N	0.16632000	0.22582100	-2.10096800
C	-1.34885000	0.40699800	-4.07809800
H	-0.51812300	0.89608700	-4.58610900
H	-1.53215300	-0.54188900	-4.59721600

H	-2.23946500	1.02340900	-4.21445200
C	2.10730800	-0.89487700	-0.04426600
H	2.53028100	-0.98545300	-1.05477000
H	2.85108100	-0.35213500	0.55404600
C	1.84312500	-2.29795600	0.52447200
H	1.72742000	-2.22609600	1.61823800
C	2.98108000	-3.29088900	0.25135100
H	3.10391500	-3.39123300	-0.83562800
H	3.91793400	-2.84859700	0.61256700
C	2.76602700	-4.65706200	0.88000700
H	3.60357800	-5.33288400	0.68859200
H	2.64894800	-4.57917000	1.96638400
H	1.86080200	-5.13468300	0.49287700
C	0.50747500	-2.79484000	-0.00519600
C	-0.55922000	-3.11866700	0.84282200
C	0.27429300	-2.86312500	-1.38123600
C	-1.80891200	-3.45278500	0.34768900
H	-0.40802700	-3.07620500	1.91999300
C	-0.97217700	-3.19843800	-1.90163300
H	1.08163100	-2.61287200	-2.06638300
C	-2.02833900	-3.47680000	-1.03163400
H	-2.64191700	-3.66805000	1.00911600
H	-1.11469100	-3.22004900	-2.97651200
O	-3.29777600	-3.77194000	-1.42741300
C	-3.55428100	-3.76253500	-2.81317900
H	-2.96893600	-4.52579300	-3.34119700
H	-4.61482400	-3.98216100	-2.92892000
H	-3.34013400	-2.78064600	-3.25604400

TS₂

0 2

Fe	0.09002000	0.02608800	0.02111000
N	0.15055800	-0.04383400	1.96032800
C	1.36599600	0.08265900	2.77061500
C	-0.86095400	0.03662300	2.77399100
C	0.86789200	-0.21200800	4.17235700
H	2.13943200	-0.60844800	2.43281800
H	0.99220000	-1.26667400	4.44775200
N	-1.86934600	0.28144800	0.03658200
C	-2.72623500	0.24110300	1.09996000
C	-3.77074200	0.54842200	-1.46006600
C	-4.14521900	0.31420800	0.90872200
C	-4.64018600	0.47531000	-0.41385900
H	-4.13434900	0.66898900	-2.47447700
H	-5.71328800	0.53396900	-0.56726100
C	-2.25718200	0.10589100	2.44540000
C	-5.02039800	0.22685600	2.00068500
C	-4.54330000	0.08504700	3.29294900
H	-5.22770300	0.01951500	4.13107600
C	-3.17526600	0.03274000	3.50561600
H	-2.78393200	-0.07122700	4.50968300

H	-6.08793100	0.27642500	1.80611100
O	-0.54316800	0.06358600	4.09420400
C	-2.38371500	0.43061800	-1.23548500
C	-1.43114900	0.43058100	-2.28659700
C	0.84778900	0.08510100	-2.86656900
C	0.74401800	-0.85871300	-3.89731300
C	2.02099300	0.84158000	-2.76874200
C	1.78429400	-1.04290100	-4.79899000
C	3.05265600	0.66103700	-3.68003000
C	2.94500400	-0.28367400	-4.69645100
H	1.68725900	-1.78736000	-5.58297900
H	3.95126800	1.26328000	-3.59158200
H	3.75791200	-0.42738400	-5.39995600
H	-0.15963900	-1.45629800	-3.97517800
H	2.11688200	1.57176400	-1.97259500
H	1.76012100	1.10267900	2.66520900
H	1.29252400	0.41470200	4.95607300
N	-0.17297600	0.20915300	-1.90027500
C	-1.83981500	0.75672800	-3.68968200
H	-0.98517900	1.07018100	-4.28913700
H	-2.30144500	-0.09447900	-4.20629000
H	-2.56858300	1.57135500	-3.69970500
C	1.71272900	-1.21455500	-0.11907100
H	1.91879800	-1.38765800	-1.18161500
H	2.68468000	-0.99159500	0.33959100
C	1.14693100	-2.49387900	0.52322800
H	1.19697700	-2.39314800	1.61754300
C	1.99116300	-3.72050000	0.14009100
H	1.94501400	-3.85124000	-0.94921700
H	3.04224200	-3.50354000	0.36858600
C	1.55529700	-4.99730100	0.83779100
H	2.18950100	-5.84449500	0.56533400
H	1.60033000	-4.88960300	1.92675900
H	0.52467600	-5.25943100	0.58169900
C	-0.31685800	-2.68672600	0.17673900
C	-1.29736300	-2.86973400	1.15914500
C	-0.73046800	-2.70059000	-1.15606400
C	-2.63549700	-3.00093300	0.83094900
H	-1.00209500	-2.87895000	2.20663500
C	-2.06817800	-2.83339700	-1.51032000
H	0.01469000	-2.58220200	-1.93874500
C	-3.03272500	-2.95978900	-0.50813000
H	-3.39930200	-3.10316600	1.59487500
H	-2.34926400	-2.81479800	-2.55736700
O	-4.37212400	-3.04546600	-0.73339500
C	-4.80293400	-2.96479500	-2.07400600
H	-4.41937500	-3.79840500	-2.67530000
H	-5.89057800	-3.01424900	-2.04812200
H	-4.49551500	-2.01864800	-2.53823700
Si	0.51376200	2.33058500	0.19148300
H	1.49596100	0.48521600	-0.04680800

H	1.92283700	2.80142800	0.15842200
C	-0.39803600	3.32517500	-1.15916900
H	-1.46167400	3.07634700	-1.18166100
H	-0.30655600	4.39905700	-0.97495000
H	0.01411300	3.11602500	-2.14976700
H	0.00041400	2.76456900	1.51618500

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IV

0 2

Fe	0.20687500	-0.20284000	0.17138200
N	0.49156500	-0.05522600	2.04364300
C	1.75187700	0.26996300	2.71671300
C	-0.44742400	-0.12290600	2.95597200
C	1.42682700	0.05225200	4.18693100
H	2.55643600	-0.37748500	2.35818400
H	1.78363100	-0.91392400	4.55968100
N	-1.74700000	-0.55391600	0.36183000
C	-2.47890500	-0.50630000	1.50496000
C	-3.77680000	-0.79480400	-0.94614300
C	-3.90518400	-0.65439900	1.46720500
C	-4.52921000	-0.77825000	0.19245600
H	-4.24838300	-0.88517500	-1.91835800
H	-5.61084300	-0.86071900	0.14858800
C	-1.85495600	-0.33299800	2.78598700
C	-4.64740400	-0.68230600	2.65403000
C	-4.02125900	-0.55991800	3.88745200
H	-4.60179500	-0.59050300	4.80267300
C	-2.65081400	-0.38120600	3.94662800
H	-2.16027000	-0.26748000	4.90477900
H	-5.72570900	-0.79589100	2.58785100
O	-0.01063800	0.04041900	4.23015200
C	-2.37045600	-0.70872600	-0.85841500
C	-1.49673300	-0.80782200	-1.97605900
C	0.78506400	-1.02547900	-2.64375200
C	0.73017800	-2.28817900	-3.25733200
C	1.88887600	-0.20477300	-2.90657200
C	1.74331000	-2.71039500	-4.10676300
C	2.89072000	-0.62720700	-3.76958500
C	2.82930800	-1.88081500	-4.37179900
H	1.68768200	-3.69654800	-4.55706300
H	3.73141000	0.02993600	-3.96832800
H	3.62096700	-2.21036900	-5.03598000
H	-0.10340600	-2.94693200	-3.03026300
H	1.94022100	0.77027400	-2.43838000
H	2.03299900	1.30577500	2.48878500
H	1.77715500	0.84282300	4.85139800
N	-0.19656400	-0.63768200	-1.71184300
C	-2.04205500	-1.01233900	-3.35602600
H	-1.28661100	-0.81103600	-4.11467600
H	-2.41086200	-2.03074600	-3.51975800

H	-2.88441200	-0.33885300	-3.53526300
C	3.81289200	-1.59015100	-0.12484900
H	3.44465400	-1.91273100	-1.10388800
H	4.86905700	-1.33483300	-0.24936700
C	3.63426600	-2.68589100	0.92300000
H	4.12426800	-2.36038000	1.85439100
C	4.33658900	-3.97409200	0.46512900
H	3.86179100	-4.31147100	-0.46663500
H	5.37213300	-3.72740800	0.19909700
C	4.31797300	-5.09134500	1.49181700
H	4.85814000	-5.97214700	1.13719200
H	4.78602600	-4.77627100	2.43042700
H	3.29653300	-5.40293100	1.72743300
C	2.17955000	-2.93574900	1.25238300
C	1.74671300	-3.09880800	2.57230600
C	1.21885300	-3.04308600	0.24709700
C	0.41738800	-3.34152500	2.88078400
H	2.47650700	-3.03395300	3.37763700
C	-0.12275600	-3.29365600	0.53267500
H	1.51477100	-2.93806700	-0.79346500
C	-0.53170200	-3.44080300	1.85933200
H	0.08317300	-3.45070600	3.90786500
H	-0.83794700	-3.35181500	-0.28049700
O	-1.81124500	-3.67200500	2.25069400
C	-2.76120100	-3.92445800	1.23363700
H	-2.50090500	-4.82444300	0.66254300
H	-3.71287200	-4.07619000	1.74067300
H	-2.85878400	-3.07914100	0.54345000
Si	1.07204800	2.01495800	-0.22553700
H	3.27193600	-0.67306200	0.13327800
H	0.88061300	2.60945800	-1.57292900
C	0.11903100	3.14109600	1.01048500
H	0.33620500	2.86997700	2.04758600
H	0.36791800	4.19813400	0.88330500
H	-0.96047700	3.03463500	0.87371600
H	2.52403300	2.20435700	0.06464000

V

02

Fe	0.02231100	0.14987600	-0.00222500
N	0.03851200	0.13114100	1.91729800
C	1.20432500	0.16955900	2.81021400
C	-1.03095300	0.08827700	2.67154600
C	0.62615900	-0.27672500	4.14054200
H	2.00063000	-0.48007300	2.44447100
H	0.76276700	-1.34852700	4.32285000
N	-1.93166600	0.56616500	-0.07544400
C	-2.82649300	0.49403500	0.94456200
C	-3.72314900	1.09779800	-1.62083000
C	-4.22593400	0.69954800	0.71012500
C	-4.64132700	1.01224700	-0.61399700

H	-4.03735400	1.32156100	-2.63367800
H	-5.69754700	1.17318000	-0.80513800
C	-2.41022000	0.20750100	2.28660500
C	-5.14728100	0.58160500	1.75934500
C	-4.72845900	0.27540900	3.04542600
H	-5.44860700	0.17885500	3.84995600
C	-3.37930300	0.09721700	3.30057500
H	-3.04181500	-0.12771000	4.30423400
H	-6.20085000	0.72793300	1.53962100
O	-0.78603100	-0.02650600	3.99933400
C	-2.36096100	0.86412200	-1.34899500
C	-1.34117800	0.88721100	-2.34681200
C	0.96775100	0.47022000	-2.82428200
C	0.92143500	-0.28772700	-3.99753000
C	2.16230000	1.10881800	-2.47685900
C	2.04520600	-0.39424500	-4.80795100
C	3.27777600	1.00790100	-3.29441000
C	3.22550300	0.25537200	-4.46507700
H	1.99969100	-1.00074000	-5.70688400
H	4.19663800	1.51076500	-3.01102300
H	4.10234400	0.16557100	-5.09704800
H	0.01257900	-0.82530200	-4.24747200
H	2.20108900	1.67102400	-1.54792900
H	1.59955400	1.19207800	2.84221700
H	0.98099900	0.28174700	5.00625100
N	-0.12347600	0.54063600	-1.93057000
C	-1.65305700	1.33069700	-3.74149800
H	-0.75783000	1.68417400	-4.25237700
H	-2.07402100	0.52279100	-4.35027500
H	-2.38342700	2.14174000	-3.73537800
H	2.18368300	-1.93503800	-1.55935600
H	3.16868000	-0.79203000	0.25385200
Si	1.88436000	-1.40416000	-0.20605500
C	1.61808800	-2.94245200	0.92833900
H	2.48765000	-3.60556400	0.92777800
H	1.41844300	-2.66020300	1.96619700
H	0.75906400	-3.52674100	0.58964900

TS₃

0 2

Fe	0.34891300	0.14371600	0.00329100
N	0.33075600	0.54042500	1.90144400
C	1.52137700	0.68915200	2.74011300
C	-0.68732000	0.32309800	2.68686200
C	0.95407800	0.78961700	4.15043800
H	2.16907900	-0.18386000	2.59871200
H	1.43905300	0.14580500	4.88461500
N	-1.60510800	0.12885300	-0.07627000
C	-2.49080700	0.04597300	0.95599200
C	-3.46057500	0.09075500	-1.65352100
C	-3.89813500	-0.08295900	0.71331900

C	-4.35291800	-0.05853900	-0.63829000
H	-3.79798700	0.11787700	-2.68320500
H	-5.41647500	-0.15106100	-0.83260900
C	-2.05516600	0.07636000	2.31903600
C	-4.78627700	-0.23317500	1.78294200
C	-4.33898300	-0.24241100	3.09666500
H	-5.03969500	-0.36156500	3.91522300
C	-2.99079500	-0.07738500	3.35697900
H	-2.63059600	-0.05104800	4.37734800
H	-5.84399900	-0.34209800	1.56043100
O	-0.41209000	0.34920600	4.00948900
C	-2.07653700	0.18137100	-1.38009000
C	-1.07972400	0.28584200	-2.36965700
C	1.28705700	0.29727800	-2.77866700
C	1.43546500	-0.74572100	-3.69970100
C	2.29397500	1.26240900	-2.68394700
C	2.56348600	-0.81734400	-4.50814900
C	3.41202400	1.19402600	-3.50277500
C	3.55455200	0.15416100	-4.41766800
H	2.66990100	-1.64087100	-5.20720100
H	4.18174900	1.95500900	-3.42193200
H	4.43407500	0.09780700	-5.05020800
H	0.66894200	-1.51206100	-3.76400500
H	2.17765600	2.05400400	-1.95207400
H	2.09082400	1.56862300	2.43634100
H	0.93560200	1.81424300	4.53469100
N	0.18120500	0.36616600	-1.89872900
C	-1.42200300	0.34189300	-3.82551700
H	-0.62232500	0.80855700	-4.40122500
H	-1.59414800	-0.65077500	-4.25827400
H	-2.33209700	0.92271000	-3.98800600
H	1.91300600	-3.14105300	-0.25080000
H	0.39105600	-2.58053100	1.48132800
Si	0.71884500	-2.33042800	0.06205600
C	-0.69887200	-2.92951900	-1.05962800
H	-0.61375200	-2.51408900	-2.06596500
H	-0.69122000	-4.01926900	-1.14314600
H	-1.66402900	-2.61745000	-0.65732700
H	1.77861400	0.67327100	-0.02614000
H	1.57495900	-0.89933200	-0.03406700

Imaginary Frequency: -432.50

VI

0 2

Fe	-0.05526300	-0.02788200	0.51689300
N	-0.10378300	0.21249900	2.44887600
C	1.07767700	0.47288700	3.27576900
C	-1.15548600	0.28468200	3.21050400
C	0.52213600	0.48056900	4.69547300
H	1.82957600	-0.29989800	3.10578700
H	0.75106500	-0.43343200	5.25226200

N	-2.07807500	-0.10821500	0.45957500
C	-2.96608800	-0.06810300	1.48477500
C	-3.89013100	-0.48445000	-1.10372200
C	-4.37210800	-0.23659000	1.25126600
C	-4.80313400	-0.43660700	-0.08843900
H	-4.21592500	-0.63977500	-2.12543800
H	-5.86393500	-0.55691700	-0.28416200
C	-2.54090500	0.12085900	2.84039300
C	-5.27752400	-0.21486000	2.32096200
C	-4.84377000	-0.03659200	3.62457500
H	-5.55201200	-0.02766600	4.44508300
C	-3.48991100	0.12914800	3.87417000
H	-3.13672300	0.26415900	4.88862600
H	-6.33354300	-0.34759300	2.10301700
O	-0.90918500	0.53336200	4.51399300
C	-2.51814100	-0.32661200	-0.82773100
C	-1.50283300	-0.38450700	-1.83582800
C	0.82470900	-0.13382900	-2.33014800
C	1.96417700	-0.92435400	-2.15144600
C	0.79493500	0.78083800	-3.38886400
C	3.03206500	-0.82196000	-3.02992700
C	1.87495000	0.89023500	-4.25633000
C	2.99564300	0.08509800	-4.08676100
H	3.90608600	-1.44853000	-2.88298500
H	1.84118200	1.61467400	-5.06400500
H	3.83866100	0.17103600	-4.76404800
H	1.99396000	-1.60135300	-1.30534200
H	-0.07164400	1.42373100	-3.50858700
H	1.52526300	1.42701100	2.97847700
H	0.81337600	1.34380200	5.29456000
N	-0.24420000	-0.23473400	-1.41336800
C	-1.87366300	-0.67391500	-3.25753100
H	-2.28535900	0.20205400	-3.77150500
H	-1.01057400	-1.00915600	-3.83109700
H	-2.63390900	-1.45694500	-3.30509600
H	-0.65149000	-4.57580700	4.26289800
H	-1.06124200	-2.24311000	4.50627800
Si	-0.58174800	-3.27798000	3.57405100
C	-1.62104300	-3.29266600	1.99271500
H	-2.68971300	-3.25966100	2.21756800
H	-1.38687100	-2.42733500	1.36872900
H	-1.42739100	-4.19081000	1.40330300
H	1.50264400	-0.00093400	0.48904300
H	0.83058600	-2.99404100	3.26266600

Quartet

I₀

0 4

Fe	-0.00309500	-0.06838000	-0.01520100
N	0.01336800	-0.07954800	1.91413300

C	1.20776700	-0.15786500	2.75730700
C	-1.03610100	-0.10487600	2.69229600
C	0.66081100	0.04283400	4.16476200
H	1.68727800	-1.13215500	2.61503200
H	1.01219300	-0.68349500	4.89824600
N	-1.99591300	-0.09210600	-0.07568900
C	-2.87259400	-0.12366900	0.96284300
C	-3.85270300	-0.16412700	-1.64456000
C	-4.28819500	-0.16385500	0.73233900
C	-4.74652900	-0.18667700	-0.61633300
H	-4.19655300	-0.17445800	-2.67236500
H	-5.81518000	-0.22047600	-0.80308300
C	-2.42535300	-0.11838100	2.32522500
C	-5.18346400	-0.18183100	1.80714700
C	-4.73084000	-0.16551400	3.12026600
H	-5.43373100	-0.17776300	3.94538500
C	-3.37130400	-0.13508200	3.36832100
H	-3.00502300	-0.12533900	4.38696400
H	-6.24749600	-0.20842600	1.58968400
O	-0.76279100	-0.13275900	4.01653100
C	-2.46843500	-0.10732400	-1.37699100
C	-1.47556700	-0.03999500	-2.38554700
C	0.85525900	0.27986900	-2.83559200
C	2.00399400	-0.51719000	-2.78304200
C	0.81287500	1.34261500	-3.74642100
C	3.06708100	-0.27292500	-3.63956300
C	1.88644800	1.59029600	-4.59239300
C	3.01612300	0.78043900	-4.54942300
H	3.94712800	-0.90636600	-3.59152300
H	1.84145900	2.42682700	-5.28266500
H	3.85401100	0.97432900	-5.21053500
H	2.04495400	-1.31787100	-2.05332400
H	-0.05882100	1.98911400	-3.76452700
H	1.93069800	0.60166800	2.45658800
H	0.83362200	1.05090700	4.55496800
N	-0.21019000	0.03464000	-1.94331600
C	-1.84257700	-0.11748100	-3.83514500
H	-0.99235100	-0.43331100	-4.43957500
H	-2.65055300	-0.83524200	-3.99083300
H	-2.18460200	0.84239900	-4.23770600
H	1.55056100	-0.14283900	-0.01275200

I

04

Fe	0.39513400	-0.73952500	0.36558200
N	0.14491400	-0.10689700	2.18248500
C	1.18454100	0.01872000	3.20570900
C	-1.00552900	0.16699400	2.73853100
C	0.45716500	0.66117500	4.38111100
H	1.58901100	-0.97222000	3.43845000
H	0.60432100	0.15593700	5.33655200
N	-1.57343400	-0.86359200	0.05477300
C	-2.57739700	-0.41793500	0.85387100
C	-3.20205200	-1.49409000	-1.63591200
C	-3.94439300	-0.46614400	0.41997900

C	-4.21992100	-1.02596700	-0.86039500
H	-3.40588600	-1.91399600	-2.61399500
H	-5.24987400	-1.06969700	-1.19998100
C	-2.31921200	0.11587700	2.16014100
C	-4.96896500	0.01971300	1.23922700
C	-4.69649500	0.54839800	2.49518400
H	-5.49847400	0.92342800	3.12071500
C	-3.39071000	0.58615700	2.94547200
H	-3.16523100	0.98362700	3.92686200
H	-5.98936000	-0.02851500	0.86955400
O	-0.93759200	0.55053900	4.03486200
C	-1.86812800	-1.40331200	-1.18366900
C	-0.75182000	-1.81228100	-1.95501400
C	1.63745100	-1.84363100	-2.11771200
C	2.70087300	-2.46440400	-1.44856400
C	1.80654600	-1.49667000	-3.46390500
C	3.87631300	-2.76491700	-2.11915100
C	2.98839700	-1.79436900	-4.12986400
C	4.02653400	-2.43881600	-3.46597700
H	4.68230900	-3.26023900	-1.58666900
H	3.10327100	-1.49588800	-5.16785300
H	4.94637700	-2.68081700	-3.98943900
H	2.58198000	-2.69970100	-0.39703500
H	1.01908400	-0.95461800	-3.97583600
H	2.01416700	0.62051300	2.82942900
H	0.68844300	1.72382300	4.50397800
N	0.45019300	-1.55597300	-1.41366400
C	-0.95435000	-2.57232600	-3.23068300
H	-0.08794300	-3.19230300	-3.46063400
H	-1.82403200	-3.22705900	-3.15154500
H	-1.11897300	-1.92051900	-4.09570200
C	-0.47370100	1.98001100	-0.66834600
H	1.94161300	-0.68364800	0.59286600
C	0.85436400	2.16574400	-0.61324000
C	1.72133900	1.88674100	-1.77583400
C	3.03048000	1.42186200	-1.61554900
C	1.27628800	2.12387300	-3.08564000
C	3.86638200	1.19755100	-2.70238900
H	3.39850400	1.19163000	-0.62083900
C	2.09737000	1.91290400	-4.17762600
H	0.27571400	2.51698600	-3.24015500
C	3.40137300	1.44607400	-3.99300000
H	4.86115100	0.80320600	-2.53461700
H	1.75710800	2.11259700	-5.18813300
C	1.54926700	2.66358000	0.62982000
H	2.10659600	1.81633500	1.05470900
C	0.65735200	3.28166300	1.68969800
H	1.25006400	3.63318800	2.53857000
H	0.10583300	4.13946500	1.29480000
H	-0.08089200	2.57331500	2.07332900
O	4.12860600	1.25132800	-5.12688300
C	5.45910700	0.80387400	-4.96666900
H	6.05720300	1.51726400	-4.38688400
H	5.49696900	-0.17538500	-4.47415100
H	5.87434700	0.72047300	-5.96992900

H	-1.12751100	2.21565000	0.16454600
H	-0.95254300	1.57272900	-1.55320400
H	2.31821900	3.38607800	0.32824300

TS₁

0 4

Fe	0.08324200	0.22642800	0.09391500
N	0.09032300	-0.17177400	2.06718500
C	1.22305100	-0.33052200	2.97504000
C	-0.99906000	-0.12554100	2.78754400
C	0.61792100	-0.06205400	4.34808100
H	1.63617300	-1.34278800	2.88280400
H	0.88589200	-0.78776100	5.11619500
N	-1.74624400	-0.47742000	0.03026700
C	-2.70292200	-0.33267700	0.97128500
C	-3.41912000	-1.11516700	-1.59497400
C	-4.09179500	-0.47029400	0.63910400
C	-4.41311100	-0.83316500	-0.70275400
H	-3.66619100	-1.43347900	-2.60153100
H	-5.45746300	-0.91422100	-0.98652800
C	-2.35930100	-0.06607300	2.33713100
C	-5.06368300	-0.25053300	1.61848500
C	-4.71362300	0.06387300	2.93116300
H	-5.48366200	0.23452000	3.67506000
C	-3.38097300	0.13454900	3.28704800
H	-3.09638000	0.33530900	4.31273100
H	-6.10935000	-0.33418800	1.33551000
O	-0.80320200	-0.15743800	4.12619700
C	-2.06284200	-0.97759500	-1.22363100
C	-0.95346800	-1.37775500	-2.01827200
C	1.45845500	-1.55828300	-2.03825300
C	2.43721900	-1.99874900	-1.12792100
C	1.79551800	-1.52901800	-3.40172300
C	3.67426500	-2.44216800	-1.56609800
C	3.04079600	-1.96762500	-3.83300900
C	3.98438300	-2.43878600	-2.92536400
H	4.40297400	-2.79656500	-0.84308700
H	3.28138000	-1.91761500	-4.89159600
H	4.95150200	-2.79122000	-3.26976100
H	2.18855000	-1.99662100	-0.06917700
H	1.09293400	-1.11996400	-4.11834000
H	2.02154100	0.37003000	2.71229000
H	0.83347400	0.94529800	4.72082100
N	0.25187500	-1.10244400	-1.50897300
C	-1.17086200	-2.16177800	-3.27600400
H	-0.37598700	-2.89729700	-3.41354300
H	-2.12067200	-2.69588800	-3.25146600
H	-1.17280600	-1.52807100	-4.17033800
C	-0.41144400	1.84105000	-1.02979100
H	1.49653000	0.84183700	0.21691800
C	0.97914500	2.01872500	-0.80748800
C	1.92205200	1.75310200	-1.93912500
C	3.21535000	1.28242300	-1.71353500
C	1.55525200	2.02671900	-3.26111500

C	4.10968800	1.06337200	-2.75152800
H	3.51781100	1.03472100	-0.69853100
C	2.43266700	1.81480500	-4.31220400
H	0.56452000	2.41987100	-3.46822800
C	3.71235400	1.31744900	-4.06529300
H	5.08859300	0.65472500	-2.53329100
H	2.14451700	2.01801400	-5.33793800
C	1.44562500	3.12803500	0.13273700
H	2.49654600	2.95102700	0.39046800
C	0.63083500	3.29908800	1.40072900
H	1.04643700	4.09035200	2.02888900
H	-0.40932100	3.56475700	1.19523500
H	0.62070700	2.37523300	1.98755200
O	4.48702500	1.08973800	-5.16120700
C	5.77381000	0.55352900	-4.93661400
H	6.39708800	1.23060100	-4.33971000
H	5.72093900	-0.41879000	-4.43124600
H	6.22574600	0.42591800	-5.91906200
H	-1.13320800	2.42484300	-0.46307500
H	-0.77257400	1.45992000	-1.98074600
H	1.44006200	4.06061000	-0.44801700

Imaginary frequency: -627.02

II

04

Fe	0.03945000	-0.05409300	-0.01713700
N	0.01698000	-0.16596900	1.93270100
C	1.17380600	-0.20026600	2.83449600
C	-1.06217700	-0.09873100	2.67552000
C	0.58556100	0.24630100	4.16096900
H	1.57471900	-1.22052000	2.87229700
H	0.92134300	-0.31975900	5.02945400
N	-1.90075400	-0.53909100	-0.08465500
C	-2.81641200	-0.44307500	0.91018100
C	-3.67640900	-1.07068400	-1.66468800
C	-4.21932500	-0.61281200	0.64624400
C	-4.61228900	-0.93804200	-0.68727700
H	-3.97287400	-1.31223400	-2.67904900
H	-5.66765600	-1.07773300	-0.89853800
C	-2.43020600	-0.16982700	2.26577200
C	-5.15381400	-0.46388500	1.67122100
C	-4.76108900	-0.15814900	2.97275900
H	-5.50162900	-0.03915600	3.75550600
C	-3.42043500	-0.02243300	3.26180300
H	-3.09753900	0.19170600	4.27265200
H	-6.20534100	-0.59373900	1.43082500
O	-0.82917900	0.01798400	4.00271000
C	-2.30802600	-0.86302400	-1.37389700
C	-1.27510800	-0.93415300	-2.32493100
C	1.08832300	-0.63752700	-2.68848900
C	2.23226300	-1.36552100	-2.34537000
C	1.13670800	0.20916100	-3.80217300
C	3.38869300	-1.26156900	-3.10527600
C	2.29763500	0.31193800	-4.55823900
C	3.42803400	-0.42368200	-4.21654300

H	4.26680900	-1.83521000	-2.82626800
H	2.32226900	0.98038900	-5.41322600
H	4.33435700	-0.33908000	-4.80637600
H	2.19638200	-2.00342800	-1.46700500
H	0.26564000	0.80865600	-4.04904300
H	1.97124800	0.45611000	2.48122900
H	0.73508300	1.31560900	4.34972700
N	-0.03674500	-0.69253300	-1.84177000
C	-1.53059000	-1.32421700	-3.74635500
H	-0.64906600	-1.79170700	-4.18775500
H	-2.35497900	-2.03571800	-3.81490400
H	-1.78931700	-0.46939800	-4.38171100
C	1.72929800	1.02974000	-0.10079700
H	1.04027900	2.23112000	1.56388900
C	1.61953300	2.36941700	0.63469600
C	2.96168900	2.93157000	1.04961900
C	3.18429000	3.39028800	2.34434000
C	4.02554800	3.02215200	0.14142100
C	4.41076400	3.92309300	2.74267600
H	2.37360300	3.33804700	3.06919000
C	5.24814700	3.55034700	0.51255200
H	3.88923000	2.66016000	-0.87459700
C	5.45067600	4.00545800	1.81951100
H	4.54051900	4.26655100	3.76203300
H	6.07160800	3.62036200	-0.19003100
C	0.83793300	3.39394200	-0.20281700
H	0.76534200	4.33085800	0.36270300
C	-0.55214200	2.92450400	-0.60098100
H	-1.13886100	3.72888300	-1.05254300
H	-0.51506700	2.11199000	-1.33668400
H	-1.11790800	2.56346600	0.26791400
O	6.69003800	4.50374600	2.08932500
C	6.92057300	4.97442100	3.39799100
H	6.24847600	5.80210300	3.65679400
H	6.80231000	4.17807700	4.14355500
H	7.94925300	5.33087000	3.41748400
H	1.98969300	1.20370700	-1.15362000
H	2.53011700	0.40402000	0.32031600
H	1.42136600	3.63151700	-1.10270200

III

04

Fe	0.29474300	-0.13567100	-0.21658700
N	0.12758100	0.13800800	1.71134600
C	1.19665400	0.44592900	2.66455000
C	-0.95164300	-0.14723300	2.40400900
C	0.64648800	-0.07737800	3.98043300
H	2.13043600	-0.03708500	2.37160100
H	1.01390300	-1.08186600	4.22164400
N	-1.69264100	-0.08347100	-0.41182200
C	-2.62176600	-0.33058600	0.54023300
C	-3.43130100	-0.10532600	-2.11483200
C	-4.00048700	-0.54489900	0.19354900
C	-4.36878600	-0.41105400	-1.17967700
H	-3.70993000	-0.00296500	-3.15814800

H	-5.40841400	-0.55989200	-1.45500100
C	-2.27049300	-0.41439200	1.92990700
C	-4.93047300	-0.88252400	1.17481800
C	-4.56003400	-1.00499900	2.51393400
H	-5.29558500	-1.27493600	3.26337300
C	-3.25421100	-0.76445100	2.88166200
H	-2.95645700	-0.83496100	3.92013500
H	-5.96004300	-1.05152900	0.87197000
O	-0.77101500	-0.16813400	3.74672000
C	-2.07352600	0.04517000	-1.74177500
C	-1.02456500	0.27633000	-2.64420400
C	1.37361600	0.49117000	-2.85319100
C	1.65415500	-0.35545600	-3.93414700
C	2.34787500	1.41716200	-2.45972200
C	2.86506300	-0.26131800	-4.60971000
C	3.55336600	1.50909700	-3.13869500
C	3.81922500	0.67248400	-4.22042400
H	3.06729600	-0.93089600	-5.44001900
H	4.29294900	2.23744400	-2.82125100
H	4.76404600	0.74259200	-4.74840800
H	0.92422000	-1.10529700	-4.22415000
H	2.13689200	2.05574300	-1.60646600
H	1.37344600	1.52848400	2.68217200
H	0.80511400	0.57501400	4.83899900
N	0.20387400	0.37474800	-2.08240400
C	-1.27684300	0.46521400	-4.10700200
H	-0.48231600	1.04859100	-4.57402100
H	-1.34031600	-0.48442500	-4.65370800
H	-2.21758400	0.99291500	-4.27476200
C	2.09668300	-1.03778200	-0.13046300
H	2.47029700	-1.17828700	-1.15365300
H	2.86372600	-0.47901400	0.42065500
C	1.77057000	-2.39119300	0.50924100
H	1.66681300	-2.25686300	1.59869200
C	2.85714800	-3.45097600	0.27799800
H	2.96446000	-3.60609700	-0.80390400
H	3.81717500	-3.03998100	0.61423500
C	2.57791700	-4.77356600	0.97042900
H	3.38056600	-5.49694100	0.80661300
H	2.47209000	-4.64024900	2.05246900
H	1.64845200	-5.22350000	0.60901700
C	0.40937000	-2.83959000	0.00036900
C	-0.63909900	-3.17988400	0.86337100
C	0.14411100	-2.86078400	-1.37384200
C	-1.89993500	-3.49537500	0.38491800
H	-0.46494700	-3.16913800	1.93815500
C	-1.11326500	-3.17972800	-1.87575200
H	0.93753200	-2.59907400	-2.07049400
C	-2.14972100	-3.48307200	-0.98980300
H	-2.72051200	-3.71997100	1.05830200
H	-1.28019800	-3.16564000	-2.94679500
O	-3.42474300	-3.77025000	-1.36474800
C	-3.71033700	-3.73474000	-2.74617400
H	-3.13510100	-4.48835300	-3.29828700
H	-4.77269900	-3.95412900	-2.84260100

H	-3.50683700	-2.74432600	-3.17286800
TS₂			
04			
Fe	0.31465600	0.18007600	-0.10290100
N	0.14510500	0.10597900	2.01096300
C	1.31187300	0.21390800	2.88586500
C	-0.90519500	0.05619200	2.76124200
C	0.75501800	-0.16319600	4.25010200
H	2.11172000	-0.44881200	2.54620800
H	0.93740500	-1.21282500	4.50887800
N	-1.85721600	0.30164500	-0.04535800
C	-2.72741400	0.21723400	0.99964800
C	-3.74665600	0.67271500	-1.54192300
C	-4.14882600	0.27561700	0.79344700
C	-4.62790500	0.52267300	-0.52108300
H	-4.09716300	0.87094800	-2.54787500
H	-5.69932800	0.59032400	-0.68313200
C	-2.29240400	0.05381400	2.35960200
C	-5.04633400	0.10147700	1.85304700
C	-4.59869700	-0.10583300	3.14459800
H	-5.29762600	-0.24541200	3.96109000
C	-3.23348600	-0.11182200	3.38462100
H	-2.86490200	-0.24543200	4.39330400
H	-6.10975700	0.13802500	1.63340400
O	-0.66816700	0.01120300	4.09713200
C	-2.35690700	0.52261400	-1.30699000
C	-1.43240900	0.55415600	-2.38393200
C	0.81052000	0.06396300	-3.05230400
C	0.58788100	-0.91528200	-4.03463800
C	2.06529000	0.68566400	-2.99800200
C	1.59116700	-1.26156100	-4.92813600
C	3.06150100	0.33566600	-3.90007300
C	2.83492000	-0.63837700	-4.86722600
H	1.40217500	-2.02787900	-5.67349300
H	4.02527900	0.83212400	-3.84591600
H	3.61770700	-0.90950500	-5.56734500
H	-0.37579300	-1.41509400	-4.06993700
H	2.23611400	1.44726500	-2.24611000
H	1.69597200	1.24011600	2.84651900
H	1.08493500	0.46959100	5.07368500
N	-0.15250100	0.33306400	-2.06927100
C	-1.88998900	0.89016900	-3.77303800
H	-1.04273900	1.10634600	-4.42296900
H	-2.45637100	0.07464100	-4.23980500
H	-2.54071200	1.76917100	-3.77193500
C	1.87318100	-1.30324000	-0.10404800
H	1.95977900	-1.47084800	-1.18534800
H	2.89727800	-1.19173200	0.26628900
C	1.21714900	-2.51075100	0.58660400
H	1.22582600	-2.34041200	1.67460000
C	2.04057000	-3.78587600	0.32452900
H	2.03796600	-3.98500100	-0.75527400
H	3.08618600	-3.58420400	0.58865900
C	1.53815600	-5.00379800	1.08053500

H	2.16724700	-5.87883700	0.89929000
H	1.52922800	-4.82384300	2.16095200
H	0.51695100	-5.26276800	0.78741100
C	-0.23161400	-2.69308300	0.18606500
C	-1.23925700	-2.87957400	1.13634600
C	-0.60922300	-2.67593200	-1.15737100
C	-2.57067900	-2.99675100	0.77084400
H	-0.97379800	-2.90728900	2.19213400
C	-1.93896500	-2.79126400	-1.54823200
H	0.15170900	-2.54826400	-1.92363800
C	-2.93167300	-2.92873200	-0.57580500
H	-3.35452100	-3.10356100	1.51361800
H	-2.19211600	-2.75078200	-2.60177000
O	-4.26664100	-2.99578500	-0.83984700
C	-4.65758300	-2.88184500	-2.18985000
H	-4.26588500	-3.70643900	-2.79840200
H	-5.74611400	-2.91947100	-2.19641700
H	-4.32730700	-1.92915600	-2.62486900
Si	0.80512600	2.58430900	0.06327200
H	1.85768100	0.40656300	-0.05133700
H	1.82631000	3.15617000	-0.84618800
C	-0.83783700	3.50438100	-0.28549300
H	-1.58842000	3.25477300	0.46843700
H	-0.70213000	4.58964700	-0.28859000
H	-1.24408200	3.21542700	-1.25888200
H	1.24344800	2.95686500	1.43294200

Imaginary frequency: -807.21

IV

04

Fe	-0.48981000	0.36054600	-0.18495200
N	-0.51105900	-0.21433700	1.67683100
C	0.62695000	-0.30346500	2.59468400
C	-1.60125500	-0.45685400	2.36072400
C	0.03068800	-0.96807900	3.82541700
H	1.43427100	-0.88775700	2.14631100
H	0.24792200	-2.04000600	3.87855500
N	-2.48932500	0.40847300	-0.29794700
C	-3.39172100	0.08444200	0.65828700
C	-4.29145900	1.07465900	-1.79194900
C	-4.79980900	0.20098600	0.40950800
C	-5.21270200	0.74235200	-0.84858000
H	-4.59934300	1.47808000	-2.75083900
H	-6.27463000	0.87491000	-1.03171000
C	-2.97711700	-0.38234100	1.94891500
C	-5.72161700	-0.20705100	1.37440100
C	-5.30318800	-0.71158600	2.60160200
H	-6.02889200	-1.03606000	3.33852600
C	-3.95268900	-0.78329100	2.88263000
H	-3.61831300	-1.15429100	3.84293500
H	-6.78078800	-0.12344500	1.14577600
O	-1.38942200	-0.81438800	3.64838100
C	-2.91184400	0.85826900	-1.54114300
C	-1.89832300	1.02589900	-2.49290000
C	0.37138800	0.39571300	-2.98350100

C	0.11145100	-0.35637200	-4.14459600
C	1.70352500	0.73702000	-2.70428200
C	1.14348600	-0.74483300	-4.98581700
C	2.72889600	0.34885600	-3.55455100
C	2.46077800	-0.39513900	-4.70040500
H	0.91733200	-1.33806600	-5.86653500
H	3.75013900	0.62977100	-3.31553900
H	3.26580200	-0.70020400	-5.35992600
H	-0.90760300	-0.66484700	-4.35549800
H	1.91928300	1.30923700	-1.80852300
H	1.01784500	0.70163300	2.79875600
H	0.30346300	-0.50044600	4.77178800
N	-0.64772200	0.68866200	-2.06947700
C	-2.16943900	1.62735700	-3.83851800
H	-1.24406700	1.95742100	-4.31167500
H	-2.65668600	0.93480800	-4.53473100
H	-2.82433000	2.49848700	-3.74839700
C	3.10613700	-1.52617100	-0.18565300
H	3.02293600	-1.44723700	-1.27368900
H	4.16903200	-1.45483900	0.06154400
C	2.51553000	-2.83952500	0.32170100
H	2.75879600	-2.93847300	1.39187400
C	3.17143800	-4.02596400	-0.40311600
H	2.93245000	-3.94923400	-1.47256000
H	4.26080500	-3.91444500	-0.33197600
C	2.75609900	-5.38635000	0.12535800
H	3.27389400	-6.19443000	-0.39634000
H	2.98531100	-5.48560300	1.19168000
H	1.68179100	-5.55245800	0.00715800
C	1.00777200	-2.88239800	0.20827100
C	0.22036300	-3.41495800	1.23519900
C	0.34739000	-2.42090900	-0.93030900
C	-1.16098200	-3.47590400	1.14272600
H	0.71020000	-3.79647700	2.12948000
C	-1.04299400	-2.47217000	-1.04635900
H	0.91900500	-2.00889200	-1.75959100
C	-1.80668100	-3.00217800	-0.00337900
H	-1.76740200	-3.87824000	1.94824800
H	-1.51469300	-2.08965600	-1.94464500
O	-3.16037500	-3.09392900	-0.00787800
C	-3.83021400	-2.74301600	-1.20460500
H	-3.52613300	-3.39343400	-2.03403600
H	-4.89199200	-2.87890800	-1.00509800
H	-3.65073000	-1.69890200	-1.48337600
Si	0.63572700	2.45671600	0.32791100
H	2.60051700	-0.65060900	0.23590700
H	0.75146600	3.41728500	-0.79275100
C	-0.42903800	3.25671200	1.70717400
H	-0.43689000	2.63839900	2.60882600
H	-0.06558600	4.24969300	1.98509700
H	-1.46648800	3.35825600	1.37922300
H	2.01447200	2.28492000	0.86393900

Fe	-0.02047400	0.03516900	-0.02909100
N	-0.00500600	-0.04136300	1.91735800
C	1.16535800	-0.08053900	2.80517300
C	-1.06652000	0.06039500	2.67970700
C	0.55875100	-0.41030500	4.15454300
H	1.89285600	-0.81928100	2.47081700
H	0.58275800	-1.48298100	4.37792500
N	-1.95246800	0.55673000	-0.06788400
C	-2.84521900	0.53431700	0.95572400
C	-3.74398700	1.11431600	-1.61507500
C	-4.24011500	0.78292600	0.72557300
C	-4.65671600	1.07624800	-0.60458100
H	-4.05835000	1.32475500	-2.63058800
H	-5.70893000	1.26496000	-0.79177500
C	-2.43622400	0.26655300	2.30321600
C	-5.15371000	0.73873300	1.78337500
C	-4.74027100	0.45991400	3.08025500
H	-5.45838900	0.42418300	3.89141400
C	-3.40088200	0.23235400	3.33032100
H	-3.06391500	0.02320900	4.33740000
H	-6.20099900	0.92914100	1.56651000
O	-0.82074500	-0.01912100	4.00712400
C	-2.38360000	0.84923000	-1.35065900
C	-1.37485400	0.84059800	-2.34417100
C	0.95309600	0.47771300	-2.79671200
C	0.95798500	-0.31615000	-3.94614500
C	2.10156500	1.20482000	-2.46995800
C	2.08725900	-0.37389600	-4.75369000
C	3.22472200	1.14808100	-3.28254500
C	3.22352900	0.35890100	-4.42943400
H	2.08147700	-1.00606100	-5.63595600
H	4.10831900	1.71859800	-3.01530400
H	4.10522300	0.30769200	-5.05896300
H	0.08336400	-0.91376500	-4.18196600
H	2.09985500	1.80352200	-1.56336600
H	1.66115400	0.89778600	2.78921000
H	0.97568800	0.14063000	4.99696900
N	-0.14926700	0.50924800	-1.91084900
C	-1.66704400	1.24299500	-3.75508700
H	-0.78024600	1.65599900	-4.23678300
H	-2.00063600	0.40025100	-4.37104700
H	-2.45156700	1.99981800	-3.79140300
H	2.37475600	-1.77504300	-1.57199600
H	3.20337000	-0.71395200	0.36615000
Si	1.98547500	-1.36588200	-0.19959500
C	1.75955800	-3.01135600	0.78498900
H	2.69204800	-3.57857200	0.85338100
H	1.39314800	-2.84935800	1.80285700
H	1.02542000	-3.64912600	0.28652200

TS₃

04

Fe	0.39351100	-0.07314800	0.10297000
N	0.39329600	0.54720000	2.00116400
C	1.52218500	1.00533600	2.80715800

C	-0.66745600	0.54701800	2.75567200
C	0.96671200	1.02161500	4.22745300
H	2.37195800	0.32876900	2.68638600
H	1.30277300	0.17339800	4.83197100
N	-1.57701800	0.05138500	0.00478500
C	-2.45393600	0.04156500	1.04109800
C	-3.41647300	-0.13462900	-1.56285100
C	-3.85923100	-0.14300800	0.81151400
C	-4.30621400	-0.25281800	-0.53434900
H	-3.75652500	-0.19243600	-2.59004800
H	-5.36340800	-0.40887300	-0.72321400
C	-2.02577400	0.22823600	2.39742800
C	-4.75195800	-0.20722300	1.88710300
C	-4.31172900	-0.06525900	3.19636800
H	-5.01147700	-0.12115000	4.02223000
C	-2.96935800	0.16346000	3.43877400
H	-2.61735200	0.30274500	4.45295400
H	-5.80416300	-0.37056800	1.67220600
O	-0.45767000	0.89730200	4.04577800
C	-2.04341600	0.03204800	-1.29597500
C	-1.06335600	0.16918900	-2.32872000
C	1.28675100	0.25674500	-2.81874300
C	1.40148700	-0.59251800	-3.93084200
C	2.35863000	1.11274400	-2.52257100
C	2.54023400	-0.56551000	-4.72585700
C	3.48447700	1.14499400	-3.32966300
C	3.58447200	0.30670300	-4.43856500
H	2.61327100	-1.24019000	-5.57317400
H	4.29572200	1.82452400	-3.08788300
H	4.47151800	0.32501800	-5.06225400
H	0.60530400	-1.29552200	-4.15098400
H	2.28174300	1.74816100	-1.64516300
H	1.84433100	1.99476500	2.46260100
H	1.15392900	1.94353500	4.77883300
N	0.20301700	0.21239500	-1.93553000
C	-1.50249600	0.29816500	-3.75523600
H	-0.72485200	0.75710500	-4.36507700
H	-1.73540600	-0.67570200	-4.20205000
H	-2.40177700	0.91148700	-3.83327200
H	1.61615800	-3.47068000	-0.02505100
H	-0.32171700	-2.88140200	1.18746800
Si	0.43247000	-2.58171300	-0.05576000
C	-0.62491300	-3.10394300	-1.55875100
H	-0.14116200	-2.81701800	-2.49504600
H	-0.76917800	-4.18729100	-1.57604300
H	-1.60888800	-2.63185000	-1.52850000
H	1.95039500	-0.04413900	0.13959400
H	1.63717600	-1.05335200	0.03818600

Imaginary frequency: -1043.57

VI

04

Fe	0.36917000	0.72780600	-0.00053400
N	0.38064900	0.70313000	1.93079300
C	1.57051700	0.82902000	2.77270600

C	-0.63319500	0.41308000	2.70132600
C	1.00248500	0.84496800	4.18533600
H	2.23486500	-0.02261400	2.58354300
H	1.50581500	0.18129200	4.88887200
N	-1.57478200	0.29447300	-0.06999700
C	-2.43343200	0.08856500	0.96431500
C	-3.40997300	0.02623700	-1.64586900
C	-3.82180900	-0.18193100	0.72699500
C	-4.28065800	-0.19845900	-0.62262300
H	-3.75197600	0.00886500	-2.67440200
H	-5.33128600	-0.39325300	-0.81303200
C	-1.99189600	0.12917300	2.32744500
C	-4.69256400	-0.41672000	1.79617900
C	-4.24356300	-0.38427400	3.11040100
H	-4.92791900	-0.56672000	3.93097900
C	-2.91296600	-0.10999400	3.36508600
H	-2.55090500	-0.07333700	4.38463900
H	-5.73552300	-0.62417600	1.57387600
O	-0.35044400	0.37202100	4.02296900
C	-2.04454400	0.25834000	-1.37363800
C	-1.05660800	0.39934500	-2.37635200
C	1.30134500	0.45833900	-2.80097000
C	1.43235500	-0.62829200	-3.67594900
C	2.31966000	1.41727100	-2.76038000
C	2.54594800	-0.74182500	-4.49831600
C	3.42304100	1.30393500	-3.59289400
C	3.54436300	0.22584800	-4.46643500
H	2.63695300	-1.59700800	-5.16070500
H	4.19979200	2.06106800	-3.55473700
H	4.41406800	0.13599800	-5.10850600
H	0.66409000	-1.39523600	-3.68477900
H	2.22890500	2.23795600	-2.05826400
H	2.12435500	1.73170500	2.51211900
H	0.95499600	1.84949900	4.61798700
N	0.19968300	0.56223700	-1.92677900
C	-1.42324100	0.39005300	-3.82771200
H	-0.63445600	0.83130600	-4.43673300
H	-1.60063900	-0.62168600	-4.21101500
H	-2.33918300	0.96037100	-3.99770100
H	1.13688300	-3.96642200	0.67807300
H	-0.37006000	-2.24883800	1.36941600
Si	0.43241100	-2.74990200	0.24071700
C	-0.67354700	-3.12768800	-1.24968300
H	-0.09597500	-3.56785500	-2.06511800
H	-1.46461000	-3.83158700	-0.98378500
H	-1.14747300	-2.21712700	-1.62158200
H	1.85398900	1.18873000	0.01846300
H	1.44150700	-1.73002300	-0.10522300

Sextet

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Fe	0.12335100	0.50705300	-0.02247500
N	0.01084700	-0.31866100	1.90250100

C	1.19151500	-0.56897100	2.72623800
C	-1.01916800	-0.26021900	2.68827400
C	0.67589100	-0.42950100	4.15562600
H	1.58340100	-1.57043800	2.51270900
H	0.93368900	-1.25946500	4.81451500
N	-1.99186700	0.07259900	-0.06474000
C	-2.85926000	-0.00027000	0.97359500
C	-3.84705200	-0.13071100	-1.61489000
C	-4.27974300	-0.01751800	0.75664100
C	-4.74160500	-0.07692000	-0.58740700
H	-4.19480800	-0.20280000	-2.63849000
H	-5.81081900	-0.09968000	-0.77333000
C	-2.40692000	-0.07653700	2.33356700
C	-5.16809200	0.00306100	1.83695300
C	-4.70582100	0.00717400	3.14483500
H	-5.40071600	0.03177600	3.97624200
C	-3.34214800	-0.05186500	3.38018800
H	-2.96968700	-0.09702100	4.39566000
H	-6.23409500	0.00869500	1.62702900
O	-0.75849600	-0.41129000	4.00860600
C	-2.46162100	-0.04205700	-1.35258800
C	-1.49304700	-0.04274300	-2.40694500
C	0.82682300	0.36031400	-2.94469100
C	2.08871900	-0.13147700	-2.56963000
C	0.73114000	1.10190800	-4.13454900
C	3.20066800	0.07273700	-3.37092300
C	1.85044100	1.30631900	-4.92838800
C	3.08863100	0.78690900	-4.56071800
H	4.16245600	-0.32401500	-3.06247700
H	1.75664200	1.89078700	-5.83832500
H	3.95938500	0.95168800	-5.18572000
H	2.17613600	-0.68711200	-1.63868800
H	-0.21572600	1.55287800	-4.40863300
H	1.97430800	0.15272500	2.47677100
H	0.97508700	0.50846100	4.63295700
N	-0.23048300	0.17852700	-2.05502100
C	-1.91554500	-0.36087500	-3.80956400
H	-1.06608200	-0.70272600	-4.40101600
H	-2.67297700	-1.14675200	-3.81985900
H	-2.34326400	0.50464200	-4.32786600
H	1.19558200	1.67998100	0.38396000

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Fe	0.58425900	-0.51186200	0.34999100
N	0.00649600	-0.19167200	2.33342400
C	1.01056700	-0.05542100	3.38727800
C	-1.14620400	0.15923600	2.82131400
C	0.24885100	0.60175100	4.53610500
H	1.40882500	-1.04284400	3.64510700
H	0.30711900	0.05988600	5.48155700
N	-1.58860400	-0.81350000	0.08471400
C	-2.62479800	-0.39499500	0.85323800
C	-3.17698900	-1.54212200	-1.60904100
C	-3.98554700	-0.46648900	0.38835100

C	-4.22217800	-1.06489300	-0.87967700
H	-3.35146800	-1.99861000	-2.57570900
H	-5.24199500	-1.13422200	-1.24489300
C	-2.42665900	0.14357600	2.17203900
C	-5.03889500	0.02852500	1.16241200
C	-4.81300200	0.58835700	2.41381500
H	-5.63669900	0.97431700	3.00340200
C	-3.52437200	0.62919300	2.90892300
H	-3.33371200	1.03310700	3.89492500
H	-6.04626100	-0.03967500	0.76103200
O	-1.12742500	0.58965800	4.10572800
C	-1.85223700	-1.40079300	-1.13481700
C	-0.74120500	-1.82395600	-1.92391200
C	1.63874200	-1.79457900	-2.21132400
C	2.75257100	-2.31452900	-1.53367800
C	1.75902200	-1.51981900	-3.58195400
C	3.92546500	-2.59647900	-2.21786000
C	2.93586900	-1.80468700	-4.26021500
C	4.02235200	-2.35480200	-3.58614400
H	4.76937400	-3.01458900	-1.67799400
H	3.00953000	-1.57395800	-5.31893500
H	4.93687900	-2.59143600	-4.12122400
H	2.67596700	-2.49155200	-0.46660200
H	0.93111400	-1.05377100	-4.10534600
H	1.85451700	0.53703600	3.02347500
H	0.53527600	1.64345100	4.70964600
N	0.47481300	-1.51198400	-1.48080200
C	-0.98089500	-2.66617500	-3.14405100
H	-0.08898500	-3.23491200	-3.40501600
H	-1.79318500	-3.37433200	-2.97184900
H	-1.25124900	-2.07267200	-4.02436400
C	-0.31813500	1.86739300	-0.55455300
H	2.22004900	-0.37174300	0.72565900
C	1.00369000	2.13542500	-0.55846100
C	1.82552200	1.86577500	-1.75563700
C	3.14538200	1.41546300	-1.65112400
C	1.31266200	2.08766200	-3.04314400
C	3.92786100	1.18862600	-2.77617100
H	3.55394200	1.18827000	-0.67199900
C	2.08301600	1.87935400	-4.17117500
H	0.29997800	2.46491900	-3.15139700
C	3.39894600	1.42587200	-4.04470200
H	4.93311800	0.80435900	-2.65461500
H	1.69312800	2.06692200	-5.16579800
C	1.71639100	2.74690400	0.62086200
H	2.43274800	2.00280500	0.99477300
C	0.83039400	3.22777800	1.75346100
H	1.43067700	3.64242100	2.56720400
H	0.13865000	4.00729900	1.42221000
H	0.22762200	2.41586000	2.16758300
O	4.07228400	1.23297200	-5.20960600
C	5.41726300	0.80929700	-5.11312900
H	6.03011300	1.53733800	-4.56830200
H	5.49606300	-0.16544700	-4.61742400
H	5.78308900	0.72623900	-6.13539000

H	-0.95941200	2.11568300	0.28499500
H	-0.80718200	1.43319800	-1.42059000
H	2.33083400	3.57620000	0.24724700

TS₁

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Fe	0.27518700	-0.01455500	0.10212000
N	-0.03714100	-0.18433800	2.17858600
C	0.96521500	-0.28062500	3.23776100
C	-1.18208400	0.07213500	2.74528900
C	0.26808600	0.33684600	4.44152400
H	1.22581800	-1.33494100	3.39826700
H	0.38746800	-0.21497600	5.37402200
N	-1.75131900	-0.76843700	0.02317200
C	-2.75813500	-0.40561700	0.83613100
C	-3.34103200	-1.56376900	-1.61184500
C	-4.13047200	-0.52848500	0.42680200
C	-4.37991300	-1.12791300	-0.83933900
H	-3.53369200	-2.02551000	-2.57347300
H	-5.40715500	-1.23899300	-1.17250100
C	-2.49640100	0.10212000	2.15607600
C	-5.15899600	-0.08163600	1.26202100
C	-4.88091700	0.46297500	2.51122100
H	-5.68588900	0.81224400	3.14791300
C	-3.57032100	0.53305100	2.95335200
H	-3.35148100	0.91408700	3.94323500
H	-6.18508200	-0.17534500	0.91729400
O	-1.12834000	0.29931100	4.08186200
C	-2.01048700	-1.36596700	-1.17877200
C	-0.86881400	-1.74734600	-1.95893000
C	1.53569300	-1.67957700	-2.13371400
C	2.60159300	-2.07299400	-1.30748800
C	1.76536700	-1.57564700	-3.51398100
C	3.83115400	-2.41261900	-1.84978300
C	3.00142100	-1.91246400	-4.04939600
C	4.03619500	-2.34615100	-3.22619600
H	4.63459300	-2.73467300	-1.19454800
H	3.16092900	-1.81269300	-5.11927600
H	4.99745600	-2.61827000	-3.65067600
H	2.43379500	-2.11983700	-0.23443000
H	0.98027000	-1.19678800	-4.15874600
H	1.88109300	0.24057600	2.94733400
H	0.54578100	1.38374700	4.60728800
N	0.32285400	-1.35153000	-1.51652300
C	-1.05252500	-2.63175200	-3.15381400
H	-0.15960400	-3.23051100	-3.33646000
H	-1.89375300	-3.31093800	-3.01106300
H	-1.24667300	-2.06126500	-4.06902700
C	-0.23323700	1.95270100	-0.56537400
H	1.77747300	0.76048100	0.38894400
C	1.19271100	1.97134500	-0.48453300
C	1.96847100	1.74367100	-1.75155100
C	3.28165300	1.27230600	-1.71296900
C	1.43762800	2.06621800	-3.00541000
C	4.04223200	1.11249700	-2.86220800

H	3.70537700	0.98500800	-0.75335700
C	2.17712900	1.90535300	-4.16653400
H	0.43105200	2.46627400	-3.06963700
C	3.48245100	1.41867500	-4.10376600
H	5.04645700	0.71386300	-2.78528600
H	1.76102600	2.14908000	-5.13821400
C	1.84045000	2.99868600	0.44013700
H	2.90060800	2.75135500	0.56535900
C	1.18318400	3.14333800	1.79772400
H	1.74227500	3.83096900	2.43689800
H	0.16105000	3.52352000	1.72521900
H	1.13788800	2.17378400	2.30062200
O	4.11799800	1.25231600	-5.29725100
C	5.44598900	0.77574900	-5.25545400
H	6.10470700	1.45869400	-4.70514000
H	5.50373500	-0.21864500	-4.79539700
H	5.78002000	0.71358400	-6.29012500
H	-0.83313100	2.50967900	0.14572200
H	-0.72175800	1.70961300	-1.50343500
H	1.81232100	3.95810000	-0.09597700

Imaginary Frequency:-1298.75

II

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Fe	0.34793200	-0.16497200	-0.24781300
N	0.22666400	-0.63009100	1.79482700
C	1.40866800	-0.74659600	2.64839600
C	-0.73918900	-0.13389100	2.51445000
C	0.99118500	-0.07594000	3.95615700
H	1.66997300	-1.80269600	2.77872300
H	1.12699700	-0.69654600	4.84322200
N	-1.76956900	-0.45118200	-0.20759800
C	-2.60618500	-0.17501300	0.81413500
C	-3.66563600	-0.94277800	-1.63094500
C	-4.02997900	-0.14411500	0.62316100
C	-4.52760400	-0.55665200	-0.64656500
H	-4.04529400	-1.27428700	-2.59050600
H	-5.60116100	-0.56955500	-0.80761500
C	-2.11099700	0.10021800	2.13370300
C	-4.87445100	0.26414100	1.65809900
C	-4.36513300	0.62281300	2.90161900
H	-5.02844100	0.95105900	3.69354700
C	-3.00528600	0.52148500	3.13447500
H	-2.60537700	0.74361100	4.11577100
H	-5.94436400	0.29355400	1.47109800
O	-0.42115800	0.16243300	3.79603900
C	-2.27002400	-0.86154300	-1.42256700
C	-1.32059900	-1.15458800	-2.44740000
C	0.99984200	-0.96682700	-3.07092600
C	2.24621900	-1.45546300	-2.64457900
C	0.90671200	-0.42410400	-4.36395200
C	3.34683400	-1.43140400	-3.48656500
C	2.01463200	-0.39887400	-5.19901700
C	3.23859600	-0.90703200	-4.77213500
H	4.29738500	-1.82100100	-3.13643100

H	1.92411600	0.03530100	-6.18991200
H	4.10096900	-0.88282200	-5.42926800
H	2.32572000	-1.85907400	-1.63815100
H	-0.02970500	0.01455500	-4.69110200
H	2.26542200	-0.25046200	2.17995400
H	1.47888500	0.88941700	4.12052900
N	-0.04209000	-0.93142800	-2.14637300
C	-1.77500600	-1.75229000	-3.74528800
H	-0.94554100	-2.23498500	-4.26245700
H	-2.55037400	-2.50322000	-3.57828000
H	-2.19440600	-1.00726900	-4.43080000
C	1.88128100	1.20025600	-0.23982500
H	1.12336500	1.95045200	1.64113600
C	1.64734800	2.34337200	0.74926300
C	2.91275200	2.99468800	1.27037400
C	2.99775800	3.43700500	2.58803000
C	4.02378000	3.21061100	0.44632400
C	4.13684000	4.06712500	3.08784200
H	2.14287300	3.29629100	3.24769600
C	5.16279100	3.83874400	0.91830700
H	3.99058200	2.86822000	-0.58440600
C	5.22897400	4.27041000	2.24607500
H	4.16108200	4.39074600	4.12166200
H	6.02340400	4.00545000	0.27930400
C	0.71251700	3.40710100	0.15071300
H	0.55737800	4.20105000	0.89166300
C	-0.63018800	2.85451100	-0.29544000
H	-1.31534900	3.64866400	-0.60433400
H	-0.53073600	2.17417700	-1.15002600
H	-1.12079800	2.30177000	0.51543400
O	6.39507600	4.86959600	2.62014400
C	6.48472100	5.32051700	3.95249700
H	5.72181600	6.07592000	4.17881200
H	6.38643100	4.49534000	4.66916500
H	7.47182900	5.76804100	4.05781900
H	2.05719600	1.58704100	-1.25447800
H	2.78398500	0.62914700	0.02762200
H	1.22476000	3.88316600	-0.69640800

III

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Fe	0.51013700	-0.00512100	-0.14506500
N	0.06062900	0.55328700	1.82184900
C	1.06697000	0.97857000	2.79360500
C	-0.90824300	-0.01888600	2.48047400
C	0.64050800	0.28341000	4.08122600
H	2.06684500	0.68402900	2.46222800
H	1.22883000	-0.61441300	4.29850900
N	-1.63300900	-0.08406700	-0.35228700
C	-2.52751100	-0.43897600	0.59303400
C	-3.39289500	-0.10555400	-2.01775900
C	-3.88252700	-0.77506200	0.25057800
C	-4.28576500	-0.57142600	-1.09861300
H	-3.70274300	0.06654000	-3.04250300

H	-5.31196900	-0.79286100	-1.37637200
C	-2.16365200	-0.51306800	1.98010800
C	-4.75460400	-1.28201200	1.21631600
C	-4.34863700	-1.44115900	2.53715200
H	-5.02904600	-1.84711200	3.27702800
C	-3.07769500	-1.04063000	2.90967000
H	-2.76883800	-1.11114600	3.94520100
H	-5.76193500	-1.55210900	0.91155700
O	-0.71407100	-0.12879800	3.81835500
C	-2.04213800	0.09757300	-1.65263200
C	-1.03723400	0.42554200	-2.60972100
C	1.33926900	0.53997900	-2.97441900
C	1.48614600	-0.22229600	-4.14664500
C	2.43855400	1.29528100	-2.53248000
C	2.67960300	-0.20503100	-4.85469100
C	3.62447900	1.31284300	-3.24909200
C	3.75348600	0.56599100	-4.41773300
H	2.77625200	-0.81080700	-5.75044900
H	4.45777700	1.90898100	-2.89089200
H	4.68407100	0.57448300	-4.97453000
H	0.66933100	-0.85841200	-4.47277300
H	2.33477600	1.86664500	-1.61350100
H	1.05630100	2.07174400	2.88303900
H	0.63200100	0.92386000	4.96361700
N	0.21416500	0.47478600	-2.15758600
C	-1.42002200	0.73609300	-4.02600000
H	-0.61298400	1.25285400	-4.54538700
H	-1.65331600	-0.16621500	-4.60496400
H	-2.30631900	1.37396000	-4.06181500
C	2.21078800	-1.16944100	0.04419100
H	2.64198300	-1.30545900	-0.95897200
H	3.00936300	-0.74383000	0.66628400
C	1.72997200	-2.51137300	0.60516000
H	1.55609300	-2.39221700	1.68836200
C	2.75458500	-3.64449600	0.43216300
H	2.92737500	-3.78814000	-0.64310300
H	3.71287000	-3.30300300	0.84303300
C	2.34673000	-4.95874500	1.07540700
H	3.11537100	-5.72665700	0.95549500
H	2.17075300	-4.83661400	2.14976900
H	1.42148000	-5.34741400	0.63967800
C	0.38610900	-2.87275800	-0.00403400
C	-0.69437000	-3.29578500	0.77839100
C	0.17893500	-2.76964600	-1.38356700
C	-1.93016000	-3.57805100	0.22118200
H	-0.56588300	-3.38139900	1.85579400
C	-1.05355500	-3.05369000	-1.96531700
H	0.99762900	-2.44706200	-2.02273500
C	-2.12153000	-3.44543100	-1.15658800
H	-2.77394000	-3.87396900	0.83591100
H	-1.17453700	-2.94616600	-3.03743000
O	-3.37831600	-3.71137700	-1.61109800
C	-3.59349000	-3.59328600	-2.99962100
H	-2.97517500	-4.29986600	-3.56723600
H	-4.64503200	-3.82360500	-3.16627800

H	-3.38699900	-2.57496300	-3.35446800
TS₂			
0 6			
Fe	0.07705200	0.22614900	-0.10093600
N	-0.08997300	0.29911400	1.99822300
C	1.03710300	0.41431100	2.92735200
C	-1.15548000	0.09175200	2.71346900
C	0.49412600	-0.20904300	4.19863500
H	1.92510500	-0.08795800	2.53414800
H	0.73199700	-1.27696700	4.28375800
N	-2.07766400	0.36246700	-0.09587400
C	-2.95334500	0.21615800	0.92972300
C	-3.94194000	0.62189300	-1.63476600
C	-4.37482400	0.20249600	0.69871400
C	-4.83544200	0.43602000	-0.62526200
H	-4.29000300	0.79504700	-2.64603100
H	-5.90523900	0.45638300	-0.81021800
C	-2.52934100	0.04253000	2.29389600
C	-5.27875000	-0.03258500	1.73795400
C	-4.84004400	-0.24618600	3.03740400
H	-5.54591400	-0.43522500	3.83789800
C	-3.48442800	-0.19849700	3.30035900
H	-3.12681300	-0.34412500	4.31129300
H	-6.33905000	-0.04524200	1.50125000
O	-0.93140500	-0.08051800	4.04436100
C	-2.55426000	0.54338700	-1.37824300
C	-1.61206700	0.56682100	-2.45002300
C	0.61830500	0.11304300	-3.13917200
C	0.41617600	-0.94749000	-4.03817500
C	1.83173100	0.80838000	-3.19600900
C	1.40009400	-1.30405600	-4.94940800
C	2.80897600	0.45231500	-4.11597000
C	2.60501400	-0.60828000	-4.99327300
H	1.22644400	-2.13490100	-5.62629700
H	3.73914700	1.01110100	-4.14573800
H	3.37441600	-0.88901100	-5.70430100
H	-0.51786400	-1.50007300	-3.99675900
H	1.99237200	1.63855700	-2.52003100
H	1.29379400	1.47238000	3.06133600
H	0.78181200	0.29574200	5.12043200
N	-0.32541100	0.41085800	-2.14381800
C	-2.09013400	0.79490300	-3.85577700
H	-1.25784700	1.01791000	-4.52207100
H	-2.61399700	-0.07504700	-4.27006200
H	-2.78707300	1.63542100	-3.90043700
C	1.92997400	-1.14308000	-0.09453000
H	1.98740400	-1.32898000	-1.17582400
H	2.96895500	-1.03643400	0.24072000
C	1.28504900	-2.32857300	0.64018500
H	1.26755900	-2.10391200	1.71859600
C	2.11931700	-3.61082000	0.46242400
H	2.14631300	-3.86022600	-0.60658200
H	3.15617000	-3.38817700	0.74340500
C	1.60664300	-4.79529400	1.26286300

H	2.24781200	-5.67184600	1.14192900
H	1.56715300	-4.56359100	2.33290000
H	0.59618600	-5.07996000	0.95631100
C	-0.15698400	-2.54852400	0.22211900
C	-1.17391200	-2.76828100	1.16041200
C	-0.51533400	-2.57260100	-1.12696500
C	-2.48905700	-2.95781800	0.77626300
H	-0.92613800	-2.76938500	2.22057900
C	-1.83351900	-2.75543800	-1.53619200
H	0.25121700	-2.43703100	-1.88511800
C	-2.83271600	-2.92640300	-0.57838100
H	-3.27893000	-3.09160700	1.50792000
H	-2.07089800	-2.74730700	-2.59403900
O	-4.15675000	-3.05862900	-0.85888400
C	-4.53445500	-2.97967100	-2.21618000
H	-4.10313700	-3.79796000	-2.80601400
H	-5.62042700	-3.05902800	-2.23498000
H	-4.23510000	-2.02110200	-2.65957900
Si	1.84865900	2.27636800	0.15107400
H	1.84633100	0.37178800	0.05249100
H	2.72755300	2.85754200	-0.88956300
C	0.18066500	3.23819900	0.10115700
H	-0.51108500	2.87976800	0.86902700
H	0.33578100	4.30806000	0.26692100
H	-0.31226600	3.11737500	-0.86710800
H	2.50330000	2.59689100	1.44221800

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IV

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Fe	-0.30596100	0.44426300	-0.14569300
N	-0.59560900	-0.29490200	1.76943300
C	0.49827300	-0.51416200	2.71615200
C	-1.71055200	-0.34419100	2.43168400
C	-0.21139800	-1.01524500	3.96536200
H	1.21532700	-1.23628600	2.31851300
H	-0.15527200	-2.10321400	4.07927800
N	-2.42412200	0.37873600	-0.34965100
C	-3.37648400	0.25252000	0.61044400
C	-4.16299700	0.68584000	-2.02244300
C	-4.77178300	0.41238200	0.29657100
C	-5.12736700	0.65404600	-1.06109000
H	-4.43433800	0.82361800	-3.06216300
H	-6.17589300	0.77823200	-1.31281600
C	-3.05278000	-0.08088100	1.96931000
C	-5.75026300	0.29095200	1.28665400
C	-5.41106800	-0.01227800	2.59767000
H	-6.17579700	-0.10765900	3.35975100
C	-4.08023300	-0.20487600	2.92044400
H	-3.80334800	-0.46298900	3.93407900
H	-6.78946900	0.43060600	1.00159300
O	-1.59105600	-0.66730300	3.74104500
C	-2.80145400	0.54469500	-1.67061000
C	-1.76711400	0.55854400	-2.65236500
C	0.59741900	0.36295500	-3.05596800

C	0.68433600	-0.67754400	-3.99453200
C	1.70590400	1.20341800	-2.87705800
C	1.84733800	-0.86847800	-4.72949300
C	2.86021700	1.01081600	-3.62327500
C	2.94095700	-0.02634900	-4.54875600
H	1.90090500	-1.68435800	-5.44363800
H	3.70565400	1.67560800	-3.47753300
H	3.84799500	-0.17836900	-5.12368000
H	-0.16146800	-1.34865800	-4.12000000
H	1.63721900	2.00597400	-2.14945800
H	1.03459800	0.43033500	2.87467500
H	0.10763100	-0.54054200	4.89370600
N	-0.51107400	0.51499800	-2.21126800
C	-2.10513800	0.69788800	-4.10715900
H	-1.22206800	0.95140900	-4.69228700
H	-2.52749500	-0.22042500	-4.52996600
H	-2.84321700	1.48781700	-4.26154200
C	2.78178400	-1.32899600	-0.32231000
H	2.41576400	-1.03717300	-1.31281300
H	3.86986700	-1.21727600	-0.34029400
C	2.37588900	-2.76265800	0.01302500
H	2.80589000	-3.02699800	0.99158600
C	2.95753300	-3.73496000	-1.02386700
H	2.56047000	-3.46578300	-2.01287700
H	4.04031800	-3.56945400	-1.08525700
C	2.67024800	-5.19492000	-0.72553300
H	3.13311200	-5.85608900	-1.46165400
H	3.05356300	-5.48118500	0.25953400
H	1.59577600	-5.39934100	-0.72612800
C	0.87517300	-2.90830800	0.13027200
C	0.27108200	-3.48645000	1.25052300
C	0.03691300	-2.48712300	-0.90199300
C	-1.10580500	-3.60807800	1.35301300
H	0.89917600	-3.84439600	2.06463600
C	-1.34903600	-2.60987800	-0.82735300
H	0.47382800	-2.06820200	-1.80495000
C	-1.92967000	-3.16242300	0.31513500
H	-1.57332500	-4.04427500	2.23013900
H	-1.95917700	-2.25783100	-1.65187500
O	-3.26560800	-3.30217400	0.51287000
C	-4.11468400	-2.97518900	-0.57003600
H	-3.94275900	-3.64205000	-1.42424200
H	-5.13292300	-3.10403600	-0.20596600
H	-3.98333600	-1.93818000	-0.89664100
Si	0.94842700	2.46762500	0.74748400
H	2.38668200	-0.60354900	0.39749300
H	1.21307700	3.61012400	-0.16957600
C	-0.16819800	3.15533000	2.16698100
H	-0.28700700	2.41810100	2.96744200
H	0.23519800	4.06663100	2.61636100
H	-1.17119500	3.38266900	1.79575600
H	2.27499600	2.21094800	1.38518800

Fe	0.26789900	0.00815000	-0.22099300
N	0.19786800	0.43388100	1.83101000
C	1.37304200	0.54114500	2.69369000
C	-0.82660300	0.15603600	2.58004000
C	0.85114000	0.18023600	4.08477800
H	2.15542900	-0.14012500	2.34158800
H	1.24375400	-0.76467200	4.46962400
N	-1.80358800	0.44309400	-0.17216500
C	-2.66779200	0.25514300	0.85232100
C	-3.65331400	1.04225200	-1.61887600
C	-4.08715400	0.31957900	0.64541900
C	-4.54738800	0.72970900	-0.63791300
H	-4.00110800	1.37852900	-2.58856300
H	-5.61635800	0.80635900	-0.81008600
C	-2.20860000	0.00225100	2.18775700
C	-4.97040200	0.01053300	1.68465200
C	-4.50203600	-0.32638300	2.94723300
H	-5.19389700	-0.57577000	3.74335100
C	-3.13922000	-0.30361600	3.19382500
H	-2.76561500	-0.50640900	4.18947100
H	-6.03738400	0.04692900	1.48304400
O	-0.57036700	0.02503800	3.90031100
C	-2.26811600	0.87277400	-1.39447900
C	-1.29662500	1.09150200	-2.41812900
C	1.01434500	0.70937600	-3.03156600
C	0.89404800	0.27495600	-4.36307400
C	2.30122400	1.00266400	-2.54522900
C	2.01464500	0.17603600	-5.17488800
C	3.41484400	0.90403700	-3.36402100
C	3.27908700	0.49713100	-4.68853000
H	1.90016900	-0.17199500	-6.19671000
H	4.39535700	1.14208500	-2.96477000
H	4.15000800	0.41441000	-5.32918400
H	-0.07472000	-0.02861200	-4.74217900
H	2.40759600	1.32097600	-1.50975900
H	1.77993000	1.55694100	2.64346600
H	1.00593400	0.95715500	4.83565900
N	-0.04153400	0.74991400	-2.12535200
C	-1.69748500	1.73762700	-3.70917400
H	-0.83425300	2.18659700	-4.20117500
H	-2.14124000	1.02901500	-4.41756500
H	-2.43569200	2.52355800	-3.53850200
H	1.59868100	-3.12250300	-0.95863600
H	2.99120700	-1.93004100	0.51912000
Si	1.56165600	-2.13081600	0.14543900
C	0.75439600	-3.00754300	1.66436300
H	1.21008700	-3.97800200	1.87747800
H	0.84940600	-2.39568700	2.56642400
H	-0.31466200	-3.17041500	1.50335000

TS₃

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Fe	0.39800500	0.50718500	-0.01603300
N	0.16372500	0.35866400	2.01248400
C	1.30141100	0.46080100	2.92652500

C	-0.91159300	0.18719600	2.72457800
C	0.72314200	-0.01323000	4.25157800
H	2.13312900	-0.15532200	2.57553900
H	0.96652600	-1.05740000	4.47371400
N	-1.75696000	0.32026200	-0.10533300
C	-2.66340100	0.21512900	0.89707300
C	-3.56582900	0.33205300	-1.72940100
C	-4.07623400	0.15787900	0.62090800
C	-4.49267000	0.23257700	-0.73618500
H	-3.87840000	0.36939000	-2.76566600
H	-5.55415400	0.19691400	-0.95993900
C	-2.27660100	0.12973700	2.28040500
C	-5.00931800	0.02628600	1.65276400
C	-4.60831600	-0.06233000	2.97970200
H	-5.33919500	-0.16854100	3.77290000
C	-3.26089300	-0.01419100	3.27783400
H	-2.93130100	-0.08304700	4.30644800
H	-6.06276100	-0.00898500	1.38964000
O	-0.70313000	0.07449200	4.05679500
C	-2.19086100	0.36351500	-1.41504900
C	-1.19606000	0.40065100	-2.44153700
C	1.14288300	0.21258200	-2.93690200
C	1.16440200	-0.88375800	-3.81209000
C	2.26751400	1.04391900	-2.86713600
C	2.27783300	-1.13108300	-4.60138300
C	3.37541200	0.79110300	-3.66426800
C	3.38867900	-0.29497800	-4.53435600
H	2.28251500	-1.99009300	-5.26484500
H	4.23747000	1.44758500	-3.60223100
H	4.25969500	-0.49297400	-5.14960900
H	0.31206800	-1.55597400	-3.83958500
H	2.25595800	1.88067300	-2.17634900
H	1.65143500	1.49935100	2.95611400
H	0.98263600	0.60427900	5.11140000
N	0.07283000	0.42217800	-2.05370800
C	-1.60499900	0.45643400	-3.88337600
H	-0.76090000	0.71913500	-4.51931000
H	-2.00339200	-0.49847600	-4.24252000
H	-2.38622500	1.20468200	-4.03502700
H	2.70146800	-2.19592800	-1.16760800
H	2.34057800	-2.32907900	1.18059800
Si	1.74793100	-1.84317300	-0.09272000
C	0.11662400	-2.81334200	-0.36972700
H	-0.35996000	-2.49877200	-1.30122400
H	0.28104000	-3.89375700	-0.41672100
H	-0.59034400	-2.61022200	0.43852900
H	2.01237800	1.17377200	0.08441700
H	2.05082700	0.04189700	0.06841700

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VI

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Fe	0.23814600	0.87596300	0.02194600
N	0.08581000	0.04573500	1.94533500
C	1.22986100	-0.21483100	2.81683300

C	-0.98048000	0.06500400	2.68539800
C	0.65428100	-0.06968300	4.22036600
H	1.62098600	-1.22275700	2.62461200
H	0.91464800	-0.87626400	4.90615100
N	-1.86415700	0.36323500	-0.10915200
C	-2.76196700	0.30148500	0.90063000
C	-3.67058600	0.25331000	-1.72206100
C	-4.17722100	0.29594200	0.63901100
C	-4.59612700	0.27175900	-0.71965100
H	-3.98983100	0.19752900	-2.75562500
H	-5.65910700	0.24899600	-0.93872100
C	-2.35528300	0.22478400	2.27702700
C	-5.10053600	0.30126500	1.68879900
C	-4.68196800	0.29042600	3.01239400
H	-5.40417800	0.30524800	3.82042200
C	-3.32771300	0.23840400	3.29191900
H	-2.98925400	0.19422500	4.31919200
H	-6.15892900	0.31277000	1.44355600
O	-0.77166200	-0.10740300	4.01304000
C	-2.29466900	0.30647600	-1.41402400
C	-1.28715200	0.27885500	-2.43569500
C	1.06856500	0.16289200	-2.88145900
C	1.14045900	-0.90175000	-3.79536900
C	2.19557800	0.98507700	-2.71986600
C	2.29446200	-1.11752200	-4.53686600
C	3.34013800	0.76619300	-3.47064100
C	3.39791500	-0.28389800	-4.38487200
H	2.33492100	-1.95170000	-5.23045800
H	4.19760300	1.41845600	-3.33859100
H	4.29793400	-0.45664700	-4.96502000
H	0.29696200	-1.57814000	-3.89338200
H	2.14583800	1.79109000	-1.99181800
H	2.03508400	0.49463300	2.60498400
H	0.90047900	0.88889700	4.68786100
N	-0.02587700	0.36805200	-2.03715600
C	-1.69437300	0.22536900	-3.87865400
H	-0.86530400	0.49742700	-4.53048500
H	-2.04210000	-0.76787200	-4.18296700
H	-2.51360300	0.92128100	-4.07096300
H	3.11568400	-2.06035700	-1.55846000
H	3.09250700	-2.44072000	0.80733100
Si	2.35418900	-1.84791800	-0.32128600
C	0.61272700	-2.58759600	-0.41640800
H	0.06726200	-2.20013100	-1.27872000
H	0.65441000	-3.67531000	-0.50291400
H	0.03192200	-2.33968700	0.47557300
H	1.05163600	2.28381000	0.27750800
H	2.27185000	-0.39069300	-0.06222400

I'(Doublet)

0 2			
Fe	0.95187700	-0.84004400	-0.18716500
N	0.89581400	-0.87967600	1.75399500
C	2.03580100	-1.07009200	2.65114600
C	-0.10138100	-0.43079700	2.46738700

C	1.58820400	-0.39811300	3.94420400
H	2.23292800	-2.14113300	2.76941700
H	1.75420500	-0.98736100	4.84648000
N	-1.00644800	-0.88288900	-0.24754700
C	-1.87447800	-0.44922000	0.70118500
C	-2.85935700	-1.19708900	-1.78943600
C	-3.26573000	-0.26590200	0.40144100
C	-3.72637700	-0.65697300	-0.88992200
H	-3.20636800	-1.51330600	-2.76667500
H	-4.77698000	-0.52895100	-1.13050300
C	-1.43328800	-0.14232600	2.02826800
C	-4.11985100	0.28680100	1.36031200
C	-3.65492400	0.64372100	2.62044100
H	-4.33122500	1.07369200	3.35175700
C	-2.33101100	0.41706700	2.95313400
H	-1.96125100	0.66637900	3.94028500
H	-5.16495500	0.42813500	1.09868800
O	0.16670300	-0.23306200	3.77832600
C	-1.48572900	-1.31702800	-1.47098800
C	-0.50192100	-1.83505900	-2.33524200
C	1.85672500	-2.23158800	-2.60813100
C	2.79956900	-3.10500100	-2.05327200
C	2.08823900	-1.72710400	-3.89452400
C	3.93360900	-3.46665100	-2.76505700
C	3.23248700	-2.08319400	-4.59928600
C	4.15962500	-2.95545800	-4.04082700
H	4.64932800	-4.15048600	-2.31975000
H	3.40019200	-1.67048200	-5.58915000
H	5.05139100	-3.23299900	-4.59268800
H	2.61768800	-3.48415500	-1.05387100
H	1.37463300	-1.03923000	-4.33557000
H	2.93344700	-0.62201100	2.21835300
H	2.02576300	0.59664000	4.08319200
N	0.74839800	-1.83993000	-1.82377900
C	-0.85878600	-2.39993300	-3.67439200
H	-0.12697800	-3.14101300	-3.99817600
H	-1.83427500	-2.88875700	-3.63978200
H	-0.91029200	-1.63565800	-4.45881300
C	2.40865500	0.53415700	-0.57459600
H	2.33896600	-1.38738800	-0.05006200
C	1.14322700	1.14364400	-0.80594300
C	0.46821800	1.96455500	0.21725500
C	-0.83705600	2.44095700	0.01704700
C	1.06290400	2.28662700	1.45231500
C	-1.52828300	3.15972400	0.98388000
H	-1.35166900	2.21235300	-0.91171800
C	0.38752100	2.99086000	2.43053300
H	2.08029500	1.96542500	1.65639900
C	-0.92416700	3.42265300	2.21237700
H	-2.54508500	3.47481900	0.78226500
H	0.85293400	3.21799800	3.38426300
O	-1.51984700	4.07314400	3.24885900
C	-2.86138400	4.47099900	3.06454100
H	-2.96136200	5.19596000	2.24733300
H	-3.50925600	3.61020300	2.85599000

H	-3.17123200	4.94018400	3.99709200
H	3.01722300	0.27599100	-1.43857300
H	2.99778600	0.77942400	0.30478100
C	0.69055800	1.30948200	-2.24170200
H	1.24779000	0.59819900	-2.85722700
H	-0.36676400	1.03500900	-2.36265200
C	0.92486700	2.71985000	-2.77549800
H	1.98342900	2.98790500	-2.71225100
H	0.62106500	2.80338900	-3.82254800
H	0.36633200	3.46705400	-2.20598700

TS₁ (Doublet)**

0 2

Fe	0.36290600	-0.15464500	0.13016000
N	0.33382000	-0.21799100	2.07069200
C	1.47725400	-0.39521400	2.96560300
C	-0.66512500	0.22904400	2.78596600
C	1.02839700	0.27697000	4.25855500
H	1.68469800	-1.46395800	3.08871100
H	1.20100900	-0.31044300	5.16091800
N	-1.57114200	-0.23870700	0.07482400
C	-2.43864200	0.19366200	1.02386600
C	-3.42563600	-0.59084200	-1.45637400
C	-3.83173000	0.36593000	0.72509600
C	-4.29339600	-0.04740900	-0.56024500
H	-3.77436100	-0.92288200	-2.42783700
H	-5.34622100	0.06711800	-0.79782100
C	-1.99594700	0.51300800	2.34774300
C	-4.68425100	0.92808400	1.67837000
C	-4.21713400	1.30384500	2.93405400
H	-4.89378600	1.74229600	3.66008300
C	-2.89402500	1.08327900	3.26831000
H	-2.52285700	1.34407000	4.25204500
H	-5.73071500	1.06177500	1.41826900
O	-0.39311800	0.43308200	4.09622000
C	-2.04797800	-0.69061100	-1.14654200
C	-1.05997100	-1.19533800	-2.00831600
C	1.31233000	-1.53876400	-2.27743900
C	2.29841900	-2.34687500	-1.69701700
C	1.52201000	-1.06398800	-3.57971400
C	3.45184500	-2.67174900	-2.39558900
C	2.68328000	-1.38563700	-4.27277000
C	3.65331000	-2.19130000	-3.68718300
H	4.20035900	-3.30420800	-1.92868600
H	2.83168800	-0.99630200	-5.27515500
H	4.55845700	-2.44098200	-4.23043600
H	2.13211800	-2.70669200	-0.68726900
H	0.77873000	-0.42292800	-4.04134200
H	2.37168000	0.06028300	2.53261200
H	1.46184200	1.27393100	4.39490000
N	0.19454800	-1.17633000	-1.49628800

C	-1.40835300	-1.77947000	-3.34145400
H	-0.66884700	-2.51806600	-3.65413900
H	-2.37842700	-2.27865700	-3.30150300
H	-1.46742500	-1.02785200	-4.13751900
C	1.89996800	1.11510600	-0.24908900
H	1.81823900	-0.52023200	0.21823100
C	0.64183200	1.76650500	-0.49229600
C	-0.01135600	2.60629900	0.53076400
C	-1.31448200	3.09239800	0.33627200
C	0.59204100	2.92652500	1.76191100
C	-1.99565500	3.81668300	1.30565600
H	-1.83595300	2.86243700	-0.58849300
C	-0.07371200	3.63686300	2.74263100
H	1.60738100	2.59682300	1.96352500
C	-1.38394300	4.07633200	2.53127500
H	-3.01225300	4.13600100	1.10975700
H	0.39793600	3.86107000	3.69400200
O	-1.97045400	4.73005100	3.57064600
C	-3.31648000	5.11930500	3.39981000
H	-3.42944500	5.84366400	2.58377600
H	-3.96003800	4.25369000	3.19783500
H	-3.61977800	5.58663600	4.33543500
H	2.51229800	0.88463800	-1.12056700
H	2.50343500	1.40045700	0.61041100
C	0.20811900	1.95620100	-1.93153000
H	0.76045500	1.24276500	-2.54900200
H	-0.85167100	1.69452300	-2.06403600
C	0.46439700	3.36790100	-2.45080500
H	1.52551700	3.62326000	-2.37596500
H	0.17136500	3.46424000	-3.49978600
H	-0.09032700	4.11677400	-1.87972100

Imaginary Frequency: -477.63

II" (Doublet)

0 2

Fe	-0.24336100	-0.22109400	-0.35470900
N	0.10378400	-0.12061400	1.54289100
C	1.35667500	0.19603600	2.22748500
C	-0.86949900	0.00764700	2.41336400
C	0.89982200	0.77239500	3.56422200
H	1.95834500	-0.71330700	2.33980300
H	1.41521200	0.36264800	4.43368500
N	-1.93950000	-0.98375600	-0.09353000
C	-2.74738100	-0.79433000	0.97858600
C	-3.74587900	-2.09681000	-1.27739800
C	-4.13883800	-1.14371700	0.91245900
C	-4.60439800	-1.81306500	-0.26219700
H	-4.09439700	-2.61613100	-2.16337700
H	-5.64992200	-2.09882800	-0.31697200
C	-2.25787600	-0.22232400	2.19815400
C	-4.98478000	-0.82176200	1.97272600

C	-4.50558600	-0.18685400	3.11992700
H	-5.18434300	0.06161400	3.92920900
C	-3.16051700	0.09169900	3.23683500
H	-2.76662800	0.55775700	4.13222000
H	-6.03637700	-1.08163800	1.88851500
O	-0.48498600	0.40048600	3.65234100
C	-2.39395400	-1.67924900	-1.21641400
C	-1.43270800	-1.86281700	-2.21226100
C	0.85662800	-1.32508900	-2.82136900
C	2.14917200	-1.57155800	-2.33250100
C	0.71806100	-0.97134700	-4.17306500
C	3.25895400	-1.46169100	-3.15721300
C	1.83324900	-0.86377600	-4.99519100
C	3.10871100	-1.10602500	-4.49531700
H	4.24768300	-1.66093000	-2.75568900
H	1.70330800	-0.57660800	-6.03409100
H	3.97576900	-1.01934400	-5.14126000
H	2.25045700	-1.85211800	-1.28779300
H	-0.26652800	-0.75224000	-4.57087400
H	1.94847500	0.90705700	1.64256800
H	0.95924600	1.86578600	3.59688800
N	-0.20535300	-1.35294700	-1.90321400
C	-1.71729500	-2.64191900	-3.45671600
H	-0.81252300	-3.12147300	-3.83553400
H	-2.44840900	-3.42836000	-3.26022300
H	-2.11930800	-2.02841300	-4.27195600
C	0.98175400	1.48677700	-1.06943100
H	1.36554700	0.46657400	-0.67176300
C	-0.51134400	1.59463700	-1.07638300
C	-1.20809200	2.31334500	0.01089800
C	-2.61334700	2.33807200	0.04765300
C	-0.55249700	2.92093600	1.09900500
C	-3.32639800	2.88529300	1.10496400
H	-3.17303200	1.86818500	-0.75598800
C	-1.24640800	3.46672500	2.16316500
H	0.53322100	2.95270900	1.12843800
C	-2.64353500	3.43710300	2.18826800
H	-4.40869100	2.83685000	1.09309700
H	-0.72607700	3.91752100	3.00215300
O	-3.23429600	3.95300100	3.29955200
C	-4.63969600	3.84280900	3.38197400
H	-5.13885900	4.40977300	2.58658800
H	-4.96089300	2.79486600	3.32728700
H	-4.92173200	4.26012300	4.34736300
H	1.41566200	1.50589900	-2.07327200
H	1.51544800	2.19584300	-0.43178800
C	-1.16994500	1.62350700	-2.44380200
H	-0.55366300	1.04322500	-3.13611800
H	-2.13592200	1.10133000	-2.41433300
C	-1.35654700	3.03329100	-2.99676800
H	-0.39709400	3.55468200	-3.07421000

H	-1.80471900	3.01574900	-3.99386100
H	-2.00119500	3.63484200	-2.35044800

III'' (Doublet)

0 2

Fe	0.50565100	-1.16071300	-0.36300300
N	0.69673600	-1.83924300	1.51249600
C	1.72850900	-2.70798100	2.07819800
C	-0.03195700	-1.40847000	2.49855200
C	1.62178700	-2.47017300	3.57993800
H	1.52664100	-3.74679500	1.79025700
H	1.60101500	-3.37763900	4.18459200
N	-1.40190200	-0.72718800	0.02366700
C	-1.93146900	-0.35797700	1.21646800
C	-3.44337200	-0.05934600	-1.09662000
C	-3.20778700	0.28723900	1.28690700
C	-3.94308900	0.43282100	0.07347200
H	-4.01114700	0.02917700	-2.01603700
H	-4.91262600	0.92000500	0.10558600
C	-1.23964500	-0.61578300	2.44199500
C	-3.69836400	0.74011800	2.51772900
C	-2.98562800	0.53346800	3.69016700
H	-3.37454400	0.88791300	4.63855300
C	-1.78193200	-0.15654300	3.64961500
H	-1.23246700	-0.35125000	4.56281700
H	-4.65831000	1.24871700	2.53720500
O	0.35528200	-1.80466700	3.73692200
C	-2.15817100	-0.64871400	-1.12359800
C	-1.54403900	-1.18961800	-2.28620800
C	0.46683400	-2.21173800	-3.14157300
C	1.26599900	-3.30640900	-2.78401600
C	0.52377100	-1.74767800	-4.46357700
C	2.07465300	-3.93226400	-3.72034800
C	1.34484000	-2.37134500	-5.39444700
C	2.11941100	-3.46887900	-5.03323500
H	2.68025500	-4.78252900	-3.42260200
H	1.38838700	-1.98653900	-6.40856100
H	2.75949600	-3.95164800	-5.76370900
H	1.23892600	-3.64332800	-1.75012400
H	-0.03878800	-0.86398000	-4.74389200
H	2.71062000	-2.43792900	1.68222600
H	2.40223000	-1.80205300	3.95822300
N	-0.27232700	-1.58559700	-2.12495200
C	-2.33380300	-1.38577900	-3.54223500
H	-1.97299100	-2.25143100	-4.09975800
H	-3.38858900	-1.54888600	-3.31714200
H	-2.27599900	-0.52493600	-4.21833500
C	3.51563800	-1.29863800	-1.00339800
H	3.52871400	-2.01939900	-0.17896200
C	2.32842500	-0.36394400	-0.95045000
C	2.16810500	0.41408600	0.28631200

C	1.06778100	1.29319200	0.42572300
C	2.96365400	0.22600400	1.44269000
C	0.72266500	1.86769900	1.64836300
H	0.47750900	1.55093800	-0.44852200
C	2.62438700	0.78356600	2.65834000
H	3.86432900	-0.37678300	1.37432500
C	1.47801400	1.58309400	2.78178000
H	-0.14946100	2.50905700	1.70464700
H	3.23936500	0.63388300	3.54061800
O	1.20218800	2.03655200	4.03526900
C	0.13021100	2.94975900	4.16337600
H	0.30381400	3.85545200	3.56936200
H	-0.82367700	2.50153100	3.86156500
H	0.08367700	3.21584400	5.21837300
H	3.50276500	-1.87778400	-1.93141900
H	4.48191600	-0.76993600	-0.97071900
C	2.16737100	0.43243200	-2.24276000
H	2.24370400	-0.25836500	-3.08870200
H	1.16052700	0.86549400	-2.31597000
C	3.20232000	1.54299100	-2.40632100
H	4.22145100	1.14510400	-2.38709600
H	3.07870600	2.07490100	-3.35405900
H	3.12472300	2.27776200	-1.59905700

TS₂^o (Doublet)

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Fe	-0.52393900	-2.11823100	-0.28731200
N	-0.75429800	-2.85572400	1.59277200
C	-0.08670600	-3.85857600	2.44102900
C	-1.50499500	-2.16340600	2.41157900
C	-0.10994100	-3.21310300	3.80501800
H	-0.68580300	-4.77907900	2.40689300
H	-0.24911500	-3.89618800	4.64215800
N	-2.50298300	-1.86897100	-0.26426300
C	-3.20530900	-1.37297100	0.78346800
C	-4.48874600	-1.70490800	-1.64350000
C	-4.53794100	-0.87505000	0.62099700
C	-5.16654700	-1.08259900	-0.64012100
H	-4.96768000	-1.87708600	-2.59954800
H	-6.18985800	-0.74829400	-0.77836500
C	-2.62895000	-1.33161400	2.09032200
C	-5.16857700	-0.21851900	1.68338100
C	-4.54054700	-0.07932900	2.91477600
H	-5.03655900	0.44375500	3.72466700
C	-3.29901700	-0.65843200	3.12293100
H	-2.83926800	-0.63445900	4.10325900
H	-6.16718900	0.17879100	1.52586100
O	-1.27705200	-2.36186000	3.73148000
C	-3.13103600	-2.06886500	-1.46896100
C	-2.27938900	-2.49922500	-2.51202500
C	-0.10320300	-2.87122600	-3.26885300

C	0.28711000	-4.15212800	-3.66456300
C	0.39347100	-1.76613700	-3.96604800
C	1.18661800	-4.32020800	-4.71149400
C	1.29082000	-1.93802400	-5.01228900
C	1.69793300	-3.21545200	-5.38498100
H	1.48767200	-5.32161600	-5.00273500
H	1.67802100	-1.06891900	-5.53465200
H	2.40333400	-3.34938500	-6.19795500
H	-0.12134800	-5.01026300	-3.13945600
H	0.08612100	-0.77002100	-3.65951400
H	0.91583600	-4.09483500	2.10473700
H	0.77060400	-2.58305400	3.97944100
N	-0.99211800	-2.68423000	-2.17690100
C	-2.77577700	-2.64285900	-3.91769100
H	-2.25576200	-3.44554100	-4.44310100
H	-3.84243900	-2.86327200	-3.94541500
H	-2.61455200	-1.72951200	-4.50291800
C	1.52093700	-4.10894000	-0.46044500
H	0.70275300	-4.57175600	0.09537300
C	1.66167700	-2.61082900	-0.21439600
C	2.22200600	-2.23941100	1.14525200
C	2.02103700	-0.97349100	1.70410200
C	3.06480600	-3.09926400	1.87156400
C	2.59601500	-0.57765400	2.90932500
H	1.38930400	-0.25537600	1.19294100
C	3.64098000	-2.73389000	3.07779000
H	3.27949300	-4.09161700	1.48709800
C	3.41195700	-1.46399800	3.61070700
H	2.39568600	0.41747500	3.28831700
H	4.28803600	-3.41491900	3.62072000
O	4.01562500	-1.19211900	4.80069600
C	3.80434300	0.09195200	5.34658100
H	4.17308900	0.88177900	4.68094600
H	2.74315300	0.27448700	5.55668800
H	4.36338100	0.12164900	6.28037100
H	1.32816800	-4.28957700	-1.51717500
H	2.43528500	-4.67287500	-0.22326600
C	2.60555900	-2.00792700	-1.28568800
H	2.12263400	-2.07304700	-2.26303300
H	2.73408100	-0.93668700	-1.08415400
C	3.97910100	-2.66038400	-1.37683200
H	3.91367100	-3.70187700	-1.70519100
H	4.60575700	-2.13565700	-2.10284300
H	4.50604500	-2.64440600	-0.41764200
Si	-0.39923100	0.27923200	-0.73844200
H	0.69403400	-1.26672000	-0.59446900
H	0.83662700	0.93524100	-1.22722700
H	-0.64575500	0.85148800	0.60739900
C	-1.81559100	0.83110700	-1.89487600
H	-1.66825500	1.87158200	-2.19526700
H	-1.87408200	0.22674200	-2.80299300

H -2.78069000 0.75592500 -1.38962300
Imaginary Frequency:-731.04

IV'' (Doublet)

0 2

Fe	0.34987000	0.02059900	0.60108400
N	0.16044800	0.21935300	2.50730300
C	1.21782700	0.44894700	3.50456600
C	-0.98217000	0.22056800	3.14171400
C	0.44726600	0.97024300	4.70297200
H	1.73234200	-0.49840600	3.70848200
H	0.76059200	0.55982600	5.66216400
N	-1.51243100	-0.68125200	0.40504900
C	-2.51516600	-0.62483000	1.32109800
C	-3.03623100	-1.65880000	-1.20968100
C	-3.84020400	-1.05903100	0.98906500
C	-4.06192300	-1.59009500	-0.31223900
H	-3.20345600	-2.04947400	-2.20668400
H	-5.05886400	-1.92961100	-0.57472300
C	-2.28952200	-0.12683800	2.64468700
C	-4.87880300	-0.94767000	1.92305800
C	-4.64832000	-0.42961000	3.18767000
H	-5.45894300	-0.33922800	3.90170800
C	-3.36817300	-0.03267400	3.53975500
H	-3.17331200	0.35561100	4.53124400
H	-5.87349600	-1.27022100	1.62906200
O	-0.90889300	0.53264700	4.45312300
C	-1.75680800	-1.18794700	-0.85109000
C	-0.64718900	-1.16570700	-1.74497000
C	1.60148200	-0.42941000	-2.08990800
C	2.84940800	-0.80032100	-1.57694700
C	1.53937800	0.14811100	-3.36234800
C	4.00209400	-0.61382800	-2.32527100
C	2.69772000	0.33917600	-4.10533900
C	3.93327400	-0.04278000	-3.59425500
H	4.96145300	-0.90846000	-1.91234800
H	2.63415400	0.80479800	-5.08369300
H	4.83681700	0.11281900	-4.17377700
H	2.89573500	-1.22332600	-0.57759400
H	0.58185600	0.48401200	-3.74680600
H	1.96328800	1.15643800	3.13909300
H	0.44491800	2.06453500	4.76311200
N	0.45819900	-0.58035900	-1.27699100
C	-0.74297500	-1.82245900	-3.08667000
H	0.24272900	-2.09018600	-3.46632700
H	-1.34221600	-2.73287600	-3.02800300
H	-1.21220700	-1.17624200	-3.83687400
C	5.09321700	-1.59591900	5.57325700
H	4.05755200	-1.84783900	5.32875200
C	5.60666200	-0.44653700	4.71452000
C	4.73799100	0.79220900	4.77412800

C	4.73805400	1.68846700	3.70610200
C	3.94436500	1.11470500	5.88058700
C	3.97403400	2.85127200	3.71081200
H	5.33425700	1.46304500	2.82490400
C	3.17862600	2.27031000	5.90989900
H	3.91732000	0.45086100	6.73991400
C	3.17760400	3.14260500	4.81883100
H	3.97939200	3.49490300	2.83971400
H	2.55872100	2.51483800	6.76658200
O	2.35221000	4.21970300	4.91892500
C	2.30598700	5.09845300	3.80918100
H	3.28349900	5.55782300	3.62031100
H	1.97085400	4.58209800	2.90179700
H	1.59042600	5.87620400	4.07041900
H	5.70032400	-2.49200500	5.41910300
H	5.12823300	-1.36706700	6.64186500
C	7.07689900	-0.10942200	5.03315600
H	7.68152300	-1.01214100	4.87824800
H	7.43145300	0.62115500	4.29642900
C	7.31303600	0.43473000	6.43202200
H	7.03526800	-0.28623200	7.20628100
H	8.36611100	0.68036800	6.58649300
H	6.73405200	1.34592300	6.60839800
Si	2.02575600	1.78451700	0.46804000
H	5.59029700	-0.78877100	3.67022200
H	3.36493700	1.33342200	0.95779100
H	1.65509100	2.84018300	1.46670700
C	2.36639000	2.71863200	-1.17368300
H	2.88712100	3.66149100	-0.98452400
H	2.99046700	2.12343300	-1.84378000
H	1.44131000	2.95098800	-1.70712900

TS₃^o (Doublet)

0 2

Fe	0.09085500	-1.86118600	-0.35873500
N	0.46624900	-1.99280400	1.51218800
C	1.61155600	-2.65838400	2.13853600
C	-0.14628600	-1.29332200	2.43481200
C	1.71822100	-1.97356700	3.49364900
H	1.41012700	-3.73352300	2.21756400
H	1.85288500	-2.65280200	4.33600500
N	-1.62480000	-0.86654700	-0.07160600
C	-2.08801100	-0.35892200	1.09910100
C	-3.55430600	0.01302400	-1.24054200
C	-3.31419400	0.38215600	1.14048300
C	-4.03801600	0.53625000	-0.07523700
H	-4.09653200	0.14650400	-2.16977000
H	-4.97331400	1.08706900	-0.05774900
C	-1.35887500	-0.52558700	2.32563400
C	-3.76582600	0.94432900	2.34233600
C	-3.03853800	0.79281600	3.51418400

H	-3.39240700	1.23157900	4.44048600
C	-1.85750500	0.06861800	3.50044900
H	-1.29628600	-0.06917900	4.41618500
H	-4.69441700	1.50770200	2.33403400
O	0.43811900	-1.32272600	3.65546800
C	-2.32760100	-0.68167800	-1.23950100
C	-1.71163000	-1.20526100	-2.41823000
C	0.29073000	-2.19879200	-3.30597900
C	0.94935200	-3.43082800	-3.20282900
C	0.55120400	-1.39011600	-4.41899900
C	1.82110300	-3.85188700	-4.19466500
C	1.43930600	-1.80955300	-5.40245100
C	2.07421900	-3.04220800	-5.30063700
H	2.31531700	-4.81359000	-4.10048400
H	1.64339900	-1.16110100	-6.24872000
H	2.76766800	-3.36599600	-6.06919100
H	0.76921600	-4.04092000	-2.32210700
H	0.08957000	-0.41001100	-4.48399000
H	2.50325400	-2.52567900	1.52170700
H	2.49301000	-1.20039600	3.51980900
N	-0.51897100	-1.77552400	-2.23658200
C	-2.41711400	-1.14151600	-3.73660200
H	-2.00725200	-1.86736200	-4.43871000
H	-3.48152700	-1.35306400	-3.61386300
H	-2.34035600	-0.15461900	-4.20670300
C	4.83543700	-1.91053700	0.05241700
H	4.79361600	-2.41190500	1.02928300
C	3.76671500	-0.87161200	-0.12190400
C	3.49791400	0.01638900	0.99373400
C	2.24058600	0.62558500	1.18522100
C	4.44585500	0.21494800	2.02434400
C	1.93549600	1.36480100	2.32096800
H	1.45322000	0.47683400	0.45261000
C	4.15960500	0.95936600	3.15325800
H	5.43203500	-0.22945600	1.93183300
C	2.89467100	1.53367500	3.32057800
H	0.93921600	1.77901100	2.42661100
H	4.89828300	1.10208000	3.93499300
O	2.69048900	2.21268800	4.48270900
C	1.37940900	2.67931000	4.72293500
H	1.07114400	3.42874000	3.98372800
H	0.65416500	1.85593900	4.71465700
H	1.39570400	3.13867300	5.71002700
H	4.76471300	-2.67720600	-0.72279500
H	5.84414500	-1.48234300	-0.02035800
C	2.94320200	-0.93573300	-1.24354900
H	3.24527600	-1.68355900	-1.97858000
H	1.68476000	-1.77527200	-0.83093600
C	2.30756400	0.28686800	-1.87492100
H	2.67180400	0.39399300	-2.90103700
H	1.21505900	0.23255200	-1.92952300

H 2.57047800 1.19925000 -1.33649900
Imaginary Frequency:-1000.82

V" (Doublet)

0 2

Fe	-0.00525200	-1.72578000	-0.24547600
N	0.05493800	-2.27083900	1.61915200
C	0.91376600	-3.33549200	2.14195100
C	-0.56815400	-1.72138600	2.61608300
C	0.80105400	-3.17506800	3.65507900
H	0.55039400	-4.30292100	1.78002800
H	0.52293400	-4.08560700	4.18820400
N	-1.44322700	-0.36500000	0.17396400
C	-1.99683800	-0.04779400	1.37164600
C	-2.93644100	1.18972000	-0.93718500
C	-3.03084400	0.94270100	1.46652600
C	-3.50329800	1.52880100	0.25914200
H	-3.28085900	1.64721100	-1.85770900
H	-4.30832900	2.25536300	0.31074700
C	-1.55725600	-0.66700300	2.58642300
C	-3.54011700	1.31699400	2.71770200
C	-3.06778500	0.73907000	3.88363100
H	-3.46059600	1.04209400	4.84742300
C	-2.09372400	-0.24735600	3.81030800
H	-1.73111100	-0.71912900	4.71481600
H	-4.31732800	2.07559600	2.75141300
O	-0.26491400	-2.21795000	3.83496500
C	-1.87678800	0.26048000	-0.97652900
C	-1.15803800	-0.06620700	-2.16838100
C	0.73226500	-1.21711100	-3.07476900
C	0.98065000	-2.52424900	-3.50676900
C	1.46891100	-0.16684900	-3.63699500
C	1.92508200	-2.76696200	-4.49273800
C	2.42623900	-0.41910600	-4.61256600
C	2.65602300	-1.71912900	-5.04946700
H	2.10195900	-3.78599800	-4.82261000
H	2.99819300	0.40485200	-5.02796300
H	3.40331100	-1.91636400	-5.81070200
H	0.43305900	-3.33382900	-3.03762400
H	1.29740700	0.84653500	-3.28403800
H	1.93213300	-3.21178400	1.76382900
H	1.70230600	-2.75706300	4.11364200
N	-0.19181900	-0.98103900	-2.03711200
C	-1.52759700	0.56333400	-3.47566200
H	-1.09207600	0.01892600	-4.31289300
H	-2.61264100	0.57053000	-3.60767000
H	-1.19200400	1.60398600	-3.55357600
C	5.11857300	-2.08358100	2.25037500
H	4.54049700	-2.62716100	3.00845900
C	4.29009400	-1.75787200	1.03467200
C	3.20820500	-0.77450900	1.23239800

C	2.59216000	-0.06735700	0.18639800
C	2.77134500	-0.45869700	2.53506200
C	1.60901100	0.89116700	0.41935500
H	2.90283400	-0.22624800	-0.83810700
C	1.78604800	0.47906700	2.78241900
H	3.22398500	-0.95495900	3.38664700
C	1.19866400	1.17463400	1.72350500
H	1.17197700	1.41187900	-0.42576700
H	1.45889400	0.70133500	3.79322600
O	0.25848000	2.09296400	2.06073400
C	-0.24490900	2.91236600	1.02350600
H	0.55338700	3.51253300	0.56955000
H	-0.73965000	2.32453200	0.24291700
H	-0.97730900	3.57121800	1.48774000
H	5.96769400	-2.71426100	1.98435800
H	5.50305800	-1.18339100	2.74147600
C	4.59436000	-2.39114400	-0.11836000
H	5.45740300	-3.05419600	-0.06261700
H	0.94055800	-2.88775000	-0.68226100
C	3.92486100	-2.34958800	-1.44906000
H	4.14831300	-3.25710800	-2.01540500
H	2.83663300	-2.27468200	-1.36930000
H	4.27035300	-1.51103700	-2.06838300

I''(Quartet)

0 4

Fe	0.70180300	-0.30962700	0.19811900
N	0.31873800	-0.33348100	2.27815600
C	1.38090100	-0.57015900	3.25247000
C	-0.69531400	0.16282000	2.90996500
C	0.87531400	0.13056700	4.50933900
H	1.51963700	-1.64873400	3.38584800
H	0.93796600	-0.46463500	5.42073500
N	-1.50152000	-0.37082200	0.15354100
C	-2.38162000	0.16644700	1.03595700
C	-3.31164600	-0.63873000	-1.44629500
C	-3.74916900	0.41634700	0.67420900
C	-4.18395300	-0.01010700	-0.60975100
H	-3.63524600	-0.98395100	-2.42144400
H	-5.21638600	0.16093800	-0.89850200
C	-1.99407800	0.49562500	2.37698700
C	-4.62228700	1.04256600	1.57337200
C	-4.20351900	1.40552100	2.84217900
H	-4.88790300	1.88546100	3.53339300
C	-2.90453400	1.11717100	3.23847900
H	-2.57067000	1.37351600	4.23653800
H	-5.64413500	1.22851800	1.25342700
O	-0.52019400	0.37417900	4.23535800
C	-1.95873000	-0.79952300	-1.06479800
C	-0.99116400	-1.36201500	-1.94834600
C	1.34533800	-1.60148000	-2.40862500
C	2.40810300	-2.37341400	-1.91940200
C	1.42829000	-1.09057100	-3.71401200

C	3.51328400	-2.63082300	-2.71985500
C	2.53952400	-1.34878700	-4.50398900
C	3.58775300	-2.12241500	-4.01267500
H	4.32537800	-3.23410000	-2.32658800
H	2.58963800	-0.93727900	-5.50721500
H	4.45511400	-2.32404300	-4.63222200
H	2.34346100	-2.75355100	-0.90719000
H	0.62151900	-0.47078800	-4.09328500
H	2.32905800	-0.17531000	2.87743700
H	1.35331500	1.10026000	4.68485900
N	0.27849400	-1.27316500	-1.55612200
C	-1.42555300	-2.05384100	-3.20586200
H	-0.63992900	-2.71002700	-3.58028500
H	-2.31722800	-2.65977700	-3.02986900
H	-1.66880700	-1.35209900	-4.01198700
C	2.00289300	1.28855800	-0.20970300
H	2.14395100	-1.00234000	0.54697100
C	0.71638100	1.82077000	-0.41756800
C	0.00023500	2.59347800	0.60909000
C	-1.29447100	3.08577300	0.37844300
C	0.55480800	2.87524300	1.87400000
C	-2.00483500	3.80074500	1.33453200
H	-1.78242000	2.88571100	-0.57034900
C	-0.14304700	3.57040000	2.84190900
H	1.55826300	2.53247600	2.10833700
C	-1.43650400	4.03549400	2.58514300
H	-3.00852100	4.13772100	1.10467600
H	0.29187400	3.76938500	3.81603000
O	-2.05279700	4.68494200	3.61069400
C	-3.36734300	5.14214900	3.37675100
H	-3.40151300	5.88147100	2.56704900
H	-4.04208600	4.31336200	3.12777300
H	-3.69670600	5.61109500	4.30268700
H	2.60412700	0.99719000	-1.06680100
H	2.57692100	1.49483400	0.68672900
C	0.21345400	1.90178000	-1.84364800
H	0.77805000	1.18675600	-2.44829300
H	-0.83572400	1.58284100	-1.91711900
C	0.38035000	3.29464000	-2.44628200
H	1.43213400	3.59385800	-2.43895100
H	0.03259600	3.32154300	-3.48260500
H	-0.17611100	4.05148200	-1.88800700

TS₁^o (Quartet)

0 4

Fe	0.51905400	-0.11265800	0.15426900
N	0.31585200	-0.33661800	2.19726800
C	1.39575600	-0.60098100	3.14235100
C	-0.69339100	0.14254100	2.86750900
C	0.91787800	0.06724600	4.42787400
H	1.53764400	-1.68251300	3.25048300
H	1.01383200	-0.54613400	5.32416200
N	-1.54538500	-0.30274400	0.12945300
C	-2.40725400	0.21786300	1.03374400
C	-3.36447100	-0.52712700	-1.46416700

C	-3.77589600	0.48655700	0.69010800
C	-4.22355500	0.08791600	-0.60376900
H	-3.70312800	-0.84722700	-2.44351000
H	-5.25730300	0.27180400	-0.87896800
C	-1.99015900	0.51203400	2.37403000
C	-4.62196100	1.10661400	1.61342100
C	-4.17671800	1.44430600	2.88734300
H	-4.84765700	1.92211600	3.59352100
C	-2.88211100	1.13529100	3.26455700
H	-2.53103700	1.37112000	4.26182100
H	-5.64583400	1.31608900	1.31504600
O	-0.48387400	0.30025000	4.19723300
C	-2.00908100	-0.71534000	-1.10583200
C	-1.04136300	-1.27822500	-1.96793100
C	1.32926600	-1.56562100	-2.31193700
C	2.40583100	-2.23793600	-1.70896800
C	1.46826600	-1.15827600	-3.65116700
C	3.56884400	-2.49710400	-2.42023200
C	2.63652700	-1.41959000	-4.35337300
C	3.69399700	-2.09185300	-3.74594800
H	4.38489800	-3.02313100	-1.93445300
H	2.72487500	-1.08562900	-5.38267600
H	4.60458000	-2.29477200	-4.29920700
H	2.29762800	-2.55229400	-0.67644900
H	0.66311100	-0.60795900	-4.12662400
H	2.33822400	-0.19033500	2.76575900
H	1.39414100	1.03740700	4.60794500
N	0.22729800	-1.22197700	-1.52606800
C	-1.44481600	-1.94821800	-3.24602700
H	-0.68879200	-2.66834100	-3.56218700
H	-2.38851000	-2.48390300	-3.12470900
H	-1.58003000	-1.24327000	-4.07502800
C	1.97465000	1.29872000	-0.35532200
H	2.10298200	-0.28062900	0.25610200
C	0.65927000	1.85158200	-0.55153600
C	-0.00904000	2.63165700	0.49839500
C	-1.30951000	3.13532500	0.31187500
C	0.57568000	2.87824000	1.75901200
C	-1.98968600	3.83261300	1.29964100
H	-1.82318500	2.95201300	-0.62670600
C	-0.09223100	3.56143400	2.75615200
H	1.57740700	2.51460000	1.96917500
C	-1.38744800	4.04225300	2.54037900
H	-2.99874000	4.17489300	1.10412800
H	0.36681900	3.73462600	3.72405100
O	-1.96962400	4.68148200	3.58979100
C	-3.29555700	5.13129700	3.40710900
H	-3.36274400	5.88070400	2.60900600
H	-3.97000700	4.29865700	3.17128500
H	-3.59559100	5.58587300	4.34994700
H	2.54025700	1.05258700	-1.25174000
H	2.60642700	1.67628400	0.44377100
C	0.13961400	1.94691900	-1.96851200
H	0.67938700	1.21876700	-2.58182500
H	-0.91573400	1.64379900	-2.02363400

C	0.31856100	3.33745700	-2.57281400
H	1.37495500	3.62055400	-2.58921600
H	-0.05209900	3.37317900	-3.60070400
H	-0.21293700	4.10118300	-1.99946800

Imaginary Frequency: -669.77

II" (Quartet)

0 4

Fe	-0.46576100	-0.09062600	-0.36201500
N	-0.35565800	-0.06758500	1.65467800
C	0.76799600	0.40654800	2.46249100
C	-1.43461000	-0.00514400	2.39165100
C	0.11808500	0.90959600	3.75037400
H	1.47299000	-0.41490400	2.63457300
H	0.52838600	0.46722100	4.65999200
N	-2.22559600	-1.10719500	-0.18384800
C	-3.12538600	-1.01986400	0.81628000
C	-3.80186900	-2.36429000	-1.52111900
C	-4.46107000	-1.52168700	0.65407500
C	-4.76161100	-2.19300700	-0.57016400
H	-4.03195500	-2.89679100	-2.43696400
H	-5.76488700	-2.58136200	-0.71627800
C	-2.77516600	-0.41739400	2.07054100
C	-5.40261900	-1.34691200	1.66881600
C	-5.06132800	-0.71208100	2.86017300
H	-5.80240200	-0.58453600	3.64166600
C	-3.76674400	-0.26974000	3.06000500
H	-3.48522900	0.18117200	4.00330600
H	-6.40935500	-1.72567200	1.51564000
O	-1.25529800	0.49359400	3.63892800
C	-2.50395800	-1.82659300	-1.32734500
C	-1.43020600	-1.95715000	-2.24191700
C	0.88771300	-1.33805400	-2.63370800
C	2.12451600	-1.41485500	-1.97052300
C	0.89546000	-1.07262700	-4.01330000
C	3.31743300	-1.25623500	-2.65603400
C	2.09635600	-0.90928600	-4.69457800
C	3.31225900	-1.00397800	-4.02708300
H	4.25852300	-1.32744100	-2.11982600
H	2.07787700	-0.69300400	-5.75837300
H	4.24495500	-0.87452700	-4.56510400
H	2.11677600	-1.60523900	-0.89923400
H	-0.04144000	-0.95558000	-4.54520400
H	1.30444200	1.20011900	1.93073500
H	0.12913100	1.99966500	3.84242800
N	-0.26250500	-1.41165900	-1.83824800
C	-1.58944300	-2.73994600	-3.50809600
H	-0.63716500	-3.16484100	-3.82936100
H	-2.28732500	-3.56685300	-3.36673200
H	-1.97229900	-2.13752200	-4.34059400
C	0.94760800	2.02019000	-1.84569400

H	1.71330500	1.79136100	-1.09357100
C	-0.45764600	1.72132800	-1.36699600
C	-0.91027600	2.46949700	-0.18091800
C	-2.24386800	2.40117800	0.27410400
C	-0.01701300	3.20924700	0.62887500
C	-2.64813800	2.94886400	1.48411800
H	-2.98083000	1.86345200	-0.31605400
C	-0.40886300	3.75842700	1.83578100
H	1.00930900	3.34769300	0.30537300
C	-1.72046000	3.60483900	2.29376700
H	-3.67765500	2.82618000	1.79988800
H	0.29050800	4.31466500	2.45278900
O	-1.98480100	4.10684100	3.53365400
C	-3.28110400	3.88263700	4.04630900
H	-4.04890000	4.38163400	3.44250300
H	-3.51253300	2.81121000	4.09812200
H	-3.28905700	4.30379800	5.05043500
H	1.19140900	1.42773000	-2.73146300
H	1.08632600	3.07968800	-2.11371800
C	-1.46296300	1.56866400	-2.50246300
H	-1.02500200	0.90433700	-3.25841300
H	-2.37042300	1.04935500	-2.16377000
C	-1.85542900	2.89252600	-3.15403200
H	-0.98066200	3.40684700	-3.56267600
H	-2.56374700	2.74538700	-3.97394200
H	-2.32025600	3.56534800	-2.42745600

III'' (Quartet)

0 4

Fe	0.48654800	-1.39217800	-0.40052000
N	0.44231000	-1.89933100	1.55391400
C	1.48732000	-2.60378300	2.29658000
C	-0.27358900	-1.22124200	2.41350900
C	1.34810200	-2.08246100	3.72585000
H	1.32970300	-3.68585800	2.22135500
H	1.22956900	-2.86521500	4.47729700
N	-1.45057100	-0.77944300	-0.21103400
C	-2.04704300	-0.27492500	0.88771700
C	-3.34548600	-0.12596400	-1.56587500
C	-3.29538600	0.42853900	0.79333800
C	-3.91560000	0.48731000	-0.49180200
H	-3.83550700	-0.09701200	-2.53249600
H	-4.86039900	1.01336200	-0.58849900
C	-1.44739500	-0.42164500	2.18289600
C	-3.85429000	1.01771300	1.92787600
C	-3.23198300	0.91252100	3.16902200
H	-3.67803400	1.37397600	4.04324700
C	-2.05802800	0.19277000	3.29372900
H	-1.59678200	0.06893200	4.26551300
H	-4.79333300	1.55471700	1.82656600
O	0.13574900	-1.30708400	3.70247000

C	-2.09664600	-0.78402300	-1.42970900
C	-1.42121500	-1.45903600	-2.47570200
C	0.60804500	-2.67693300	-3.02495300
C	1.33471400	-3.78423300	-2.55475200
C	0.89695000	-2.19855900	-4.31388300
C	2.29154800	-4.40151300	-3.34334000
C	1.86197800	-2.81966900	-5.09839000
C	2.56123300	-3.92418300	-4.62505300
H	2.83307600	-5.25951300	-2.95753900
H	2.07694900	-2.42537600	-6.08686700
H	3.31341400	-4.40323000	-5.24220900
H	1.12116800	-4.14425700	-1.55040800
H	0.39218200	-1.31489800	-4.68643600
H	2.46956600	-2.37960500	1.86626200
H	2.16311500	-1.41645300	4.02375300
N	-0.26448300	-2.05895600	-2.12053700
C	-2.03018900	-1.56679600	-3.83938400
H	-1.68653600	-2.46621100	-4.35265500
H	-3.11816800	-1.62095800	-3.77363400
H	-1.79124100	-0.71393300	-4.48590500
C	3.09126500	-0.74932800	-1.60654000
H	3.38165600	-1.63001700	-1.01953400
C	1.90403700	-0.01387100	-1.02028700
C	2.08784800	0.53260500	0.33607900
C	1.12344300	1.36941300	0.93552200
C	3.18441500	0.16834400	1.15208300
C	1.19131100	1.74954700	2.26919200
H	0.26700400	1.69748200	0.35288700
C	3.26234800	0.54156800	2.48121700
H	3.98846700	-0.42772300	0.73341500
C	2.24927800	1.30803400	3.06424400
H	0.39597500	2.35783100	2.68403800
H	4.10487100	0.24545500	3.09901700
O	2.37460400	1.54966500	4.40039400
C	1.31498100	2.24502600	5.02256200
H	1.20823900	3.26231400	4.62658600
H	0.36131900	1.71583800	4.90106900
H	1.56603300	2.29996400	6.08070800
H	2.86919400	-1.10490400	-2.61610400
H	3.98942400	-0.11512500	-1.67456400
C	1.19341300	0.88387900	-2.02666900
H	1.03179000	0.30537000	-2.94527600
H	0.18462100	1.14910900	-1.68055900
C	1.96331300	2.16002300	-2.35794600
H	2.95116200	1.93055700	-2.76811400
H	1.43484900	2.77143500	-3.09449200
H	2.11472500	2.77104500	-1.46331800

TS₂" (Quartet)

04

Fe	-0.32932700	-1.96824600	-0.38889200
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N	-0.49626900	-3.07347600	1.37005800
C	0.14300100	-4.26224700	1.94072300
C	-1.17334200	-2.51465300	2.33511500
C	0.06785800	-4.01643900	3.43817600
H	-0.41432900	-5.15523300	1.62787600
H	-0.21268500	-4.88696400	4.03118000
N	-2.30942600	-1.73348100	-0.15668200
C	-2.84662600	-1.27535100	0.99657200
C	-4.38293400	-1.26332400	-1.30167900
C	-4.11373200	-0.60988400	1.01573300
C	-4.86821400	-0.62186400	-0.19650500
H	-4.98630700	-1.32039000	-2.20041500
H	-5.84714600	-0.15353200	-0.20967900
C	-2.17319500	-1.48585500	2.23888600
C	-4.55450800	-0.01214400	2.19991800
C	-3.81745600	-0.11472800	3.38046400
H	-4.17152900	0.36786600	4.28475400
C	-2.66430700	-0.87699900	3.40911500
H	-2.13378500	-1.04239800	4.33977100
H	-5.49397400	0.53338900	2.18705400
O	-0.98329100	-3.03647700	3.56851000
C	-3.08351700	-1.81631900	-1.29902700
C	-2.42068000	-2.37714800	-2.41932600
C	-0.36870100	-3.16799400	-3.30969300
C	-0.48259500	-4.52150400	-3.65044200
C	0.58285200	-2.38626000	-3.97697700
C	0.34349300	-5.07624200	-4.61981500
C	1.40389600	-2.94480100	-4.94876800
C	1.29234800	-4.29378000	-5.27248800
H	0.24954300	-6.12998800	-4.86417300
H	2.13583400	-2.32239500	-5.45465500
H	1.93747900	-4.73136000	-6.02666900
H	-1.20963500	-5.13407100	-3.12505800
H	0.67163800	-1.33598400	-3.71322200
H	1.17058900	-4.37363200	1.59365700
H	0.99056900	-3.58227200	3.83922700
N	-1.11682200	-2.60856600	-2.26240900
C	-3.11186400	-2.61035200	-3.72587700
H	-3.30889600	-3.67425000	-3.89404500
H	-4.06635500	-2.08973900	-3.78770600
H	-2.48777600	-2.27632800	-4.56040900
C	1.88518200	-3.52293300	-0.87410600
H	0.99725400	-4.09578000	-0.58405600
C	1.88607900	-2.08031300	-0.37701200
C	2.20888300	-1.86489400	1.07998500
C	1.74341500	-0.72923800	1.75120800
C	3.04077100	-2.72527000	1.81176000
C	2.03545500	-0.47684400	3.08701700
H	1.10663100	-0.02070500	1.22662100
C	3.35548500	-2.48824900	3.14117800
H	3.46021900	-3.60545300	1.33306700

C	2.84335100	-1.36639600	3.79618700
H	1.62486900	0.40635300	3.56130900
H	4.00066500	-3.16175700	3.69569200
O	3.17644000	-1.23439500	5.10832600
C	2.64706500	-0.11960300	5.79525400
H	2.98967400	0.82605700	5.35845000
H	1.55025400	-0.13159400	5.79960500
H	3.01046400	-0.19283200	6.81876500
H	1.93189300	-3.54607200	-1.96475700
H	2.75361300	-4.09014300	-0.51457500
C	2.85875400	-1.24356200	-1.24111400
H	2.49640400	-1.23508400	-2.27720500
H	2.83861000	-0.20138200	-0.90190200
C	4.29505600	-1.74698400	-1.21610900
H	4.38186700	-2.75344200	-1.63523000
H	4.94354000	-1.09449700	-1.80572600
H	4.69494500	-1.77304800	-0.19827200
Si	-0.31524200	0.40093700	-1.24633700
H	0.79200100	-0.99613800	-0.91329800
H	0.92991900	1.15378600	-1.52264300
H	-0.87005500	0.99935200	-0.01089200
C	-1.48255200	0.70171200	-2.71702100
H	-1.39198800	1.74460900	-3.03125400
H	-1.23402700	0.06947200	-3.57167700
H	-2.52224200	0.51536200	-2.44900000

Imaginary Frequency: -867.75

IV" (Quartet)

0 4

Fe	0.36054200	0.12818600	0.51366200
N	0.34875700	0.15767800	2.46850700
C	1.47474300	0.45427800	3.36978800
C	-0.66225400	-0.20433800	3.21735500
C	0.81202100	0.56542400	4.72849500
H	2.20592100	-0.36310800	3.31563800
H	1.34293200	0.07096400	5.54174300
N	-1.38985000	-0.84892600	0.45598500
C	-2.27271100	-1.04970600	1.46997800
C	-2.97874200	-1.82369800	-1.10817400
C	-3.56610400	-1.62125400	1.22419400
C	-3.88668600	-2.00382400	-0.10966600
H	-3.22053500	-2.10403300	-2.12655800
H	-4.86130700	-2.43789100	-0.30850700
C	-1.94968400	-0.70934700	2.82229600
C	-4.47576600	-1.79855800	2.27142000
C	-4.15232500	-1.43912800	3.57321400
H	-4.86648500	-1.57690500	4.37691400
C	-2.90336100	-0.90942200	3.83840300
H	-2.63184200	-0.63824700	4.85038000
H	-5.44658000	-2.22851000	2.04154600
O	-0.45302700	-0.10878600	4.54602000

C	-1.72543200	-1.23682100	-0.82921200
C	-0.74480500	-0.98180800	-1.81669700
C	1.40479700	-0.03640200	-2.27822700
C	2.71163200	-0.41177400	-1.94883900
C	1.18616300	0.68157400	-3.45848700
C	3.76976200	-0.08687900	-2.78539600
C	2.24862800	1.00435100	-4.29311900
C	3.54443900	0.62132900	-3.96344300
H	4.77719600	-0.38552500	-2.51402400
H	2.06332200	1.57312900	-5.19877300
H	4.37338900	0.87957000	-4.61353500
H	2.88061900	-0.95288500	-1.02249500
H	0.18125400	1.01316300	-3.69873500
H	1.98858200	1.37017300	3.07798600
H	0.60535700	1.60195200	5.01609200
N	0.35681600	-0.34791000	-1.38293400
C	-0.91923600	-1.47103900	-3.22063300
H	0.04459400	-1.64517400	-3.69940500
H	-1.47488500	-2.40947700	-3.23777100
H	-1.46492400	-0.76043700	-3.85158100
C	4.09083100	-1.34528500	6.11593700
H	3.13219100	-1.48063500	5.60714400
C	5.06428700	-0.53675700	5.26538500
C	4.54906000	0.83727500	4.89188200
C	4.90680900	1.40147700	3.66787000
C	3.75002100	1.61114800	5.74168200
C	4.49532400	2.67386600	3.28640500
H	5.51672100	0.82267300	2.97739100
C	3.32036500	2.87934500	5.37949800
H	3.45190000	1.21946300	6.71060200
C	3.68968700	3.42259100	4.14579300
H	4.77857200	3.05659300	2.31397700
H	2.69874200	3.47440600	6.04039100
O	3.21408100	4.66410700	3.87215900
C	3.61343000	5.25279300	2.64796800
H	4.70295000	5.36616400	2.59594700
H	3.26804100	4.66583600	1.78946300
H	3.14849100	6.23677900	2.62190200
H	4.49476300	-2.33969400	6.32553200
H	3.88553600	-0.87507100	7.08146800
C	6.45956200	-0.45528300	5.91565600
H	6.83858900	-1.47669500	6.04851300
H	7.14130000	0.03030400	5.20733700
C	6.50352900	0.28346800	7.24245300
H	5.88388000	-0.20062900	8.00297700
H	7.52145300	0.32254900	7.63674000
H	6.15323500	1.31431800	7.13870700
Si	2.06694500	1.88931800	0.42497100
H	5.19992000	-1.08429800	4.32201400
H	3.44929100	1.37853400	0.67076400
H	1.85270500	2.85042000	1.54987200

C	2.20313900	3.00006100	-1.13833800
H	2.72350600	3.93266500	-0.89986700
H	2.76213500	2.50479500	-1.93442800
H	1.22266700	3.26588500	-1.54142400

TS₃" (Quartet)

0 4

Fe	0.10510100	-1.93563800	-0.38860400
N	0.52617900	-2.06428600	1.49711500
C	1.71578700	-2.67838400	2.08947600
C	-0.10505200	-1.40559900	2.43741800
C	1.79335100	-2.03849700	3.46838200
H	1.58584700	-3.76668100	2.12788500
H	1.96066700	-2.73814600	4.28777800
N	-1.53246600	-0.84719400	-0.07620400
C	-1.99683300	-0.37233100	1.10830200
C	-3.36217500	0.24568300	-1.24647300
C	-3.17580400	0.44430500	1.15954400
C	-3.84408400	0.73103300	-0.06979800
H	-3.86090600	0.47888300	-2.18053200
H	-4.73575900	1.34932900	-0.04298200
C	-1.31723400	-0.63691500	2.34502700
C	-3.63946400	0.94448500	2.37874500
C	-2.97158600	0.67522500	3.56970900
H	-3.34536200	1.06466000	4.51001600
C	-1.82857500	-0.09876000	3.54568900
H	-1.30294700	-0.32032800	4.46611100
H	-4.53922200	1.55357800	2.37709000
O	0.48611400	-1.45116700	3.65132300
C	-2.19521900	-0.55254400	-1.26237300
C	-1.61567200	-1.09653300	-2.42470900
C	0.27201400	-2.37414800	-3.25301200
C	0.76436300	-3.68077400	-3.12596000
C	0.67132000	-1.61686800	-4.36239000
C	1.61512300	-4.21577300	-4.07995300
C	1.52992200	-2.15652600	-5.31328100
C	2.00474300	-3.45662700	-5.18231200
H	1.97927500	-5.23168000	-3.96352800
H	1.83698000	-1.54883700	-6.15895800
H	2.67520700	-3.87337300	-5.92600400
H	0.46768600	-4.26261200	-2.25665000
H	0.33501300	-0.58970900	-4.45457300
H	2.59271100	-2.46673700	1.47247000
H	2.53084800	-1.23077700	3.52036500
N	-0.50989400	-1.84724700	-2.20988400
C	-2.23448200	-0.91476200	-3.77462200
H	-1.96288300	-1.73203200	-4.44431500
H	-3.32333900	-0.89433000	-3.70208800
H	-1.92905100	0.01683900	-4.26552400
C	4.83515400	-1.65232100	-0.09865100
H	4.84877400	-2.18019200	0.86374900

C	3.70570400	-0.67142600	-0.21481000
C	3.40774700	0.15912500	0.93966000
C	2.11717500	0.67084800	1.18085400
C	4.36709000	0.38417500	1.95287000
C	1.79110800	1.34532800	2.35052500
H	1.32392000	0.49560200	0.46112300
C	4.06065900	1.06659900	3.11460100
H	5.37844700	0.01269100	1.81972100
C	2.76306400	1.54474200	3.33247700
H	0.77210300	1.68605200	2.49452500
H	4.80779500	1.23377000	3.88314900
O	2.54368700	2.16463400	4.52147500
C	1.21071200	2.53936200	4.80904100
H	0.83847600	3.29141600	4.10323500
H	0.53932600	1.67246300	4.78937900
H	1.22512900	2.96585400	5.81057100
H	4.78760900	-2.39876400	-0.89464400
H	5.81309000	-1.16081600	-0.18555500
C	2.87774800	-0.73278200	-1.32776600
H	3.19277700	-1.44793300	-2.08927400
H	1.66185600	-1.66119100	-0.87449700
C	2.13594600	0.45654500	-1.89576600
H	2.47867200	0.63751600	-2.91897700
H	1.05132500	0.31038100	-1.94485900
H	2.32682200	1.36459200	-1.32131900

Imaginary Frequency: -940.95

V'' (Quartet)

0 4

Fe	-0.09621300	-1.74500700	-0.29032300
N	0.07901500	-2.28346200	1.55560700
C	0.94131200	-3.35344000	2.05739500
C	-0.50747900	-1.71263500	2.57080500
C	0.87843700	-3.18309900	3.57223100
H	0.55734100	-4.31971100	1.71486800
H	0.59103800	-4.08451100	4.11623500
N	-1.46598600	-0.37474400	0.14643900
C	-1.97390200	-0.04882700	1.36368500
C	-3.01778700	1.16863900	-0.92056400
C	-3.00644200	0.93866000	1.48845800
C	-3.53529400	1.51064300	0.29191200
H	-3.40439800	1.61220000	-1.83149900
H	-4.34601700	2.22813500	0.37288100
C	-1.48876400	-0.65837900	2.56585600
C	-3.46443600	1.32720500	2.75048800
C	-2.94539200	0.76219600	3.90883500
H	-3.30027900	1.07908500	4.88277900
C	-1.97906400	-0.22220900	3.80933400
H	-1.58018400	-0.68367800	4.70397300
H	-4.23865400	2.08763100	2.80624700
O	-0.15474000	-2.19714300	3.78076900

C	-1.94538900	0.25018600	-0.99745900
C	-1.25720000	-0.06759000	-2.18686200
C	0.68840400	-1.15436100	-3.07402200
C	1.04885800	-2.44722900	-3.47357200
C	1.33982500	-0.06175200	-3.66489800
C	2.01708100	-2.63584400	-4.44877400
C	2.31714200	-0.25870900	-4.63185100
C	2.65842100	-1.54639800	-5.03353400
H	2.27981300	-3.64524000	-4.74999500
H	2.81964000	0.59923500	-5.06764400
H	3.42172300	-1.69999200	-5.78884300
H	0.56480400	-3.28893000	-2.99123400
H	1.08709800	0.94284400	-3.33787000
H	1.94973600	-3.24124200	1.64941500
H	1.80394800	-2.78996100	4.00305700
N	-0.25922700	-0.96539500	-2.05028700
C	-1.66071800	0.51598300	-3.50552800
H	-1.26931300	-0.07684500	-4.33266000
H	-2.74902800	0.54379800	-3.59889500
H	-1.30296100	1.54208100	-3.64732200
C	5.19986000	-1.99100100	2.31566100
H	4.66335300	-2.48923600	3.13295200
C	4.31769300	-1.77760500	1.11388000
C	3.23355100	-0.78928500	1.27185700
C	2.62905600	-0.12163800	0.19538200
C	2.78903300	-0.42509900	2.55861700
C	1.64327600	0.84398800	0.38195600
H	2.95473400	-0.31722400	-0.81893900
C	1.80532900	0.52459400	2.76164900
H	3.23642800	-0.88871000	3.43145200
C	1.22559200	1.17856300	1.67202300
H	1.21397100	1.33334700	-0.48529500
H	1.47090300	0.78668100	3.76026900
O	0.28881400	2.11336900	1.96780900
C	-0.21807900	2.88372900	0.89496100
H	0.57821400	3.46382900	0.41232300
H	-0.71371000	2.25963600	0.14360600
H	-0.95013500	3.56212800	1.33055400
H	6.05444600	-2.62092200	2.06515900
H	5.57693200	-1.04726500	2.72320000
C	4.56823100	-2.50680900	0.00626800
H	5.44008500	-3.15777600	0.06746800
H	0.74505500	-2.98544900	-0.70200500
C	3.81406800	-2.58524800	-1.27654500
H	3.96943300	-3.55795500	-1.75117600
H	2.73592000	-2.45847600	-1.14062500
H	4.14228100	-1.83502300	-2.00831500

I" (Sextet)

0 6

Fe	0.71930100	-0.71893600	0.38533900
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N	0.41912000	-0.27432500	2.39107300
C	1.51540200	-0.42171000	3.34492100
C	-0.60294900	0.21738200	3.02237700
C	1.02554300	0.35218200	4.56271200
H	1.68509600	-1.48563700	3.54550400
H	1.14850100	-0.16791100	5.51310700
N	-1.45407900	-0.34560400	0.24726200
C	-2.32062100	0.15022200	1.16952600
C	-3.28308000	-0.47417900	-1.35915600
C	-3.69992300	0.41076700	0.84113700
C	-4.14836900	0.07872000	-0.46660700
H	-3.62077700	-0.73289600	-2.35512400
H	-5.18466100	0.26742100	-0.72931600
C	-1.92096100	0.46818700	2.51484500
C	-4.57489600	0.97350400	1.77425400
C	-4.15132400	1.29604100	3.05836400
H	-4.83786100	1.72845400	3.77806200
C	-2.84175100	1.04065600	3.41288200
H	-2.49192900	1.28534900	4.40784300
H	-5.60437600	1.14553000	1.47071200
O	-0.38585900	0.51734700	4.32627100
C	-1.93003000	-0.68283600	-1.00716200
C	-1.00487700	-1.21042700	-1.95543200
C	1.29066600	-1.63420200	-2.48339600
C	2.27611200	-2.55332300	-2.09474800
C	1.41001800	-1.01682700	-3.74016300
C	3.33098600	-2.85416400	-2.94507300
C	2.47238900	-1.31918300	-4.58080500
C	3.43841400	-2.24170000	-4.19039300
H	4.07888100	-3.57434600	-2.62850000
H	2.54736400	-0.82653700	-5.54530100
H	4.26793500	-2.47734800	-4.84852800
H	2.19747800	-3.01152500	-1.11629900
H	0.66755700	-0.28583500	-4.04523400
H	2.44724600	-0.03304400	2.92435300
H	1.46924400	1.35087700	4.64503800
N	0.26892200	-1.29573300	-1.58238900
C	-1.50169100	-1.70973100	-3.28228300
H	-0.76694300	-2.36201500	-3.75248100
H	-2.42567100	-2.27866000	-3.16166700
H	-1.71379500	-0.89889400	-3.98840600
C	2.02359400	1.24623400	0.01228400
H	2.14061500	-1.57407900	0.64820700
C	0.88096900	1.89118300	-0.36365000
C	0.03526300	2.62652100	0.58885500
C	-1.27631100	2.99500700	0.26186700
C	0.48986600	2.98310100	1.87283400
C	-2.10667500	3.65833300	1.15592600
H	-1.68435700	2.72418100	-0.70693200
C	-0.32231700	3.63376300	2.77781700
H	1.50927700	2.74784800	2.16364900

C	-1.63594500	3.97139500	2.43016200
H	-3.12283100	3.89216000	0.86289400
H	0.03198600	3.89534100	3.76932600
O	-2.36524600	4.58473500	3.39489600
C	-3.68832200	4.95773300	3.06243300
H	-3.70627800	5.67688300	2.23491800
H	-4.29366700	4.08438600	2.79265200
H	-4.10367800	5.42540700	3.95347100
H	2.67489300	0.79840700	-0.73264500
H	2.42949200	1.30460900	1.01539600
C	0.50385500	1.91716100	-1.82232600
H	1.15830000	1.22490900	-2.35751000
H	-0.51538300	1.53259900	-1.96463700
C	0.62448200	3.30845400	-2.43745600
H	1.64626800	3.68656000	-2.34644700
H	0.36997200	3.28940600	-3.50012100
H	-0.03456600	4.03068500	-1.94944100

TS₁^o (Sextet)

0 6

Fe	0.57787200	-0.14957000	0.29496000
N	0.31704200	-0.19867100	2.33232500
C	1.40309200	-0.37669200	3.29124700
C	-0.73297100	0.21644600	2.98098600
C	0.86859300	0.29089200	4.55290900
H	1.60911300	-1.44542600	3.42780200
H	1.00008500	-0.28986500	5.46620600
N	-1.56938200	-0.28988400	0.21039000
C	-2.44439800	0.19104000	1.12145700
C	-3.36262500	-0.49959200	-1.40428600
C	-3.82172400	0.42817200	0.77742600
C	-4.24533300	0.06583000	-0.53050800
H	-3.68655700	-0.78730100	-2.39754700
H	-5.27997300	0.23608900	-0.81183400
C	-2.04829300	0.48683400	2.47254000
C	-4.70516600	0.98614900	1.70576800
C	-4.28598700	1.30536600	2.99351700
H	-4.97845500	1.73784600	3.70743700
C	-2.98001600	1.04645600	3.36548300
H	-2.64416500	1.28409800	4.36731300
H	-5.73441900	1.15527600	1.40085000
O	-0.54429600	0.41674600	4.30690400
C	-2.01111900	-0.66760700	-1.03255100
C	-1.03669900	-1.19264500	-1.94590900
C	1.29248200	-1.53105500	-2.40198000
C	2.32894000	-2.29780600	-1.84914900
C	1.41412500	-1.10881900	-3.73531300
C	3.43078100	-2.65359900	-2.61193800
C	2.52708200	-1.45911700	-4.48972800
C	3.53895500	-2.23669600	-3.93688700
H	4.21559500	-3.25715700	-2.16693000

H	2.60531700	-1.11356900	-5.51583700
H	4.40660100	-2.50818900	-4.52844100
H	2.24650300	-2.60196500	-0.81089800
H	0.64138300	-0.48122000	-4.16745000
H	2.32432500	0.08294500	2.92058500
H	1.27327300	1.29688200	4.70760900
N	0.23380200	-1.13699500	-1.57467700
C	-1.49776400	-1.82485100	-3.22592400
H	-0.74041100	-2.50044300	-3.62268800
H	-2.41523500	-2.39511000	-3.07076300
H	-1.70727000	-1.08194500	-4.00404100
C	2.11398500	1.30912700	-0.28897300
H	2.23026100	-0.29353500	0.14293600
C	0.83992800	1.89261100	-0.56393000
C	0.09697500	2.61042200	0.46898200
C	-1.21661600	3.07098700	0.24008800
C	0.62196500	2.87200800	1.75723200
C	-1.96404100	3.72009300	1.21322200
H	-1.68375000	2.88992300	-0.72317800
C	-0.11562500	3.50568900	2.73773300
H	1.63445400	2.56202400	1.99888700
C	-1.42258100	3.93053900	2.48084700
H	-2.97654800	4.02927100	0.98126300
H	0.30008200	3.69100300	3.72332800
O	-2.07993100	4.51315600	3.52366100
C	-3.39349300	4.96471900	3.27526900
H	-3.41546400	5.73433500	2.49340000
H	-4.05415200	4.14006100	2.97996200
H	-3.74990400	5.39517900	4.21014400
H	2.74165700	1.08410600	-1.14816200
H	2.69585300	1.64637800	0.56473100
C	0.38574000	1.99550300	-2.00131800
H	0.96682100	1.28644800	-2.59896300
H	-0.66088900	1.67700700	-2.11624400
C	0.55999600	3.39733800	-2.58000600
H	1.61021200	3.70180600	-2.54888300
H	0.22750300	3.44847100	-3.62103300
H	-0.00808900	4.13950200	-2.01242200

Imaginary Frequency: -867.29

II" (Sextet)

0 6

Fe	-0.49355100	-0.00059600	-0.35943400
N	-0.45770800	-0.06446800	1.71532500
C	0.64607700	0.32106600	2.59391800
C	-1.56092400	0.00578300	2.40429100
C	-0.04656800	0.82392200	3.85907500
H	1.29117200	-0.54581100	2.78030500
H	0.30616200	0.35450700	4.77876900
N	-2.25964200	-1.14627600	-0.18705100
C	-3.19547400	-1.02554200	0.77400000

C	-3.72158700	-2.59583500	-1.45003800
C	-4.51039100	-1.57789400	0.60137100
C	-4.73533300	-2.36758100	-0.56370900
H	-3.88483200	-3.22960000	-2.31428900
H	-5.71653400	-2.80709600	-0.71475600
C	-2.90200500	-0.36872300	2.01557600
C	-5.50105300	-1.35025700	1.55960900
C	-5.22342600	-0.63020500	2.71694500
H	-5.99966300	-0.45570400	3.45342500
C	-3.93629400	-0.17303600	2.94674500
H	-3.69806600	0.32592400	3.87795100
H	-6.49355500	-1.75756500	1.38781900
O	-1.42554100	0.44768300	3.67624700
C	-2.46715600	-1.97107500	-1.26599700
C	-1.36910000	-2.13451700	-2.16817100
C	0.82521500	-1.31980500	-2.74696000
C	2.09294600	-1.21237000	-2.14751500
C	0.74046700	-1.18658900	-4.14458900
C	3.22996000	-1.00901200	-2.91273200
C	1.88310000	-0.97199600	-4.90285400
C	3.13431000	-0.88860200	-4.29746400
H	4.19789200	-0.93684900	-2.42671400
H	1.79333600	-0.85586000	-5.97855500
H	4.02260100	-0.72037100	-4.89635600
H	2.15586600	-1.29670100	-1.06460600
H	-0.23251700	-1.20731100	-4.62382900
H	1.25653800	1.09471500	2.11651400
H	-0.01115200	1.91156400	3.97070200
N	-0.27850300	-1.41723200	-1.90655500
C	-1.45614400	-3.13711200	-3.27930300
H	-0.46158800	-3.42491100	-3.62130300
H	-1.97474000	-4.04058700	-2.95208100
H	-1.99940900	-2.75386400	-4.15062000
C	1.06495400	2.15068300	-1.82720800
H	1.83725800	1.89177300	-1.09249900
C	-0.33946700	1.83881700	-1.34990800
C	-0.79127200	2.54829100	-0.14688500
C	-2.14093600	2.52728100	0.27442100
C	0.11374600	3.19986100	0.72818400
C	-2.54826100	3.02561200	1.50576800
H	-2.89293300	2.07408300	-0.36514800
C	-0.28253900	3.70054000	1.95348700
H	1.15414100	3.30300200	0.43741700
C	-1.61269700	3.59246700	2.37096100
H	-3.59214000	2.94522200	1.78707600
H	0.42658300	4.18933600	2.61532300
O	-1.88405000	4.05337800	3.62817800
C	-3.21538700	3.92728700	4.07722400
H	-3.91056900	4.50421300	3.45472500
H	-3.54027100	2.87946400	4.09017400
H	-3.23460700	4.32213800	5.09199300

H	1.29872500	1.58419500	-2.73331900
H	1.21015400	3.21759500	-2.06370600
C	-1.34653300	1.72320700	-2.49068100
H	-0.92293900	1.05922500	-3.25542500
H	-2.26747800	1.22096500	-2.16104700
C	-1.71286900	3.06242600	-3.12712400
H	-0.82688600	3.56131700	-3.53057700
H	-2.42567200	2.94291300	-3.94803900
H	-2.16038300	3.73716100	-2.39121400

III'' (Sextet)

0 6

Fe	0.53987900	-1.30443800	-0.38278200
N	0.38110200	-1.82775000	1.62057300
C	1.33927300	-2.59450800	2.41626600
C	-0.34634300	-1.12347000	2.43984400
C	1.16749200	-2.04594600	3.83132000
H	1.10755000	-3.66396800	2.34545400
H	0.98902800	-2.81048100	4.58907200
N	-1.49800500	-0.77180300	-0.22080800
C	-2.09185800	-0.21500100	0.85206400
C	-3.46532900	-0.33940600	-1.55358700
C	-3.36476100	0.44092100	0.73739200
C	-4.02620400	0.35914600	-0.52265300
H	-3.98931400	-0.43316500	-2.49801200
H	-4.99519300	0.83571900	-0.63529700
C	-1.48870800	-0.28549000	2.15213500
C	-3.91519600	1.10641100	1.83547500
C	-3.26980400	1.10685700	3.06762700
H	-3.70286200	1.62941900	3.91306500
C	-2.08966800	0.39834100	3.22261200
H	-1.61972800	0.33669700	4.19638700
H	-4.86635600	1.61647400	1.71052100
O	-0.01565700	-1.22720600	3.74814000
C	-2.17944800	-0.90715300	-1.40626700
C	-1.51284000	-1.62300800	-2.45013700
C	0.59139500	-2.59692500	-3.11760400
C	1.47643300	-3.58814000	-2.65645800
C	0.72696200	-2.15500100	-4.44596300
C	2.43641000	-4.13446800	-3.49269200
C	1.69843700	-2.70017400	-5.27423600
C	2.55399800	-3.69580400	-4.80986500
H	3.10290700	-4.90323200	-3.11443200
H	1.79645800	-2.33330600	-6.29132800
H	3.31077800	-4.11624000	-5.46296800
H	1.38324300	-3.91678600	-1.62331600
H	0.09625700	-1.34983300	-4.80735300
H	2.35380700	-2.44666100	2.03185900
H	1.99361000	-1.40437800	4.15136800
N	-0.27090600	-2.02480900	-2.18893100
C	-2.24431700	-1.95645200	-3.71535400

H	-1.77842200	-2.80242600	-4.22171100
H	-3.28432000	-2.21777600	-3.50963900
H	-2.25823000	-1.12204400	-4.42588500
C	3.26051500	-0.72978100	-1.60030900
H	3.54403000	-1.62987200	-1.04135600
C	2.06529400	-0.01076500	-1.00678200
C	2.22409000	0.49959300	0.36008700
C	1.29178200	1.38763500	0.94427700
C	3.25645700	0.04360800	1.21817800
C	1.32104900	1.72238900	2.29250300
H	0.49454400	1.80257500	0.33418400
C	3.29472000	0.37251800	2.55948500
H	4.03854600	-0.59348600	0.81822700
C	2.30993700	1.19153400	3.12035400
H	0.55507000	2.37959500	2.68815700
H	4.08839900	0.00621500	3.20423700
O	2.39920800	1.39733600	4.46824500
C	1.39346000	2.19243200	5.05670400
H	1.39968500	3.21524700	4.65991000
H	0.39651900	1.76079400	4.90360000
H	1.61239400	2.22304200	6.12307900
H	3.04545200	-1.05645400	-2.62188000
H	4.16233300	-0.09729100	-1.64381800
C	1.36772200	0.91193000	-2.00212200
H	1.19781000	0.34970300	-2.92968300
H	0.36224400	1.18821500	-1.65301900
C	2.15079200	2.18511900	-2.31611300
H	3.13372800	1.94901200	-2.73410000
H	1.62860700	2.81749600	-3.03977900
H	2.31498000	2.77782200	-1.41123600

TS₂" (Sextet)

0 6

Fe	-0.56278600	-2.44335000	-0.37364000
N	-0.84645800	-3.08559700	1.54273100
C	-0.14183400	-4.09535400	2.33639900
C	-1.54305400	-2.35779200	2.38874200
C	-0.13632500	-3.48487200	3.72400000
H	-0.69794500	-5.04198700	2.29885700
H	-0.29257700	-4.19028900	4.53961200
N	-2.60042500	-1.86164000	-0.25925500
C	-3.21128900	-1.34411700	0.82124400
C	-4.55263300	-1.38339800	-1.60530600
C	-4.47687300	-0.67634400	0.71172400
C	-5.13330400	-0.73524100	-0.55528200
H	-5.06697400	-1.44308900	-2.55749700
H	-6.10900200	-0.27097700	-0.65924100
C	-2.61248700	-1.44364900	2.12099600
C	-5.01456800	-0.01881900	1.81756900
C	-4.36023000	-0.02854600	3.05114800
H	-4.78323100	0.50311300	3.89615300

C	-3.19429300	-0.75007100	3.20408600
H	-2.71462300	-0.81584200	4.17284100
H	-5.95921500	0.50532600	1.70159500
O	-1.26899000	-2.59052800	3.69242600
C	-3.25422600	-1.93060700	-1.47233100
C	-2.49461100	-2.46963000	-2.53672700
C	-0.38464500	-3.25596300	-3.30741100
C	-0.17616500	-4.62922000	-3.47159900
C	0.31104900	-2.36095800	-4.12529200
C	0.72264800	-5.09413700	-4.42364500
C	1.21600100	-2.83090400	-5.07043600
C	1.42850300	-4.19780900	-5.22144200
H	0.87845200	-6.16230300	-4.53855900
H	1.75955300	-2.12471300	-5.69043400
H	2.13757900	-4.56248900	-5.95678600
H	-0.71609000	-5.31944300	-2.82974000
H	0.14335800	-1.29603500	-3.99282900
H	0.86394700	-4.27783900	1.95691800
H	0.76574100	-2.89309000	3.91590400
N	-1.21492900	-2.77907400	-2.26866100
C	-3.05008100	-2.62674100	-3.91564800
H	-2.70947000	-1.82043400	-4.57729600
H	-2.71105500	-3.56114600	-4.36972700
H	-4.13878500	-2.62562800	-3.92466300
C	1.96504100	-3.52873300	-0.86489100
H	1.25197700	-4.18261300	-0.33678200
C	1.99689000	-2.10631300	-0.34388400
C	2.42930000	-1.95922700	1.06634600
C	2.31992500	-0.72496000	1.72814700
C	2.98392100	-3.01690800	1.81251500
C	2.71118000	-0.54976700	3.05009600
H	1.91734100	0.13075300	1.19546000
C	3.38933000	-2.85753300	3.12734100
H	3.12268600	-3.98898100	1.34899400
C	3.25021400	-1.62176800	3.76337900
H	2.59466000	0.42351900	3.51171300
H	3.82913000	-3.67884300	3.68389100
O	3.65748800	-1.56636700	5.06173800
C	3.52902300	-0.32504600	5.72174400
H	4.12340100	0.45707700	5.23415400
H	2.48343000	0.00309800	5.76888100
H	3.90139900	-0.47843500	6.73321700
H	1.71560300	-3.55607200	-1.92684700
H	2.93968200	-4.03059300	-0.76937200
C	2.69070500	-1.16305700	-1.32392200
H	2.09435200	-1.10583900	-2.24643900
H	2.69576900	-0.14897700	-0.90982700
C	4.11655300	-1.57657500	-1.66543300
H	4.14281800	-2.52692800	-2.20684300
H	4.60476000	-0.83083200	-2.29794000
H	4.72222700	-1.69225800	-0.76095600

Si	-0.37642200	0.30740300	-0.52797200
H	0.69206200	-1.18840300	-0.40410200
H	0.77773300	1.22637100	-0.35687700
H	-1.30510800	0.64602500	0.57062700
C	-1.14726600	0.77676400	-2.21113900
H	-1.53947200	1.79673100	-2.17855200
H	-0.39087200	0.74264900	-2.99915000
H	-1.96458700	0.11147900	-2.49239800

Imaginary Frequency: -1301.77

IV" (Sextet)

0 6

Fe	0.57152600	0.14532900	0.47887100
N	0.43123300	-0.06733900	2.53235000
C	1.51177200	0.28042500	3.46180500
C	-0.66295100	-0.18025100	3.22594100
C	0.76918700	0.67532100	4.72735400
H	2.16447000	-0.59093900	3.60334900
H	1.18261700	0.26809500	5.64995900
N	-1.32731500	-0.87492900	0.43977700
C	-2.24428800	-1.00957500	1.43054400
C	-2.83522800	-2.00789900	-1.09101700
C	-3.54309400	-1.56781900	1.17200200
C	-3.80192400	-2.06936800	-0.13337100
H	-3.02307300	-2.39932000	-2.08358700
H	-4.77307000	-2.50644900	-0.34327000
C	-1.96869900	-0.60402800	2.77936200
C	-4.51240400	-1.62576400	2.17896900
C	-4.24394600	-1.16611300	3.45929000
H	-5.00325300	-1.20502800	4.23168400
C	-2.98172000	-0.67585000	3.74910800
H	-2.74593200	-0.34757700	4.75323300
H	-5.48474900	-2.04350100	1.93313100
O	-0.54880600	0.10863300	4.54041300
C	-1.59603600	-1.38985900	-0.80926300
C	-0.59168600	-1.24168500	-1.81518500
C	1.47256700	-0.12261200	-2.37384300
C	2.80630000	-0.09696300	-1.93308800
C	1.18024300	0.40704600	-3.64175800
C	3.81157200	0.41695600	-2.73791600
C	2.19236700	0.91832300	-4.44111900
C	3.51312300	0.92389800	-3.99955500
H	4.83391500	0.42718000	-2.37403400
H	1.94377800	1.33384500	-5.41264700
H	4.29832000	1.33159700	-4.62666800
H	3.03801400	-0.48689300	-0.94502600
H	0.14902100	0.45692600	-3.97367500
H	2.13120000	1.08805800	3.06194100
H	0.65851500	1.75994400	4.83164100
N	0.49114100	-0.54632200	-1.47833000
C	-0.75684000	-1.90614500	-3.14882200

H	0.20089700	-1.98465400	-3.66301100
H	-1.16280600	-2.91344200	-3.03507400
H	-1.43724600	-1.35935800	-3.81108200
C	4.02331800	-1.36256400	6.34136800
H	3.01504800	-1.42484000	5.92167800
C	4.99104500	-0.68409500	5.37900700
C	4.55353200	0.70093700	4.94968300
C	4.97508500	1.20974300	3.72102200
C	3.76582600	1.53613700	5.74913500
C	4.63544200	2.48736400	3.28919600
H	5.58366900	0.58379900	3.07147300
C	3.40714800	2.81110000	5.33622500
H	3.42188200	1.18930800	6.71973900
C	3.84069400	3.30029600	4.10107400
H	4.97177000	2.83189400	2.31956000
H	2.79649700	3.45504700	5.96048800
O	3.44503300	4.55783500	3.78383700
C	3.92424800	5.09944300	2.56580200
H	5.01947000	5.15702400	2.55980000
H	3.58567600	4.51315800	1.70426800
H	3.51085200	6.10439200	2.50144100
H	4.35167000	-2.38147900	6.56368900
H	3.94646200	-0.83678500	7.29685400
C	6.42799600	-0.66575100	5.93695200
H	6.74080900	-1.70075800	6.12519100
H	7.09665100	-0.28551400	5.15558800
C	6.60681300	0.16311000	7.19770000
H	6.00948400	-0.22055400	8.02986000
H	7.64894800	0.16225100	7.52485500
H	6.31457300	1.20463800	7.03553900
Si	1.79439400	2.37314300	0.45871600
H	5.02474600	-1.29789500	4.46730200
H	3.27335400	2.18864500	0.57811000
H	1.47576500	3.22274300	1.64736800
C	1.56151900	3.47286600	-1.10149500
H	2.10331300	4.41963600	-1.02034000
H	1.93091900	2.95115700	-1.98845500
H	0.50822500	3.70512600	-1.27387000

TS₃^o (Sextet)

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Fe	0.17562100	-2.04153300	-0.48688200
N	0.43219600	-2.16361100	1.54864700
C	1.61023200	-2.79653700	2.14669800
C	-0.10341200	-1.39273900	2.44719400
C	1.77329100	-2.07146800	3.47778900
H	1.43018600	-3.87220900	2.26154600
H	1.90749200	-2.72596400	4.33967000
N	-1.54515600	-0.86390900	-0.07786600
C	-1.97203200	-0.32992500	1.09550400
C	-3.48748600	0.07369200	-1.19959400

C	-3.14993900	0.49156900	1.15327100
C	-3.89609400	0.66939300	-0.04586400
H	-4.05664600	0.20177400	-2.11271400
H	-4.79396200	1.27873100	-0.01659200
C	-1.27180800	-0.54995000	2.32921700
C	-3.55519100	1.08419000	2.35369200
C	-2.84267000	0.88625400	3.52705700
H	-3.16428500	1.34622800	4.45454400
C	-1.72307800	0.07157300	3.50563600
H	-1.17478300	-0.11874800	4.41972400
H	-4.44937600	1.70132400	2.34632900
O	0.51908700	-1.37359000	3.64590300
C	-2.29550900	-0.68698500	-1.22423300
C	-1.80435800	-1.26915000	-2.42877300
C	0.13672800	-2.30871600	-3.43150900
C	0.89362800	-3.48682200	-3.31106100
C	0.31312400	-1.52043900	-4.58149000
C	1.77058100	-3.87568000	-4.31156300
C	1.19773300	-1.91355100	-5.57517300
C	1.92760100	-3.09359700	-5.45279600
H	2.33915600	-4.79315400	-4.19803400
H	1.32906500	-1.28351000	-6.44940300
H	2.61850800	-3.39366600	-6.23291500
H	0.77421000	-4.09276000	-2.41560800
H	-0.21167100	-0.57461400	-4.66405500
H	2.47223100	-2.66978000	1.48471100
H	2.56944400	-1.31981000	3.46058600
N	-0.63537700	-1.91088300	-2.34282500
C	-2.60923700	-1.20473200	-3.69170200
H	-2.25300100	-1.93823200	-4.41507300
H	-3.66349500	-1.41294800	-3.49481900
H	-2.56325700	-0.22230400	-4.17515800
C	5.04782300	-1.73547900	0.21458100
H	4.95216800	-2.25797400	1.17690000
C	3.93721900	-0.75562300	-0.02827000
C	3.54735400	0.10233900	1.07535100
C	2.23883500	0.61094000	1.20825200
C	4.42830600	0.36900500	2.14921500
C	1.83005600	1.33238400	2.32331400
H	1.49959200	0.40138300	0.44118100
C	4.03591300	1.09068100	3.26052400
H	5.44787800	-0.00102400	2.10399000
C	2.72795900	1.57633500	3.36342000
H	0.80272200	1.67447900	2.38168000
H	4.72526500	1.28898000	4.07458100
O	2.42551700	2.25265200	4.50598400
C	1.08512300	2.66709800	4.66313500
H	0.78655600	3.38460200	3.88881200
H	0.39526100	1.81442300	4.63616100
H	1.02765000	3.14948900	5.63773200
H	5.08457900	-2.48857400	-0.57598300

H	6.03306000	-1.25133500	0.23373400
C	3.18735800	-0.86877300	-1.19045400
H	3.54577300	-1.62186700	-1.89205600
H	1.86841700	-1.79228000	-0.76503400
C	2.47212900	0.27944600	-1.86389800
H	2.88301500	0.42365800	-2.86821800
H	1.39588900	0.11026500	-1.98954900
H	2.60244700	1.21603300	-1.31854900

Imaginary frequency:-1301.77

V'' (Sextet)

0 6

Fe	-0.03016400	-2.01454200	-0.34672700
N	0.16669000	-2.22904600	1.69646700
C	1.03699800	-3.25179600	2.27339200
C	-0.50906800	-1.68409000	2.65597200
C	0.91909300	-3.01501700	3.77565700
H	0.68051000	-4.23952700	1.95910900
H	0.69441200	-3.90919100	4.35911700
N	-1.44901000	-0.43693200	0.13928600
C	-2.01786400	-0.12725800	1.33203700
C	-2.89380000	1.17447600	-0.96670500
C	-3.08340700	0.83697000	1.41651300
C	-3.53102300	1.44305600	0.20864600
H	-3.19646400	1.67456500	-1.87909100
H	-4.35796500	2.14520300	0.25124200
C	-1.56810600	-0.70551200	2.56842900
C	-3.64033500	1.18958700	2.64943000
C	-3.17613600	0.63056700	3.83075200
H	-3.60583700	0.91499900	4.78431000
C	-2.15321500	-0.30017600	3.77888500
H	-1.78022300	-0.74272900	4.69348900
H	-4.44378900	1.92115100	2.66043600
O	-0.19637000	-2.11130300	3.90459300
C	-1.82239600	0.25541700	-0.99510100
C	-1.04942300	0.03550500	-2.18101300
C	0.82144400	-1.12149600	-3.14236800
C	1.00220100	-2.42846800	-3.61580000
C	1.65154900	-0.10145500	-3.63010000
C	1.97228200	-2.69694900	-4.57116300
C	2.62746400	-0.38277700	-4.57796700
C	2.79003800	-1.67965100	-5.05714600
H	2.09560700	-3.71231400	-4.93492400
H	3.26704000	0.41566300	-4.94119800
H	3.55132300	-1.89586800	-5.79897400
H	0.37659100	-3.21596600	-3.20711900
H	1.53479500	0.90695000	-3.24186600
H	2.06011300	-3.14274900	1.90009500
H	1.79819100	-2.52263900	4.20371100
N	-0.10962800	-0.89593500	-2.11931400
C	-1.34906900	0.80849900	-3.43086400

H	-0.83910800	0.37698700	-4.29118900
H	-2.42078500	0.80693800	-3.64233200
H	-1.04138300	1.85741100	-3.35608900
C	5.37360900	-1.79847000	2.00210600
H	5.00301100	-2.24463500	2.93302800
C	4.29929300	-1.72422000	0.95108300
C	3.21093600	-0.75916400	1.19723700
C	2.49120300	-0.13249200	0.16861000
C	2.88441900	-0.37892200	2.51307900
C	1.50658900	0.81778200	0.42877900
H	2.73550000	-0.33895800	-0.86856500
C	1.89611100	0.54619500	2.78933800
H	3.42604300	-0.81662200	3.34555800
C	1.20163700	1.16489400	1.74629600
H	0.98689200	1.28119200	-0.40272100
H	1.64713000	0.82072900	3.80939000
O	0.27613800	2.08464100	2.11397400
C	-0.29188000	2.87680600	1.08841400
H	0.47837200	3.45805600	0.56643100
H	-0.84025800	2.27172100	0.36015700
H	-0.98874700	3.55344400	1.58078700
H	6.20868400	-2.41410800	1.66476000
H	5.75909300	-0.80820900	2.26502200
C	4.38105600	-2.54528400	-0.11492700
H	5.26952700	-3.17403800	-0.16101400
H	-0.00970500	-3.62787500	-0.76229100
C	3.40712500	-2.74709900	-1.22300100
H	3.47439800	-3.76206100	-1.62276100
H	2.36774700	-2.60666800	-0.90071500
H	3.57341400	-2.06986100	-2.07079700

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Fe	0.07293900	0.03153700	0.09166700
N	-0.03549000	0.05422300	2.02796400
C	1.08964700	0.06075300	2.98208000
C	-1.14444200	-0.00687500	2.71613600
C	0.39369800	0.38736700	4.29951900
H	0.72197000	-0.21763700	5.14749500
N	-1.81432900	-0.62949800	-0.06510700
C	-2.78186900	-0.59780100	0.89336500
C	-3.44396900	-1.43587900	-1.67713700
C	-4.13755600	-0.94862000	0.58475900
C	-4.43258600	-1.38289100	-0.73729900
H	-3.66006300	-1.76856900	-2.68569600
H	-5.45176900	-1.66731800	-0.97876700
C	-2.48408200	-0.23015700	2.24610000
C	-5.13540500	-0.86513100	1.56572200
C	-4.83415800	-0.46392700	2.85844100
H	-5.61354300	-0.39525600	3.60895000
C	-3.52423400	-0.16451600	3.19157700

H	-3.27296400	0.12196600	4.20480600
H	-6.15371900	-1.12077700	1.28750600
O	-0.99331300	0.08873500	4.05987200
C	-2.13587400	-1.03830800	-1.34140900
C	-1.06032900	-1.00162600	-2.27714200
C	1.21670700	-0.46992300	-2.68909800
C	1.98848400	-1.64382300	-2.79534500
C	1.56312800	0.69771700	-3.39521800
C	3.11510800	-1.62311100	-3.61685500
C	2.69761100	0.66628600	-4.20683300
C	3.46937700	-0.48083300	-4.32038600
H	3.72338400	-2.51683200	-3.71058700
H	2.98318500	1.55654000	-4.75731800
H	4.34846200	-0.48473000	-4.95672100
H	1.79072900	0.85433100	2.71040500
H	0.47177100	1.44649000	4.56922300
N	0.07423900	-0.46327100	-1.83729800
C	-1.22292600	-1.57056100	-3.65352500
H	-0.40319500	-1.27573800	-4.30825100
H	-1.24762000	-2.66650600	-3.62697700
H	-2.15743000	-1.24384900	-4.11588700
C	1.68150900	1.23575900	0.06557600
H	0.95617000	2.40338100	1.74089000
C	1.50867600	2.57521200	0.80405900
C	2.84347200	3.16668700	1.20030800
C	3.16711000	3.40012100	2.53365600
C	3.81421300	3.48376600	0.23969600
C	4.40193600	3.92483700	2.91912800
H	2.43028100	3.17540900	3.30343400
C	5.04126900	4.01091600	0.59667200
H	3.60188100	3.30115100	-0.81066900
C	5.34612500	4.23408300	1.94341700
H	4.60961300	4.08976000	3.96968600
H	5.79050100	4.25703600	-0.14813400
C	0.66614800	3.58739400	0.01446000
H	0.73051700	4.56244500	0.51340900
C	-0.79741300	3.19812500	-0.12153300
H	-1.36530100	3.94734800	-0.68143900
H	-0.92787700	2.24079600	-0.64125700
H	-1.27168100	3.09302700	0.86102800
O	6.58251300	4.75115100	2.19517200
C	6.91408900	4.98783500	3.54427500
H	6.23496500	5.71359300	4.00920100
H	6.89923800	4.06336100	4.13534000
H	7.92426800	5.39443100	3.54402300
H	2.09965400	1.41172900	-0.93542200
H	2.43867800	0.62620900	0.58977100
H	1.11608900	3.73492800	-0.97523400
C	0.70943100	1.94358200	-3.27931200
H	0.37522700	1.98281200	-2.23628100
C	1.47204700	3.22822200	-3.57876700

H	0.85949100	4.09869400	-3.32690400
H	2.40243800	3.29576600	-3.00733100
H	1.72654700	3.31579900	-4.64018700
C	-0.54346300	1.87109900	-4.15432200
H	-1.12611100	2.79325600	-4.06445900
H	-0.27972900	1.74546600	-5.21015000
H	-1.19781500	1.04537400	-3.87060600
C	1.63329500	-2.87963900	-1.99073200
H	0.54097200	-2.92544100	-1.90597700
C	2.09034100	-4.18334500	-2.63296500
H	3.18010600	-4.28091500	-2.63309300
H	1.69593500	-5.03859700	-2.07803900
H	1.74932600	-4.26763300	-3.66878400
C	2.18393900	-2.74815000	-0.57120600
H	1.80855100	-1.83784600	-0.09051700
H	1.89641800	-3.60131800	0.05133500
H	3.27724800	-2.68444500	-0.58105200
C	1.86114900	-1.26575700	2.95354000
H	2.22402400	-1.36731900	1.92267700
C	3.07423400	-1.18262400	3.87008100
H	2.78226700	-1.09492900	4.92273400
H	3.69313500	-2.07908600	3.78610000
H	3.70209400	-0.31985300	3.62590400
C	0.98087200	-2.46647200	3.26762500
H	0.15039400	-2.55082900	2.56051300
H	1.55546300	-3.39469100	3.21388400
H	0.55706900	-2.40733000	4.27653100

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Fe	0.09586900	0.02684400	-0.09563300
N	0.26029700	0.08854100	1.89498600
C	1.42126600	0.05409800	2.83964200
C	-0.75924500	0.50935000	2.60076900
C	0.96356700	1.02000500	3.91306100
H	1.28002200	0.76404000	4.92405100
N	-1.83542800	-0.45373300	0.08424600
C	-2.67274700	-0.06443900	1.07517600
C	-3.70555800	-1.47620300	-1.07533200
C	-4.09055400	-0.24847400	0.96656000
C	-4.57890400	-0.98205200	-0.15284400
H	-4.06161300	-2.05894200	-1.91770300
H	-5.64735500	-1.14953700	-0.24394100
C	-2.15959900	0.54192800	2.26324400
C	-4.93913500	0.28667000	1.94162500
C	-4.42785600	0.96882200	3.03760000
H	-5.09655300	1.39271200	3.77844600
C	-3.05669000	1.07367900	3.20562200
H	-2.64979100	1.54570700	4.09079700
H	-6.01110100	0.15771600	1.82226400
O	-0.46978000	0.92694100	3.85685300

C	-2.32471400	-1.19740700	-0.96243200
C	-1.35512400	-1.61361400	-1.90940500
C	0.93257100	-1.43545500	-2.62395800
C	1.99988900	-2.28577700	-2.24391500
C	0.95232200	-0.78635500	-3.88107800
C	3.10012700	-2.40326200	-3.08756500
C	2.09143500	-0.92923400	-4.68011800
C	3.16350600	-1.71110400	-4.29045500
H	3.92459200	-3.04714800	-2.80137000
H	2.12388200	-0.41899800	-5.63912600
H	4.03620800	-1.80185300	-4.92905900
H	1.24200500	2.05707600	3.68913200
N	-0.10423000	-1.21217000	-1.67436800
C	-1.74641600	-2.49710500	-3.05285900
H	-0.86877000	-2.85510800	-3.59192000
H	-2.29717400	-3.37120900	-2.69196500
H	-2.39700600	-1.98595500	-3.77009500
C	-0.30164100	1.75480000	-1.16172300
H	1.57484900	-0.16215500	-0.14733600
C	0.98261900	2.07357800	-0.69319600
C	2.15356500	1.95664500	-1.65383600
H	-1.19336500	2.21568800	-0.74689200
H	-0.41691400	1.39450600	-2.17720900
C	1.90044200	-3.11073300	-0.97721200
H	1.47693400	-2.45448700	-0.20523500
C	3.24101600	-3.63981200	-0.48269800
H	3.99733300	-2.85323300	-0.41790400
H	3.13118800	-4.07887600	0.51268900
H	3.63219500	-4.42595000	-1.13714800
C	0.92377100	-4.27477900	-1.16755700
H	-0.08004100	-3.92891500	-1.42060700
H	1.26339500	-4.93892900	-1.96969000
H	0.84641400	-4.87014400	-0.25289600
C	-0.20912100	0.00781500	-4.46448000
H	-1.01736300	0.04687100	-3.72532300
C	0.15497900	1.44693200	-4.83821300
H	0.96978700	1.46948700	-5.56820100
H	-0.70374900	1.94551200	-5.29729500
H	0.46416500	2.04806300	-3.98258200
C	-0.74456700	-0.68787900	-5.72322300
H	-0.94569600	-1.74873400	-5.56750300
H	-1.66814200	-0.21245600	-6.06698300
H	-0.01844500	-0.61418600	-6.53887700
C	1.11195200	2.96054100	0.48178100
C	0.01528400	3.25017400	1.32144000
C	2.31360300	3.60870400	0.79769400
C	0.11785500	4.09821900	2.40514100
H	-0.94920100	2.79442400	1.12675400
C	2.43902700	4.46171400	1.89167500
H	3.18613600	3.46163800	0.17222400
C	1.33992500	4.70510100	2.71294200

H	-0.73744700	4.29484100	3.04368300
H	3.39565000	4.93163800	2.08725900
O	1.35434300	5.49759100	3.81981900
C	2.58521200	6.09674500	4.16100500
H	2.40465600	6.66940200	5.06916600
H	3.36045500	5.34481000	4.35672400
H	2.94052900	6.77299000	3.37395200
H	1.78999800	1.45284500	-2.55267800
H	2.40478300	2.98121500	-1.97301800
C	3.43861600	1.24360700	-1.24404500
H	4.19843300	1.37785300	-2.02018300
H	3.86560200	1.60425300	-0.30478800
H	3.26679100	0.17021500	-1.13339100
H	1.43537000	-0.96514800	3.26092500
C	2.79361400	0.34747700	2.22834200
H	2.61508600	1.01901900	1.38363000
C	3.43403800	-0.93086400	1.71238400
H	4.34876700	-0.72041000	1.15027700
H	3.70119200	-1.59637100	2.54228900
H	2.75311600	-1.46797100	1.05335300
C	3.73693900	1.04003100	3.20835500
H	4.71172000	1.19722900	2.73745000
H	3.37558400	2.02136200	3.52745900
H	3.90893900	0.43132000	4.10406100

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Fe	0.08924500	-0.11882900	-0.03577400
N	0.30247200	-0.15564400	1.93632700
C	1.48312900	-0.02545800	2.84469700
C	-0.75369100	-0.04045600	2.70472500
C	0.87517400	0.75746300	3.99180300
H	1.70022200	-1.04743400	3.20104200
H	1.29144600	0.53613100	4.97403900
N	-1.69060200	-1.01407200	0.14282400
C	-2.55809500	-0.88208300	1.17179100
C	-3.35575600	-2.26379200	-1.09638700
C	-3.91521300	-1.33356800	1.06099000
C	-4.28577300	-2.02573400	-0.12730500
H	-3.61798600	-2.81975500	-1.98971100
H	-5.30756700	-2.37642500	-0.23186700
C	-2.13675900	-0.29553800	2.40729800
C	-4.81824800	-1.08570200	2.10018800
C	-4.41356000	-0.43442600	3.25868500
H	-5.12636200	-0.23879600	4.05204700
C	-3.08907100	-0.06297900	3.41623100
H	-2.75719800	0.39509500	4.33913200
H	-5.84671600	-1.41481300	1.98267100
O	-0.49891200	0.34228800	3.98334300
C	-2.04424200	-1.75917700	-0.95429700
C	-0.99835900	-1.97246400	-1.89114400

C	1.30436200	-1.56464600	-2.43492200
C	2.38325500	-2.33253600	-1.93100000
C	1.39749400	-0.93959500	-3.69583900
C	3.56331100	-2.38949100	-2.66762500
C	2.60755500	-1.02726800	-4.39064600
C	3.68772300	-1.72645100	-3.88361300
H	4.39965100	-2.96884200	-2.29169400
H	2.69485300	-0.53053600	-5.35377800
H	4.61924800	-1.77526700	-4.43929200
H	0.90588400	1.84277000	3.81905400
N	0.16960900	-1.40340700	-1.59177200
C	-1.21975900	-2.84912800	-3.08412700
H	-0.27531600	-3.10209700	-3.56702700
H	-1.71076200	-3.78317400	-2.79655400
H	-1.85950000	-2.36881300	-3.83258700
C	-0.73826400	1.49702200	-1.01810900
H	1.55961900	0.05995300	-0.07670300
C	0.43472400	2.03585400	-0.47058800
C	1.56871700	2.40710600	-1.38592000
C	2.64150900	1.60025000	-1.75354800
C	1.50498400	3.68339300	-1.97665900
C	3.58718100	2.00988800	-2.69305500
H	2.72962200	0.60796100	-1.32538400
C	2.42957600	4.10754100	-2.91243400
H	0.67901000	4.34272600	-1.71951900
C	3.47587600	3.26065300	-3.29103900
H	4.38676900	1.32898200	-2.95867400
H	2.35266500	5.08228500	-3.38199700
C	0.35313400	2.89635000	0.78711900
H	1.02519900	2.50023300	1.55627700
C	-1.02805100	3.10752300	1.38205000
H	-0.96603100	3.69368600	2.30314300
H	-1.68207100	3.64815900	0.69202000
H	-1.53025500	2.16910800	1.62887900
O	4.31657800	3.73863500	-4.25047300
C	5.31963600	2.85937800	-4.70973100
H	6.02900300	2.59839200	-3.91470100
H	4.88998000	1.93337100	-5.11435600
H	5.84941900	3.38688200	-5.50146600
H	-1.70847900	1.66724400	-0.55862000
H	-0.76806200	1.21727200	-2.06763400
H	0.78159900	3.87662300	0.53804400
C	2.77815800	0.54815600	2.25539600
H	2.50477000	1.28187300	1.48954900
C	3.61074800	1.24129600	3.33175300
H	3.10812600	2.10787400	3.76963600
H	3.86266400	0.55229800	4.14634200
H	4.55397200	1.59645700	2.91025400
C	3.60679200	-0.53727200	1.58657800
H	3.02955900	-1.04923600	0.81855900
H	4.49567000	-0.11460200	1.10880800

H	3.94345100	-1.28133200	2.31834700
C	0.24869800	-0.20574000	-4.36648500
H	-0.62113500	-0.24179900	-3.70068100
C	-0.13221900	-0.88822800	-5.68489300
H	-1.03659400	-0.43891200	-6.10602400
H	0.66367100	-0.76790900	-6.42657100
H	-0.30749700	-1.95980000	-5.57075000
C	0.56651500	1.26399400	-4.64026800
H	-0.27591600	1.74973700	-5.14232800
H	0.78161000	1.81825800	-3.72750900
H	1.43819000	1.36401100	-5.29600000
C	2.22123300	-3.13748100	-0.65480500
H	1.71220000	-2.48940800	0.07368400
C	1.31707700	-4.35237600	-0.88783700
H	1.74435900	-5.00883800	-1.65350200
H	1.21291000	-4.93761800	0.03066700
H	0.31482600	-4.06791200	-1.20999300
C	3.53967500	-3.60920700	-0.05164900
H	3.99719600	-4.39835600	-0.65768200
H	4.27011500	-2.80330000	0.04841700
H	3.36936800	-4.02964100	0.94322800

I'''(2c)

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Fe	0.96337300	-0.49533700	0.28169500
N	0.39027500	1.04774900	1.42510500
C	-0.59446900	0.97001000	2.27491800
H	1.11503900	2.77805800	3.82597600
N	-0.96200900	-1.05151600	0.25181900
C	-1.87787500	-0.90499300	1.24036900
C	-2.56600400	-2.36740500	-1.01114400
C	-3.12288500	-1.61699500	1.21187700
C	-3.42923800	-2.37290600	0.04343500
H	-2.80492600	-2.89665400	-1.92720100
H	-4.36777100	-2.91620400	0.00118600
C	-1.65053200	-0.00365200	2.32680800
C	-3.99587100	-1.53691000	2.30205600
C	-3.70802100	-0.73217000	3.39710600
H	-4.39252800	-0.68519000	4.23659500
C	-2.56499800	0.04949100	3.39129600
H	-2.36827800	0.73886800	4.20298000
H	-4.91751200	-2.11101100	2.26825600
O	-0.66727900	1.96814600	3.18482500
C	-1.32480000	-1.70056300	-0.90462300
C	-0.35453000	-1.66277400	-1.93425200
C	1.86167100	-1.02782700	-2.55981800
C	2.61161500	-2.16353500	-2.92688700
C	2.16240900	0.24492100	-3.10795900
C	3.69209100	-1.96760400	-3.79984200
C	3.23572900	0.37054600	-3.98173400
C	4.01275900	-0.73045600	-4.32069400

H	4.31518100	-2.82505600	-4.04312500
H	3.47202100	1.34142500	-4.40396300
H	4.86306500	-0.61965600	-4.98606400
H	0.07526600	3.85866700	2.87380500
N	0.80311100	-1.08331300	-1.60646600
C	-0.66520800	-2.21202900	-3.29253300
H	0.11576300	-1.96589700	-4.01228000
H	-0.77303700	-3.30222400	-3.28255900
H	-1.61053600	-1.80628800	-3.66580200
C	1.38541900	-1.87257900	1.76076200
C	2.62104000	-1.27650400	1.45117300
H	0.83485200	-1.54908300	2.64293900
H	1.12657300	-2.86642600	1.40677600
C	1.27751500	1.43708100	-2.80489000
H	0.92481300	1.31513300	-1.77389800
C	2.00479600	2.77286800	-2.89915500
H	1.35698600	3.58446500	-2.55463600
H	2.91407100	2.78445300	-2.28930200
H	2.29024900	3.01608000	-3.92744100
C	0.04363400	1.43969800	-3.70996900
H	-0.54119400	0.52372300	-3.59962700
H	-0.61400200	2.28213500	-3.47263300
H	0.33134500	1.52650500	-4.76342300
C	1.10442000	2.30895300	1.66964800
C	0.45744700	2.83718900	2.95359300
H	2.16016900	2.08629800	1.83711200
C	1.02014000	3.23208300	0.45067800
H	1.51841500	2.67226600	-0.34793700
C	-0.41414100	3.50427300	0.02153300
C	1.80602900	4.51293000	0.69128700
H	-0.98594200	4.01454700	0.80578000
H	-0.44279600	4.14719700	-0.86255400
H	-0.93911700	2.57636000	-0.22456600
H	1.35237000	5.13087800	1.47473100
H	2.83748900	4.30133700	0.99111400
H	1.84491300	5.12491400	-0.21355900
H	2.21837600	0.27986700	-0.07899800
C	2.45207900	-3.61643200	-2.46965800
H	3.46015700	-3.88918900	-2.12338400
C	2.13738500	-4.52503400	-3.66463000
C	1.51528400	-3.96967000	-1.32020700
H	2.85923100	-4.41582800	-4.47637600
H	2.13803100	-5.57471500	-3.35531400
H	1.14753900	-4.30609100	-4.07636200
H	1.57791700	-3.26112200	-0.49985800
H	0.46923600	-4.03910600	-1.62958500
H	1.79446600	-4.95312700	-0.92916900
C	3.19327300	-0.28494300	2.45277800
C	3.64354300	-2.03587400	0.67133000
C	3.91912400	-3.36458100	1.00461900
C	4.43342600	-1.45122300	-0.33009100

C	4.91994800	-4.09668900	0.37046200
H	3.33076700	-3.84266900	1.78359000
C	5.44474400	-2.15441700	-0.95782700
H	4.21709600	-0.43435800	-0.64414400
C	5.69139300	-3.48698500	-0.61901600
H	5.08872500	-5.12831800	0.65577100
H	6.03472700	-1.70203200	-1.74747900
H	2.36198500	0.25262700	2.92317300
H	3.64064500	-0.88211400	3.26310100
C	4.24795300	0.68797300	1.95028000
H	5.17093900	0.17261000	1.67396500
H	3.90734400	1.23339000	1.06377400
H	4.50319100	1.41797000	2.72440600
O	6.67809500	-4.10750800	-1.32493000
C	6.91580200	-5.46703100	-1.03438600
H	7.71736800	-5.78565800	-1.69888500
H	7.23249500	-5.61225400	0.00574500
H	6.02658200	-6.08246700	-1.22152300

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Fe	0.35576400	-0.79852400	0.41235400
N	0.11358100	0.73009600	1.66826400
C	-0.86762900	0.77921900	2.52223200
H	1.12161000	2.29363700	4.17326300
N	-1.64205600	-0.92441200	0.32218900
C	-2.51850900	-0.66669300	1.32327300
C	-3.47528400	-1.71480600	-1.05919300
C	-3.89089800	-1.07080200	1.22967200
C	-4.33889300	-1.61544200	-0.00934300
H	-3.81114100	-2.08533900	-2.02190900
H	-5.37721500	-1.91675400	-0.10420300
C	-2.10977900	0.04953400	2.49165400
C	-4.74080000	-0.90590500	2.32881400
C	-4.29461900	-0.30414000	3.49813800
H	-4.96321600	-0.18962000	4.34391400
C	-3.00468500	0.19814300	3.56237000
H	-2.67229600	0.74359800	4.43702800
H	-5.76784700	-1.24966300	2.24395000
O	-0.73597500	1.67633900	3.52217200
C	-2.11411800	-1.37409400	-0.88812100
C	-1.12983100	-1.49912500	-1.89720200
C	1.21693600	-1.41576300	-2.40083300
C	1.69056800	-2.68382300	-2.79959900
C	1.87385200	-0.23404800	-2.83127900
C	2.87771700	-2.72278200	-3.54689400
C	3.02847200	-0.34005900	-3.59636200
C	3.54850900	-1.58205100	-3.93822500
H	3.28168800	-3.69563900	-3.81593000
H	3.53748800	0.55992900	-3.92379700
H	4.46729900	-1.65549800	-4.51097700

H	0.22554200	3.45752100	3.16859600
N	0.12326700	-1.25538500	-1.50080100
C	-1.51142700	-1.83745800	-3.30531000
H	-0.65264000	-1.77882000	-3.97491100
H	-1.93377800	-2.84407600	-3.39524100
H	-2.27457900	-1.14487200	-3.67464800
C	0.46159300	-2.39900500	1.73104900
C	1.79662700	-1.99662500	1.56686400
C	2.67469400	-2.78125100	0.61504300
H	-0.12446700	-2.09977700	2.59553700
H	0.09833100	-3.29910000	1.24634900
C	1.28770700	1.12718500	-2.51384900
H	0.85007300	1.05665000	-1.51118100
C	2.32228400	2.24580100	-2.49536200
H	1.87097300	3.17430400	-2.13373800
H	3.16812300	2.00611700	-1.84350000
H	2.71894600	2.45794900	-3.49344300
C	0.15463600	1.46957600	-3.48342700
H	-0.64272100	0.72383700	-3.45377500
H	-0.29033800	2.43897500	-3.23708600
H	0.52288700	1.52320200	-4.51378500
C	2.47838000	-1.16801400	2.58593400
C	1.90182600	-0.89335100	3.83844900
C	3.73355000	-0.59913400	2.33711300
C	2.51419800	-0.06211000	4.75852200
H	0.94681000	-1.33652800	4.10123100
C	4.36666400	0.23718500	3.25102700
H	4.21859100	-0.77703600	1.38299200
C	3.74756300	0.52671200	4.46764700
H	2.05492200	0.14645800	5.71941800
H	5.33134900	0.66308700	3.00141500
O	4.25462400	1.35608500	5.42202000
C	5.49482100	1.96942000	5.14431800
H	5.72732700	2.59147800	6.00705200
H	6.29300900	1.22953700	5.00909000
H	5.44295200	2.60104200	4.24838900
H	3.37588000	-2.11869700	0.09665900
C	1.08963500	1.76931800	2.02836700
C	0.48941400	2.40154200	3.28936900
H	2.04057800	1.28235100	2.25882100
C	1.33400900	2.73069600	0.86272700
H	1.76517300	2.10336100	0.07460200
C	0.04804000	3.34811300	0.33270700
C	2.36479100	3.78089400	1.25263700
H	-0.46640400	3.94305900	1.09669000
H	0.25037100	4.01820700	-0.50754700
H	-0.64838200	2.57800000	-0.01300200
H	1.98343200	4.46008900	2.02404200
H	3.27814500	3.31795400	1.64097600
H	2.64359800	4.39776000	0.39412600
H	1.75196700	-0.28617700	0.10469200

H	2.04818900	-3.19245500	-0.17837500
C	3.42817600	-3.91055200	1.30863300
H	4.09334000	-3.52847100	2.08863800
H	2.73596700	-4.61120400	1.78528700
H	4.03916500	-4.47477600	0.59838500
C	1.10458200	-4.07704900	-2.52977600
H	1.96438600	-4.65594800	-2.15917100
C	0.67826100	-4.73107100	-3.85054700
C	-0.00880700	-4.28491800	-1.50654900
H	0.36372000	-5.76529500	-3.68152000
H	-0.16867500	-4.19849900	-4.29343300
H	1.48089400	-4.74072000	-4.59024200
H	0.12407800	-3.70431800	-0.59800100
H	-0.99642800	-4.04326500	-1.90403100
H	-0.03676300	-5.34256200	-1.22832900

TS₁^{...}(2a)

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Fe	-0.07419900	0.22399000	-0.07104700
N	0.14314800	0.09117900	1.93148100
C	1.28966800	0.00970300	2.88672500
C	-0.90110100	0.40927500	2.65836600
C	0.78433600	0.83988500	4.05166800
H	1.08325800	0.47498800	5.03439600
N	-1.90605200	-0.45407100	0.08362200
C	-2.76769300	-0.14901600	1.08218300
C	-3.69589300	-1.57817800	-1.09987000
C	-4.17287700	-0.40632900	0.95505300
C	-4.60804300	-1.14026100	-0.18543400
H	-4.01014100	-2.17157300	-1.95117100
H	-5.66456200	-1.36334100	-0.29409100
C	-2.29295500	0.42540800	2.30244600
C	-5.05382000	0.05139900	1.93970300
C	-4.58534800	0.71722000	3.06700900
H	-5.28142200	1.07942600	3.81544000
C	-3.22411900	0.87502400	3.25817700
H	-2.84835900	1.32154300	4.16988000
H	-6.11659800	-0.13077000	1.80847900
O	-0.64277800	0.73264800	3.95074800
C	-2.33468500	-1.22380600	-0.97139000
C	-1.32997200	-1.58261800	-1.90614100
C	0.94860500	-1.35874200	-2.58501100
C	2.00550500	-2.20478100	-2.16698400
C	0.99050100	-0.74557900	-3.86019500
C	3.11850200	-2.35137700	-2.99018200
C	2.14216300	-0.91119700	-4.63533900
C	3.20455700	-1.68872000	-4.20821000
H	3.93425200	-2.99352200	-2.67562000
H	2.19252200	-0.42782300	-5.60767800
H	4.08655800	-1.79998200	-4.83064800
H	1.05616300	1.89864800	3.95402500

N	-0.10175600	-1.12421800	-1.65923300
C	-1.67367300	-2.48287700	-3.05392800
H	-0.77722000	-2.82064100	-3.57452800
H	-2.20782700	-3.37000200	-2.70059900
H	-2.32360000	-1.99264900	-3.78645000
C	-0.37967900	1.87712600	-1.14630300
H	1.40705300	0.60091300	-0.14767600
C	0.98851900	1.98948900	-0.70691400
C	2.08437300	1.93023500	-1.76988100
H	-1.14262100	2.52451600	-0.72118700
H	-0.56679800	1.59134900	-2.17711200
C	1.87577700	-3.00074200	-0.88321300
H	1.41729900	-2.33707500	-0.13668400
C	3.20587000	-3.50691300	-0.33864900
H	3.95792700	-2.71616400	-0.27459600
H	3.07138500	-3.92260600	0.66356200
H	3.61746800	-4.30727500	-0.96242600
C	0.91877200	-4.18094500	-1.07622700
H	-0.08243800	-3.85352000	-1.36039400
H	1.28809600	-4.85454600	-1.85699900
H	0.82644100	-4.76028100	-0.15269700
C	-0.16959700	0.02244100	-4.48112500
H	-0.99004400	0.06309700	-3.75572200
C	0.17336100	1.46002200	-4.88087400
H	1.03509500	1.48722200	-5.55506700
H	-0.66837000	1.91120100	-5.41441000
H	0.40003200	2.10187100	-4.02937600
C	-0.66880400	-0.70776600	-5.73572900
H	-0.84357100	-1.77109600	-5.56607200
H	-1.59988200	-0.26283700	-6.09940200
H	0.06624200	-0.62687000	-6.54281800
C	1.21975300	2.95511300	0.42247200
C	0.22586900	3.19429300	1.38814600
C	2.40724900	3.67694700	0.56366300
C	0.42020300	4.06017000	2.44584300
H	-0.72955600	2.68554900	1.31492400
C	2.62688500	4.55177500	1.62756600
H	3.19888200	3.57091200	-0.16851900
C	1.63625700	4.73627000	2.58824900
H	-0.35763700	4.22314800	3.18524500
H	3.56948700	5.08234200	1.68940400
O	1.74933400	5.53992900	3.68033300
C	2.96952400	6.22989600	3.84412600
H	2.87368100	6.80449200	4.76382300
H	3.81609000	5.53820900	3.93750400
H	3.16340600	6.91529700	3.01018600
H	1.67744700	1.41432600	-2.63968400
H	2.28133800	2.96020500	-2.09833800
C	3.38151400	1.23031000	-1.38861300
H	4.15031900	1.38959600	-2.14948600
H	3.78536000	1.56812400	-0.42988400

H	3.22307400	0.15114500	-1.31060700
H	1.35015100	-1.04770600	3.19765000
C	2.66554000	0.42369100	2.36424600
H	2.52495000	1.30758800	1.73209300
C	3.29321300	-0.68960400	1.54354900
H	4.26151100	-0.38814100	1.13357600
H	3.45857400	-1.57996600	2.16181800
H	2.65056200	-0.97031700	0.70962200
C	3.59508100	0.80366600	3.51498300
H	4.59002100	1.04578400	3.13230700
H	3.24578300	1.67535900	4.07489600
H	3.71501800	-0.02627500	4.22154300

Imaginary Frequency: -613.43

TS₁... (2b)

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Fe	-0.04969500	0.05694200	-0.00144800
N	0.25730700	-0.13546400	1.96332600
C	1.44430500	-0.06869600	2.86404900
C	-0.78997000	-0.08570700	2.75392200
C	0.85322500	0.63395500	4.06922900
H	1.67412300	-1.11294600	3.14245700
H	1.28203300	0.34933800	5.02950600
N	-1.72010700	-0.97704200	0.16591800
C	-2.58380200	-0.89521800	1.20231600
C	-3.32928700	-2.28927800	-1.07236300
C	-3.92661400	-1.38723700	1.08747900
C	-4.27222100	-2.08035100	-0.10704700
H	-3.57096600	-2.85517200	-1.96503500
H	-5.28180900	-2.46308600	-0.21751900
C	-2.17004500	-0.33194700	2.45289100
C	-4.83261100	-1.18198800	2.13340000
C	-4.44097700	-0.54168500	3.30440700
H	-5.15731300	-0.38026300	4.10238800
C	-3.12574800	-0.14565900	3.47050900
H	-2.80089700	0.29250100	4.40567600
H	-5.85106900	-1.54039200	2.01488800
O	-0.51987600	0.21801600	4.05212100
C	-2.03789600	-1.73856000	-0.92953900
C	-0.97830200	-1.92147200	-1.86342400
C	1.30830900	-1.49615900	-2.40662300
C	2.38396500	-2.25608200	-1.88153800
C	1.41095600	-0.90179200	-3.68275800
C	3.57399600	-2.31824300	-2.60265700
C	2.62879000	-0.99545100	-4.36169100
C	3.70942200	-1.67454100	-3.82770800
H	4.40761500	-2.89032900	-2.20970300
H	2.72223200	-0.52148100	-5.33574300
H	4.64780700	-1.72697900	-4.37154800
H	0.88725800	1.72901300	3.96234500
N	0.17356600	-1.32423600	-1.57219400

C	-1.18382600	-2.81453000	-3.04908100
H	-0.23577300	-3.05332500	-3.53172300
H	-1.65563300	-3.75558100	-2.75292600
H	-1.83481100	-2.35335800	-3.79988300
C	-0.77021900	1.60038600	-1.06243800
H	1.29726500	0.73660100	-0.04413000
C	0.47521000	2.04907900	-0.51617900
C	1.57857300	2.42397500	-1.47881400
C	2.65982000	1.61169500	-1.79839000
C	1.49231400	3.66641400	-2.12871600
C	3.60828700	1.98658200	-2.74938700
H	2.75358800	0.63826100	-1.32640000
C	2.42199300	4.05819400	-3.07309200
H	0.65282200	4.32218700	-1.91045200
C	3.48455800	3.20914000	-3.40149000
H	4.41574100	1.30318200	-2.98225300
H	2.33845700	5.00841700	-3.58925100
C	0.41592600	2.99435600	0.69261500
H	1.19076400	2.71158400	1.41210400
C	-0.91769200	3.12469600	1.40881600
H	-0.80555100	3.72060200	2.31865200
H	-1.66423600	3.62390800	0.78597300
H	-1.33870800	2.15997300	1.70162800
O	4.32736100	3.65664600	-4.37310600
C	5.35642000	2.77918600	-4.77525000
H	6.05471300	2.56717600	-3.95626100
H	4.95338400	1.82846100	-5.14823300
H	5.89101500	3.28341200	-5.57872600
H	-1.71375100	1.92220400	-0.62916400
H	-0.81905600	1.33714600	-2.11592500
H	0.72088900	3.98853500	0.34183600
C	2.72890900	0.55089500	2.31491900
H	2.46166500	1.45086100	1.75005800
C	3.64851700	0.95553800	3.46515500
H	3.21684100	1.73257600	4.10192800
H	3.88454200	0.09483000	4.10164300
H	4.59575700	1.34100700	3.08094400
C	3.45860600	-0.40370600	1.38500600
H	2.82182700	-0.72063600	0.55786200
H	4.35075800	0.06517700	0.95926400
H	3.78032400	-1.29709700	1.93152000
C	0.26056100	-0.20043700	-4.38449300
H	-0.61321200	-0.22320600	-3.72317900
C	-0.10194500	-0.92563600	-5.68530300
H	-1.00675100	-0.49763400	-6.12727800
H	0.69956200	-0.81833000	-6.42302700
H	-0.26808100	-1.99508800	-5.54256500
C	0.56665600	1.26233200	-4.70150800
H	-0.27571500	1.72473500	-5.22532300
H	0.76657300	1.84499500	-3.80384500
H	1.44316300	1.35129200	-5.35257600

C	2.20112800	-3.06331000	-0.60826500
H	1.66318900	-2.42902200	0.11156600
C	1.32161500	-4.29138800	-0.86646300
H	1.77275400	-4.93417900	-1.62997100
H	1.21194100	-4.88548200	0.04575600
H	0.32038500	-4.02114200	-1.20285600
C	3.51248400	-3.51915100	0.02134800
H	3.98578100	-4.30900200	-0.57147600
H	4.23452500	-2.70641000	0.12426700
H	3.33025500	-3.93474100	1.01624800

Imaginary Frequency: -491.93

TS₁^{int} (2c)

0 2

Fe	0.85734200	-0.60409200	0.34655900
N	0.35774500	0.99662600	1.46578200
C	-0.66219800	0.95594600	2.27942600
H	1.07438000	2.65420700	3.89533500
N	-1.03876700	-1.06799500	0.25035900
C	-1.98299100	-0.87028900	1.20592200
C	-2.66370300	-2.30226600	-1.06994200
C	-3.25609600	-1.52822300	1.13539800
C	-3.55735100	-2.27309900	-0.04244300
H	-2.89824000	-2.81802600	-1.99472400
H	-4.51713100	-2.77430900	-0.11459600
C	-1.75672000	0.02717700	2.29483600
C	-4.16158000	-1.40563900	2.19344300
C	-3.87808500	-0.60972100	3.29719400
H	-4.58923100	-0.53056000	4.11184100
C	-2.70486700	0.12230400	3.32903500
H	-2.50713700	0.80615900	4.14489800
H	-5.10645900	-1.93756500	2.12691100
O	-0.73066500	1.95855000	3.18812100
C	-1.39729600	-1.69211900	-0.92748900
C	-0.40125800	-1.68545400	-1.92690900
C	1.83138400	-1.08997500	-2.51480100
C	2.56173900	-2.23336400	-2.90019300
C	2.15683000	0.18393700	-3.04825600
C	3.62910000	-2.04966000	-3.79068400
C	3.22070200	0.29930200	-3.93601300
C	3.96530600	-0.81372400	-4.30522800
H	4.23390400	-2.91501800	-4.05105100
H	3.47261400	1.27069000	-4.34794700
H	4.80528000	-0.71304300	-4.98528200
H	0.11601000	3.81425900	2.95105000
N	0.76639400	-1.13234500	-1.57043600
C	-0.69039100	-2.23432600	-3.29062200
H	0.09913800	-1.98561700	-4.00016400
H	-0.79479100	-3.32529200	-3.28423500
H	-1.63078800	-1.83134300	-3.67845900
C	1.48030900	-1.88218000	1.75395900

C	2.66464000	-1.20204200	1.31568600
H	1.03981800	-1.59271400	2.70748200
H	1.29524900	-2.91569100	1.47530700
C	1.30571300	1.39232300	-2.71401600
H	0.96545700	1.26247700	-1.67901700
C	2.06212700	2.71240100	-2.80361200
H	1.43727400	3.53494600	-2.44316500
H	2.97971800	2.69895200	-2.20555900
H	2.34028100	2.96003700	-3.83272600
C	0.05626600	1.43719600	-3.59659400
H	-0.54978600	0.53547400	-3.48507800
H	-0.57476000	2.29369600	-3.33846000
H	0.32867800	1.52890600	-4.65371100
C	1.09169000	2.24394800	1.72987700
C	0.44071600	2.77192000	3.01055000
H	2.14259300	2.01134400	1.90822000
C	1.03599400	3.17921700	0.51789900
H	1.53556000	2.62079800	-0.28095900
C	-0.38792700	3.47791200	0.07275800
C	1.83927700	4.44566100	0.77767200
H	-0.95924200	3.99273400	0.85419700
H	-0.39506700	4.12665800	-0.80755300
H	-0.92553200	2.56057200	-0.18494600
H	1.38322500	5.06683300	1.55685200
H	2.86248000	4.21654900	1.09296400
H	1.90222300	5.06140900	-0.12326000
H	2.30448700	-0.08199300	0.21926600
C	2.40032700	-3.68122700	-2.42928700
H	3.41025300	-3.95082800	-2.08305600
C	2.07844500	-4.60445200	-3.61070400
C	1.46738700	-4.01404300	-1.27151400
H	2.79587700	-4.50809100	-4.42793000
H	2.07837800	-5.64992300	-3.28777700
H	1.08694600	-4.38853900	-4.01966700
H	1.55349600	-3.30549200	-0.45286000
H	0.41683400	-4.05777500	-1.57003200
H	1.72765300	-5.00408400	-0.88369800
C	3.29227500	-0.25961400	2.34603900
C	3.69760900	-1.97410600	0.54239900
C	4.01994300	-3.27623800	0.92652600
C	4.46166200	-1.39870000	-0.48088800
C	5.04319700	-3.99561200	0.31435100
H	3.45371000	-3.74365800	1.72761200
C	5.49286100	-2.08870700	-1.09111500
H	4.21891500	-0.39682700	-0.82690500
C	5.78681200	-3.39818400	-0.70397900
H	5.25042500	-5.00865400	0.63783700
H	6.06554200	-1.64401600	-1.89738800
H	2.48200400	0.23855800	2.89006300
H	3.78801800	-0.90093400	3.08805800
C	4.29936800	0.75220000	1.82364300

H	5.21948600	0.26800200	1.48828100
H	3.90591100	1.31472900	0.96848700
H	4.57341100	1.47230200	2.60004100
O	6.79440400	-4.00840300	-1.38728000
C	7.09044000	-5.34290300	-1.03806900
H	7.90409800	-5.65540100	-1.69054000
H	7.41445100	-5.42797000	0.00636700
H	6.22854100	-6.00342600	-1.19543900

Imaginary Frequency: -584.08

TS₁^{...} (2d)

0 2

Fe	0.13736800	-0.90301300	0.50958800
N	-0.10665300	0.64785300	1.78132700
C	-1.16540400	0.72814400	2.53797000
H	0.69124000	2.19435000	4.37243700
N	-1.79912400	-0.96473500	0.27970600
C	-2.74826300	-0.67170900	1.20763900
C	-3.55636900	-1.63455500	-1.26474700
C	-4.12211200	-1.02655200	0.99860000
C	-4.49281400	-1.53620300	-0.28136800
H	-3.82945100	-1.96489700	-2.26131200
H	-5.53029900	-1.79898600	-0.46059100
C	-2.41811900	0.03323200	2.40418600
C	-5.05126900	-0.84016600	2.02627900
C	-4.68440700	-0.25759600	3.23330600
H	-5.41606600	-0.12627700	4.02264000
C	-3.39212200	0.20720700	3.40226400
H	-3.11542800	0.74187300	4.30221800
H	-6.07907700	-1.14668100	1.85323600
O	-1.10817800	1.63072600	3.54354700
C	-2.19991500	-1.35049200	-0.98655000
C	-1.15566000	-1.47994500	-1.92112400
C	1.21822800	-1.46666500	-2.25501400
C	1.64927500	-2.74660700	-2.66669800
C	1.96633100	-0.31154000	-2.60192800
C	2.86324900	-2.82743900	-3.36408100
C	3.15351600	-0.45656900	-3.31061400
C	3.61437900	-1.71322000	-3.68205900
H	3.22851600	-3.81202500	-3.64585900
H	3.73006600	0.42308200	-3.57592800
H	4.55273400	-1.81933900	-4.21680400
H	-0.06784300	3.38417100	3.29210500
N	0.07651400	-1.27207300	-1.42869600
C	-1.44070500	-1.78977600	-3.35832500
H	-0.53952400	-1.71961600	-3.96873600
H	-1.85608000	-2.79420900	-3.49763600
H	-2.17614300	-1.08878500	-3.76585800
C	0.56140800	-2.36639500	1.81533600
C	1.83338200	-1.84125800	1.40905300
C	2.67388600	-2.74480300	0.51381400

H	0.12599400	-2.07421500	2.76817500
H	0.26894300	-3.35937100	1.48367300
C	1.43656700	1.06808100	-2.26535400
H	0.94622500	0.98829800	-1.28748600
C	2.52201700	2.13259000	-2.16434800
H	2.09821500	3.07319100	-1.80086100
H	3.32233500	1.83812900	-1.47742000
H	2.97994000	2.34925600	-3.13480800
C	0.36665000	1.49564900	-3.27256800
H	-0.46822800	0.79190500	-3.29659300
H	-0.03793000	2.48007100	-3.01708700
H	0.78305900	1.55652900	-4.28399800
C	2.65444000	-1.03222200	2.37137000
C	2.41458700	-1.02633900	3.74897400
C	3.70541600	-0.24204300	1.89928400
C	3.15434900	-0.22867900	4.60854500
H	1.62779100	-1.65284100	4.15678200
C	4.46602200	0.55765700	2.74426800
H	3.90944500	-0.21798100	0.83052900
C	4.17923200	0.57991800	4.11173000
H	2.96077700	-0.21933800	5.67586300
H	5.26296200	1.16511700	2.33179600
O	4.83714600	1.34206200	5.02668100
C	5.86808300	2.17840600	4.54632100
H	6.26023200	2.70627900	5.41386000
H	6.67617400	1.60117500	4.08121000
H	5.49140100	2.90968600	3.82012400
H	3.35097700	-2.15275500	-0.11348000
C	0.85225600	1.66972300	2.23655200
C	0.14904900	2.31969000	3.43199800
H	1.76447100	1.17627500	2.57230500
C	1.24270200	2.61434600	1.09758700
H	1.75841600	1.97377800	0.37130600
C	0.03447500	3.23817500	0.41486900
C	2.23448800	3.65761600	1.59347300
H	-0.55928400	3.84151000	1.11183400
H	0.33908400	3.90133000	-0.39965900
H	-0.62444800	2.47114100	-0.00353300
H	1.77015100	4.35759500	2.29766400
H	3.08284500	3.18801300	2.10325000
H	2.62878300	4.25278400	0.76541300
H	1.63828200	-0.64017100	0.39580000
H	2.00494100	-3.25468900	-0.18000300
C	3.46235000	-3.77139200	1.31313700
H	4.18228200	-3.29321100	1.98352300
H	2.79868800	-4.38498900	1.93001600
H	4.01868600	-4.44128300	0.65218100
C	0.99976300	-4.11540300	-2.41779400
H	1.82769600	-4.72447700	-2.02279100
C	0.59114700	-4.76236300	-3.74698200
C	-0.14383200	-4.27602800	-1.41772900

H	0.23757000	-5.78437000	-3.58134900
H	-0.22217000	-4.20632300	-4.22136500
H	1.41685600	-4.80499500	-4.45997800
H	-0.00736900	-3.70276900	-0.50205400
H	-1.11155400	-3.99142700	-1.83524300
H	-0.22169300	-5.33244700	-1.14407100

Imaginary Frequency: -585.89

II''(2a)

0 2

Fe	-0.18814100	0.15625400	-0.06109700
N	0.03961400	0.09026000	1.92197300
C	1.18166500	0.00503500	2.88075300
C	-1.00776100	0.41285900	2.65003000
C	0.68340300	0.84800100	4.03973300
H	0.97602700	0.48423300	5.02490800
N	-1.97469400	-0.48579600	0.07669800
C	-2.84612400	-0.18461600	1.07070900
C	-3.73951800	-1.65868800	-1.10340500
C	-4.24621400	-0.46636600	0.93325100
C	-4.66307100	-1.22128600	-0.20345900
H	-4.03714300	-2.26947400	-1.94867800
H	-5.71525500	-1.46226900	-0.31438500
C	-2.39210000	0.40568500	2.29111300
C	-5.13942200	-0.01739000	1.90780900
C	-4.69265700	0.66535500	3.03688800
H	-5.40259000	1.01842500	3.77666800
C	-3.33895500	0.84809700	3.23858300
H	-2.97646700	1.30703800	4.14953500
H	-6.19739200	-0.22270300	1.77196200
O	-0.74362300	0.75600100	3.93732000
C	-2.38222000	-1.28525500	-0.97481500
C	-1.36466200	-1.63046800	-1.88299200
C	0.93783000	-1.36742400	-2.49685500
C	1.98487800	-2.22216000	-2.06699300
C	1.01181100	-0.73552600	-3.76205000
C	3.12289400	-2.34606800	-2.85990800
C	2.18696900	-0.87973300	-4.50588100
C	3.24195200	-1.65708700	-4.06059200
H	3.93130900	-2.99329500	-2.53700800
H	2.26148900	-0.38131800	-5.46910500
H	4.14319100	-1.75091100	-4.65800200
H	0.97437700	1.90170400	3.93632100
N	-0.13886800	-1.15640700	-1.59474300
C	-1.66496300	-2.52109900	-3.04880100
H	-0.75039200	-2.85013100	-3.54338700
H	-2.20369000	-3.41612000	-2.72275400
H	-2.29371000	-2.02943300	-3.79897900
C	-0.28891800	1.83245100	-1.07630400
H	1.41612100	0.89749100	-0.13827300
C	1.14157000	1.92654000	-0.65212400

C	2.18001900	1.94246800	-1.78592600
H	-0.96959100	2.59733700	-0.70501400
H	-0.45578600	1.62050000	-2.13019000
C	1.81820000	-3.06441200	-0.81556000
H	1.33251100	-2.43477900	-0.05795000
C	3.13361100	-3.58633100	-0.25029300
H	3.88312500	-2.79816800	-0.14148300
H	2.97214800	-4.03462200	0.73380400
H	3.56382300	-4.36641700	-0.88710800
C	0.87449400	-4.24058200	-1.08386100
H	-0.12251300	-3.90568500	-1.37291800
H	1.26495000	-4.87564500	-1.88638200
H	0.76711000	-4.86186400	-0.18967300
C	-0.14241700	0.01755800	-4.41236700
H	-0.97972400	0.04960900	-3.70600900
C	0.18808400	1.45704700	-4.81659200
H	-0.64441600	1.88579400	-5.38199900
H	0.37454000	2.11396700	-3.96701000
H	1.06992200	1.49363300	-5.46399900
C	-0.59717200	-0.72591300	-5.67680300
H	-0.75212900	-1.79250100	-5.51030200
H	-1.52914100	-0.30183300	-6.06239200
H	0.15497700	-0.62898600	-6.46632900
C	1.36508700	2.98103300	0.42320000
C	0.38216700	3.23346800	1.39326400
C	2.53501100	3.73466000	0.50699900
C	0.57007300	4.15703000	2.40416800
H	-0.55858000	2.69485300	1.35924000
C	2.74625300	4.67034600	1.51997900
H	3.31948400	3.60822600	-0.22993300
C	1.76505500	4.87792700	2.48608600
H	-0.20048000	4.33861400	3.14656700
H	3.67369500	5.22990000	1.53736200
O	1.86728300	5.75078400	3.52360100
C	3.05879500	6.50222800	3.61565300
H	2.95351300	7.13286700	4.49668800
H	3.93679300	5.85612200	3.73766600
H	3.20633100	7.13724700	2.73381900
H	1.74764000	1.43000900	-2.64475000
H	2.33033300	2.98295500	-2.09949100
C	3.50132800	1.26025300	-1.46377400
H	4.22692400	1.40166200	-2.26875200
H	3.95615200	1.62088100	-0.53622300
H	3.35198500	0.18171700	-1.35515300
H	1.22847700	-1.05179300	3.19707400
C	2.56783100	0.39380800	2.37326400
H	2.47458700	1.33678700	1.82338800
C	3.13816400	-0.67861300	1.46122400
H	4.12808400	-0.40173600	1.08758300
H	3.24147500	-1.62605200	2.00272100
H	2.49375700	-0.85881600	0.59824300

C	3.51191400	0.63058400	3.54988200
H	4.52122000	0.84749100	3.19120500
H	3.20338000	1.47350000	4.17432000
H	3.57915900	-0.25709900	4.18992400

II'''(2b)

0 2

Fe	0.19309900	-0.70355900	-0.00797500
N	0.56012100	0.13315800	1.71511400
C	1.81995500	0.46413000	2.44268200
C	-0.41690100	0.58569600	2.46645600
C	1.36893000	1.64292800	3.27650400
H	2.02276700	-0.38894200	3.11433000
H	1.85981600	1.73956300	4.24435900
N	-1.65743800	-1.22220100	0.53162000
C	-2.40476200	-0.63780500	1.50502100
C	-3.60213400	-2.47983200	-0.20278200
C	-3.79828700	-0.94143300	1.64903600
C	-4.36709300	-1.90744600	0.77231800
H	-4.03087500	-3.19558300	-0.89553300
H	-5.41679700	-2.15997700	0.88318800
C	-1.82678300	0.31281400	2.40796300
C	-4.56984400	-0.28440000	2.61712300
C	-4.00326000	0.66430200	3.45542200
H	-4.60995700	1.17708100	4.19339900
C	-2.65298400	0.95193100	3.35264400
H	-2.20079300	1.67596000	4.01777000
H	-5.62674100	-0.52507000	2.68590000
O	-0.02069800	1.37076700	3.50559100
C	-2.24953500	-2.11265800	-0.33552800
C	-1.40977100	-2.57557300	-1.38828400
C	0.72421400	-2.36000100	-2.46735700
C	1.87255300	-3.08038800	-2.07048900
C	0.56307900	-1.93849400	-3.80150900
C	2.85167100	-3.35349200	-3.02183100
C	1.57598200	-2.23723100	-4.71666300
C	2.71207100	-2.93164700	-4.33846100
H	3.73914400	-3.90566800	-2.73143600
H	1.46549200	-1.91082100	-5.74746700
H	3.48808600	-3.14813800	-5.06538800
H	1.45538200	2.59079200	2.72415500
N	-0.21414700	-2.00051500	-1.46164700
C	-1.87961700	-3.64268200	-2.32486000
H	-1.06208300	-4.01449700	-2.94346500
H	-2.30480300	-4.48776000	-1.77607400
H	-2.66329900	-3.27179500	-2.99443900
C	1.25816200	0.50431800	-1.22316900
H	0.82482100	2.16965800	0.09474500
C	1.02051400	2.00361900	-0.97804200
C	2.22487800	2.85328700	-1.32457700
C	2.69716600	3.83207700	-0.45507700

C	2.90649800	2.68824300	-2.53819700
C	3.80447100	4.62497200	-0.75821400
H	2.18686300	3.98278600	0.49507500
C	4.00163700	3.46727800	-2.86419200
H	2.57302900	1.92045400	-3.23250100
C	4.46094300	4.44276500	-1.97349300
H	4.14072400	5.37114700	-0.04809400
H	4.52873600	3.33893200	-3.80355300
C	-0.22021600	2.52331800	-1.72157500
H	-0.36772500	3.57919000	-1.46110900
C	-1.48905000	1.73967800	-1.43362400
H	-2.36147500	2.19662100	-1.90973300
H	-1.41653700	0.70788300	-1.79306600
H	-1.69280800	1.69062800	-0.35669700
O	5.55115200	5.15316500	-2.38082100
C	6.03174100	6.14682400	-1.50450600
H	5.27607600	6.91831300	-1.31028100
H	6.35563000	5.72235400	-0.54576300
H	6.88785500	6.60276500	-1.99948100
H	1.00761500	0.24859000	-2.26010800
H	2.32076500	0.25387100	-1.10725300
H	-0.01396700	2.51479800	-2.80013200
C	3.06174100	0.70150200	1.59323300
H	2.78116600	1.35368900	0.76058300
C	4.13841100	1.41518500	2.40549200
H	3.82882000	2.41399500	2.72677300
H	4.40963500	0.84244300	3.30019400
H	5.04546400	1.53888500	1.80884400
C	3.59976000	-0.60958300	1.04255800
H	4.00118500	-1.23524900	1.84857400
H	2.81951800	-1.18105500	0.53555000
H	4.40323700	-0.43746200	0.32072100
C	-0.65580800	-1.17733500	-4.29043900
H	-1.33044300	-1.02551200	-3.44036700
C	-1.40652700	-1.96366500	-5.36844500
H	-2.33233900	-1.45274300	-5.64893600
H	-0.79973000	-2.05594700	-6.27481200
H	-1.66207800	-2.97543500	-5.04728500
C	-0.28503100	0.20124200	-4.83881300
H	0.28245600	0.78875200	-4.11538600
H	0.32428700	0.11330200	-5.74406300
H	-1.18332500	0.76825200	-5.10171100
C	1.99494500	-3.59545600	-0.65007700
H	1.60391600	-2.80900000	0.01765400
C	1.11768300	-4.83166400	-0.43943800
H	1.42702500	-5.64016400	-1.11004500
H	1.20142800	-5.19916800	0.58757300
H	0.06326000	-4.62383600	-0.63098400
C	3.42681700	-3.89481800	-0.22489100
H	3.82027300	-4.78113300	-0.73279600
H	4.10258800	-3.06250400	-0.43573800

H	3.46857300	-4.09841200	0.84849900
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$\Pi'''(2c)$

0 2

Fe	0.69082800	-0.39472900	0.24173600
N	0.30606000	0.98570600	1.58663500
C	-0.77351900	0.99814200	2.31639700
H	0.90353400	2.64533500	4.00046800
N	-1.13621900	-0.93096000	0.16903200
C	-2.08441100	-0.77590600	1.14402600
C	-2.71812800	-2.27529700	-1.11280100
C	-3.34724800	-1.45269500	1.06087900
C	-3.63815000	-2.20834900	-0.10984600
H	-2.92430400	-2.83188100	-2.02072300
H	-4.59873900	-2.70671800	-0.18739600
C	-1.88509300	0.09572800	2.25932300
C	-4.27633600	-1.34234500	2.10451300
C	-4.02903500	-0.54662600	3.21416000
H	-4.75726600	-0.47561600	4.01430500
C	-2.85647300	0.18414900	3.27323600
H	-2.66816200	0.85450400	4.10255700
H	-5.20974500	-1.89109100	2.01620100
O	-0.88658700	2.03794500	3.17993500
C	-1.46021900	-1.66076800	-0.96586800
C	-0.41926800	-1.77570000	-1.90997800
C	1.86850500	-1.32113700	-2.39674000
C	2.55068500	-2.49662600	-2.78191900
C	2.27012500	-0.06297400	-2.91544800
C	3.63415100	-2.36132400	-3.66002900
C	3.34441700	0.00351500	-3.79765900
C	4.03270200	-1.14198300	-4.17081100
H	4.19563500	-3.25548500	-3.92225400
H	3.64720800	0.96293500	-4.20339500
H	4.88174200	-1.07991300	-4.84410100
H	0.05877500	3.85164700	3.00560000
N	0.76691800	-1.31513500	-1.49074600
C	-0.68316600	-2.33423400	-3.27354900
H	0.15657200	-2.16555300	-3.94836500
H	-0.87069900	-3.41411600	-3.24890000
H	-1.57029900	-1.87386400	-3.71950700
C	1.46935000	-1.62469100	1.51254900
C	2.73296300	-0.89844600	1.15695500
H	1.12762100	-1.46545800	2.53993200
H	1.42044300	-2.67915400	1.25065300
C	1.48405000	1.19434100	-2.58978700
H	1.12040100	1.08856500	-1.55442400
C	2.31557900	2.46995300	-2.64968400
H	1.72460100	3.32619200	-2.31172200
H	3.20983500	2.40629100	-2.01994700
H	2.64235000	2.70060200	-3.66793500
C	0.25016800	1.31823600	-3.48484500

H	-0.40952200	0.45392700	-3.38395900
H	-0.32968200	2.21098600	-3.23023200
H	0.54282200	1.39662500	-4.53738800
C	1.03496800	2.24018800	1.84257100
C	0.32892400	2.79516900	3.08037300
H	2.07969400	2.01884600	2.07343000
C	1.03003700	3.14680900	0.60509700
H	1.56593900	2.57198000	-0.16048800
C	-0.37232700	3.43398600	0.08836700
C	1.82072300	4.42129400	0.86490500
H	-0.97651100	3.96621500	0.83207600
H	-0.33826400	4.06242000	-0.80596200
H	-0.90182800	2.51230700	-0.17186600
H	1.32630600	5.06365000	1.60189700
H	2.82713900	4.20461100	1.23715500
H	1.92682200	5.01065600	-0.04946100
H	2.46732900	-0.02691700	0.42169200
C	2.29408000	-3.94185600	-2.34802500
H	3.28797300	-4.29286800	-2.03165700
C	1.89257500	-4.81334800	-3.54411700
C	1.36550600	-4.21838800	-1.17511800
H	2.60451300	-4.74060100	-4.36911900
H	1.83398200	-5.86426000	-3.24491500
H	0.91139600	-4.52992400	-3.93362800
H	1.54055800	-3.53559600	-0.34843300
H	0.30776100	-4.14826500	-1.44023400
H	1.53753900	-5.23841900	-0.81692500
C	3.35073200	-0.18377200	2.37605600
C	3.79097200	-1.67270000	0.40294500
C	4.05699800	-3.00704900	0.69238900
C	4.60643400	-1.03780200	-0.54229400
C	5.06638400	-3.71111200	0.03759600
H	3.45627500	-3.52001800	1.43848500
C	5.61874500	-1.71305800	-1.19532600
H	4.41735300	0.00327200	-0.79562100
C	5.84069800	-3.06597600	-0.92518300
H	5.22693400	-4.75621900	0.27452600
H	6.22525100	-1.22819200	-1.95202700
H	2.53576800	0.26140400	2.95739800
H	3.77048300	-0.96808000	3.01792700
C	4.41921700	0.84862800	2.05989300
H	5.31881200	0.38612900	1.64683200
H	4.06983500	1.57957300	1.31918200
H	4.71574300	1.40347900	2.95400100
O	6.81415000	-3.66625000	-1.66573400
C	7.00646000	-5.04962500	-1.46870300
H	7.79169300	-5.35044000	-2.16039500
H	7.32530600	-5.27619800	-0.44390400
H	6.09405800	-5.61914600	-1.68850800

$\Pi'''(2d)$

0 2

Fe	-0.04881800	-0.88304900	0.49028400
N	-0.27398600	0.62538100	1.76425600
C	-1.35786400	0.72977800	2.49023300
H	0.49895700	2.04553800	4.43540900
N	-1.92291000	-0.95843100	0.21266100
C	-2.90495300	-0.63325200	1.09841800
C	-3.63060700	-1.65042300	-1.38556400
C	-4.27472200	-0.97429500	0.83676100
C	-4.60214100	-1.51363200	-0.44534200
H	-3.86765100	-2.00557400	-2.38297500
H	-5.63568000	-1.76590600	-0.65809100
C	-2.61868500	0.08244600	2.29890200
C	-5.24270800	-0.75013100	1.81633000
C	-4.92298000	-0.14981800	3.03172800
H	-5.68928800	0.00707900	3.78266700
C	-3.63450500	0.28945800	3.25453800
H	-3.38350700	0.82556600	4.16095700
H	-6.26639600	-1.04398900	1.60194600
O	-1.29228200	1.60203000	3.52256400
C	-2.28036900	-1.37101200	-1.07098900
C	-1.21146400	-1.51941000	-1.95418300
C	1.18195800	-1.47633200	-2.19011000
C	1.63332100	-2.75312800	-2.59443500
C	1.93776900	-0.31704400	-2.51130900
C	2.85556500	-2.82453200	-3.27724400
C	3.13977300	-0.45346200	-3.19799400
C	3.60708900	-1.70515900	-3.57672100
H	3.23037000	-3.80590400	-3.55775900
H	3.72012200	0.42927100	-3.44402200
H	4.55308900	-1.80403100	-4.09933000
H	-0.15674400	3.30619600	3.36986000
N	0.00739600	-1.28272400	-1.41176000
C	-1.43136300	-1.86869100	-3.39304400
H	-0.50725700	-1.80223600	-3.96862200
H	-1.82880200	-2.88167700	-3.52520600
H	-2.15598600	-1.18753500	-3.85058300
C	0.64091000	-2.20732400	1.77570600
C	1.94414100	-1.66731900	1.28518100
C	2.76067400	-2.71101400	0.50242900
H	0.32832900	-1.91426000	2.77824000
H	0.46056000	-3.26605900	1.59119000
C	1.40196200	1.06159400	-2.17538900
H	0.91351900	0.98380700	-1.19562100
C	2.47963000	2.13521500	-2.08415200
H	2.05174900	3.07053800	-1.71230400
H	3.29324000	1.84923000	-1.40935300
H	2.92277100	2.35846000	-3.05996000
C	0.32170700	1.48038500	-3.17540400
H	-0.51313600	0.77674100	-3.18365200
H	-0.07929800	2.46726000	-2.92395000

H	0.72964700	1.53303400	-4.19067800
C	2.83120000	-0.91865300	2.25831600
C	2.76932100	-1.10834000	3.64071500
C	3.77641900	-0.01893900	1.76711700
C	3.58743400	-0.39274300	4.50096700
H	2.06148000	-1.82318500	4.04940200
C	4.61051600	0.70556200	2.61164500
H	3.84644200	0.14061800	0.69159900
C	4.50680400	0.52907800	3.99359900
H	3.53599800	-0.53167300	5.57537800
H	5.32273100	1.40514000	2.19051500
O	5.25049200	1.19814100	4.91412200
C	6.17470400	2.14903400	4.42881700
H	6.65584500	2.57956900	5.30516500
H	6.93705700	1.68564600	3.79121800
H	5.67599000	2.94636600	3.86358200
H	3.50399900	-2.21242300	-0.13180400
C	0.71585500	1.58327400	2.29120700
C	-0.00143700	2.22766600	3.48075000
H	1.58921900	1.03375700	2.64492500
C	1.18888600	2.54996000	1.20125400
H	1.72191300	1.92067500	0.47614300
C	0.02893000	3.22869600	0.48701100
C	2.18463300	3.55333200	1.76710000
H	-0.58648200	3.81207300	1.18200600
H	0.38733100	3.92221900	-0.27857100
H	-0.62367800	2.49637900	0.00263000
H	1.70445000	4.25657500	2.45681400
H	2.99252500	3.05237000	2.31074700
H	2.63644500	4.14849000	0.96874600
H	1.72552200	-0.83353800	0.48644900
H	2.07956800	-3.22564700	-0.17579600
C	3.43702500	-3.72176500	1.41190500
H	4.19180500	-3.25369600	2.04990700
H	2.71130900	-4.21219200	2.06845700
H	3.93404500	-4.49998200	0.82769300
C	1.00002300	-4.12745400	-2.33501400
H	1.83625900	-4.71912000	-1.93037200
C	0.60753400	-4.80212000	-3.65480600
C	-0.13861200	-4.28540100	-1.32950500
H	0.27587200	-5.82862500	-3.47302000
H	-0.21580100	-4.27264800	-4.14079900
H	1.43663400	-4.83937600	-4.36446300
H	0.00580500	-3.71003400	-0.41521800
H	-1.10809900	-3.99810100	-1.74049100
H	-0.21536600	-5.34140900	-1.05373700

III'(Doublet)

0 2

Fe	0.27558900	0.24905500	-0.12950900
N	0.14447100	0.40824100	1.77899700

C	1.22159000	0.74601000	2.71368500
C	-0.94945500	0.24722100	2.47899900
C	0.63848400	0.34679800	4.05781600
H	2.13500200	0.20348400	2.46232800
H	0.94064400	-0.66350000	4.36008900
N	-1.71410100	0.20828800	-0.35131900
C	-2.64253400	0.00827100	0.62315900
C	-3.43996000	0.00320000	-2.04342800
C	-4.01676900	-0.22565000	0.29115600
C	-4.38290000	-0.21864300	-1.08216000
H	-3.71167500	-0.00075900	-3.09317400
H	-5.41968000	-0.40331300	-1.34635600
C	-2.28467300	0.00895300	2.01303200
C	-4.96263300	-0.47209900	1.29676600
C	-4.59539500	-0.47682500	2.63342700
H	-5.33180400	-0.66932200	3.40563400
C	-3.27657400	-0.23459300	2.98093700
H	-2.98096700	-0.23441200	4.02242800
H	-5.98982500	-0.66597500	1.00213100
O	-0.78106100	0.33738000	3.82601400
C	-2.09564400	0.20588000	-1.67273600
C	-1.03944200	0.36686400	-2.61818900
C	1.33551500	0.50205100	-2.90571600
C	1.58272200	-0.38223300	-3.96208000
C	2.31779300	1.44013800	-2.56827200
C	2.77651900	-0.31433600	-4.67145500
C	3.50110000	1.51148500	-3.28645500
C	3.73801300	0.63460800	-4.34311100
H	2.95832700	-1.01551100	-5.47990400
H	4.24921200	2.24956300	-3.01535900
H	4.66923800	0.68374700	-4.89697200
H	0.84452700	-1.14151100	-4.20301700
H	2.13478500	2.09969300	-1.72410900
H	1.44162700	1.81913300	2.64710500
H	0.84374500	1.03950000	4.87377900
N	0.18655100	0.41480400	-2.10006200
C	-1.34317100	0.50344500	-4.07710800
H	-0.52242200	0.98178600	-4.61108000
H	-1.51743100	-0.46873800	-4.55517600
H	-2.24297800	1.10187600	-4.23308800
C	2.02090500	-0.76242500	-0.10453600
H	2.40593900	-0.95840400	-1.11409000
H	2.81221500	-0.21436900	0.42890000
C	1.69747800	-2.08898000	0.59713600
H	1.60353100	-1.90675000	1.68054400
C	2.79656100	-3.14536300	0.40823400
H	2.89416100	-3.35703000	-0.66516600
H	3.75474200	-2.70369300	0.70967600
C	2.54700700	-4.43376500	1.17318500
H	3.35862800	-5.15334500	1.03789200
H	2.45214400	-4.24430900	2.24801400

H	1.61985700	-4.91557900	0.84871800
C	0.34140500	-2.59125100	0.13198100
C	-0.69625000	-2.86938500	1.02618000
C	0.06408300	-2.71540900	-1.23139100
C	-1.96350200	-3.22029300	0.58591700
H	-0.51181400	-2.77933500	2.09565500
C	-1.19806200	-3.06617100	-1.69705800
H	0.84895000	-2.49508200	-1.95174200
C	-2.22731800	-3.30319400	-0.78190100
H	-2.77502400	-3.40345200	1.28255400
H	-1.37544100	-3.12870700	-2.76524200
O	-3.51143200	-3.60809300	-1.12469000
C	-3.80797200	-3.67021300	-2.50077300
H	-3.23708900	-4.45967300	-3.00573000
H	-4.87105500	-3.89624800	-2.57430500
H	-3.60835700	-2.71290100	-3.00087000
H	-0.50525400	2.80256400	-0.15648000
H	-0.52034900	3.54498800	-0.26075700

IV' (Doublet)

0 2

Fe	0.55288800	0.65126700	0.03483700
N	0.75604000	0.92014600	1.93316300
C	2.01452500	1.16179600	2.64414100
C	-0.15219700	0.61615000	2.82565100
C	1.73391500	0.62229300	4.03793800
H	2.84215300	0.64732900	2.15049600
H	2.12108900	-0.39268000	4.18300400
N	-1.35814000	0.55394200	0.17449100
C	-2.12139400	0.42867500	1.29826700
C	-3.39545700	0.47531900	-1.18224800
C	-3.55129200	0.31007100	1.21463600
C	-4.16574800	0.36947600	-0.07175600
H	-3.84754900	0.47245400	-2.16798800
H	-5.24558000	0.28633300	-0.13848000
C	-1.54194700	0.38188900	2.60658800
C	-4.30821600	0.09822300	2.36763900
C	-3.71684500	0.00113000	3.62447700
H	-4.32358100	-0.17624000	4.50531100
C	-2.35203500	0.14758300	3.73944500
H	-1.87173900	0.10027500	4.70838800
H	-5.38431200	-0.00504400	2.25859300
O	0.29693800	0.56001600	4.10098300
C	-1.98793900	0.56413200	-1.07811900
C	-1.11821900	0.67903600	-2.15783900
C	1.19914000	0.82845900	-2.78525400
C	1.36895500	-0.24700500	-3.66539900
C	2.08887500	1.90496600	-2.86127300
C	2.40485500	-0.24469300	-4.59083100
C	3.12219200	1.90384000	-3.78912800

C	3.28730200	0.82915100	-4.65763600
H	2.52695700	-1.09077100	-5.25996400
H	3.79924700	2.75090800	-3.83826100
H	4.09561300	0.82878400	-5.38100900
H	0.68309000	-1.08631600	-3.60520800
H	1.94518800	2.74404900	-2.18725700
H	2.23908900	2.23495300	2.64187300
H	2.08039800	1.25593800	4.85420500
N	0.18562800	0.82220000	-1.79976200
C	-1.56764900	0.68758500	-3.58144700
H	-0.92075300	1.31754300	-4.19630400
H	-1.55610700	-0.31406100	-4.02921800
H	-2.58541400	1.06937100	-3.67257400
C	1.24971100	-1.27010800	0.12351200
H	1.59039500	-1.52949100	-0.88666900
H	2.14109600	-1.26291200	0.76737800
C	0.25332800	-2.28140000	0.66926600
H	-0.16164600	-1.88975800	1.61475700
C	0.97298100	-3.60179900	1.02502700
H	1.40498900	-4.01976600	0.10572600
H	1.82556800	-3.36271900	1.67395400
C	0.08678700	-4.63346200	1.70074700
H	0.65224800	-5.52592400	1.98097900
H	-0.36561300	-4.23003400	2.61300700
H	-0.73073400	-4.95050900	1.04781500
C	-0.92036100	-2.53429300	-0.24716600
C	-2.21570200	-2.65624300	0.26880900
C	-0.76326900	-2.68423900	-1.62137300
C	-3.30815900	-2.86915100	-0.55189100
H	-2.36956600	-2.55436000	1.34159400
C	-1.85032800	-2.88941600	-2.47011100
H	0.23219600	-2.63109900	-2.05322200
C	-3.13529000	-2.95935900	-1.93428100
H	-4.31422400	-2.92560000	-0.14967100
H	-1.68443200	-2.98367600	-3.53759800
O	-4.27676300	-3.09799300	-2.66916200
C	-4.13486700	-3.11130700	-4.07084100
H	-3.53746700	-3.96495600	-4.41494300
H	-5.14067500	-3.19428600	-4.48010400
H	-3.67114900	-2.18625800	-4.43909100
H	1.95284900	1.48922900	-0.16876200
H	2.18614200	0.69000400	-0.19833000

TS₄ (Doublet)

0 2

Fe	0.34017800	0.10624600	0.36202500
N	1.37627500	0.71528600	1.90750900
C	2.82114700	0.54666700	2.07654800
C	0.85836700	0.87688700	3.09761800
C	3.06232600	0.96950900	3.51877600
H	3.08336800	-0.50268900	1.89105100

H	3.71708800	0.30757600	4.08600400
N	-1.30058500	0.78866500	1.15628300
C	-1.56408400	1.03188100	2.46446600
C	-3.61021600	1.29120000	0.59459000
C	-2.89868800	1.32730400	2.90406300
C	-3.91948700	1.43191200	1.91313800
H	-4.37236100	1.41603500	-0.16628500
H	-4.93336100	1.65287200	2.23095100
C	-0.52412900	1.00981600	3.45064600
C	-3.16336400	1.50382200	4.26411700
C	-2.15002000	1.42339200	5.21312800
H	-2.37394700	1.56093600	6.26508100
C	-0.84865000	1.19620800	4.80826000
H	-0.04508000	1.17366100	5.53337000
H	-4.18524700	1.71368500	4.56710300
O	1.75309800	0.92060200	4.11617200
C	-2.28661200	0.98497100	0.20353200
C	-1.84204100	0.87727700	-1.13182800
C	0.05171500	0.67018000	-2.57135200
C	0.76062500	-0.42517500	-3.07158400
C	-0.04399600	1.82594100	-3.35507600
C	1.33138100	-0.37413300	-4.33513300
C	0.54289300	1.87629000	-4.61327400
C	1.22851500	0.77491900	-5.11481500
H	1.85974200	-1.24470700	-4.71362100
H	0.46531800	2.78438500	-5.20318000
H	1.68039800	0.81299800	-6.10028900
H	0.83803200	-1.31978700	-2.46416200
H	-0.56764000	2.69016000	-2.95791400
H	3.36632000	1.15186000	1.35048500
H	3.43419300	1.99600800	3.60546900
N	-0.52427700	0.62992900	-1.28094100
C	-2.78731200	1.00850300	-2.28620500
H	-2.93902000	2.05052600	-2.58953600
H	-2.41289200	0.47340300	-3.16065500
H	-3.77015800	0.60227900	-2.03704400
C	0.17994400	-1.96311400	0.84501300
H	0.96059900	-2.73614700	0.78587000
H	0.07660800	-1.73459500	1.91285200
C	-1.12623400	-2.50587100	0.27239600
H	-1.89333700	-1.72027600	0.34758000
C	-1.62436300	-3.70160900	1.10558900
H	-0.87786500	-4.50595800	1.04987500
H	-1.66079000	-3.39694500	2.15876700
C	-2.98313800	-4.22072800	0.66998400
H	-3.32680100	-5.03707300	1.30979900
H	-3.73853200	-3.42906900	0.71201200
H	-2.95917800	-4.59223900	-0.35836100
C	-1.00704200	-2.86230000	-1.19109700
C	-1.92657100	-2.37476800	-2.12462000
C	0.00627300	-3.69383700	-1.66332100

C	-1.81788000	-2.66321000	-3.47373000
H	-2.74067800	-1.74418600	-1.77511900
C	0.13639400	-3.99913300	-3.01692800
H	0.72951800	-4.11056200	-0.96611500
C	-0.77198700	-3.46724300	-3.93248800
H	-2.52063200	-2.26505000	-4.19802600
H	0.94673200	-4.63944800	-3.34456300
O	-0.72169600	-3.66782100	-5.27773800
C	0.33830900	-4.45617800	-5.77122000
H	0.30347800	-5.47921100	-5.37663600
H	0.21717700	-4.48698000	-6.85278700
H	1.31520700	-4.01793300	-5.53106600
H	1.66162000	-0.25586300	-0.36670900
H	1.12729500	-1.17626200	0.02797000

Imaginary Frequency: -1107.11

V' (Doublet)

0 2

Fe	-0.15242900	0.26398700	0.01647100
N	-0.41818100	-0.34043900	1.84950600
C	0.63520400	-0.92138800	2.68360600
C	-1.51932100	-0.31444100	2.53996700
C	-0.10953300	-1.38637200	3.93210400
H	1.13193000	-1.73476800	2.14672300
H	-0.21501800	-2.47363400	3.99456700
N	-2.12026900	0.71626600	-0.13412100
C	-3.08793400	0.65757800	0.81561000
C	-3.74067800	1.51644600	-1.74735500
C	-4.43500000	1.05661800	0.52211000
C	-4.72511800	1.49161200	-0.80022400
H	-3.96461600	1.82647600	-2.76126100
H	-5.74034500	1.79060200	-1.04106500
C	-2.81614500	0.17518000	2.13827800
C	-5.42322700	1.00515900	1.51456200
C	-5.13384700	0.55485100	2.79258000
H	-5.90582900	0.51942700	3.55264300
C	-3.84599600	0.13749100	3.09137800
H	-3.61085900	-0.23269200	4.08117700
H	-6.42868500	1.32480700	1.25555900
O	-1.43186200	-0.82604700	3.78728000
C	-2.42956000	1.12501000	-1.41367500
C	-1.35631600	1.08170000	-2.35980400
C	0.91229400	0.42035700	-2.73993000
C	0.75329000	-0.46514400	-3.81162200
C	2.18293900	0.94006000	-2.47121200
C	1.84173300	-0.81856400	-4.59939500
C	3.26088600	0.59913200	-3.27442500
C	3.09911000	-0.28388800	-4.34096400
H	1.70338400	-1.52713500	-5.41102200
H	4.24002900	1.01506000	-3.05869800
H	3.94919500	-0.56015100	-4.95597200

H	-0.22211100	-0.90627200	-3.99196800
H	2.30342400	1.59211300	-1.61365800
H	1.39760300	-0.16291000	2.88597800
H	0.30779900	-1.01868500	4.87051800
N	-0.16519900	0.72043100	-1.87953400
C	-1.60218800	1.44448500	-3.79050400
H	-0.66889400	1.64519700	-4.31505900
H	-2.11884400	0.64245900	-4.33279000
H	-2.22846400	2.33675600	-3.86293400
C	1.94354300	-2.93985400	-1.02868600
H	2.28855100	-3.81236500	-1.59360000
H	2.58087600	-2.85361400	-0.14370000
C	0.48061500	-3.07079600	-0.62464600
H	0.23925100	-2.19718100	0.00236200
C	0.24541200	-4.31147200	0.24876900
H	0.41851300	-5.21353400	-0.35406400
H	1.01174200	-4.32870400	1.03583700
C	-1.13639800	-4.35892100	0.87720600
H	-1.25137900	-5.21626100	1.54495800
H	-1.33412600	-3.45274900	1.46282100
H	-1.92125400	-4.42397000	0.11871400
C	-0.46200200	-3.01470200	-1.80666100
C	-1.65301600	-2.28431200	-1.72687400
C	-0.19613700	-3.67475200	-3.00455300
C	-2.51887600	-2.17591900	-2.80234100
H	-1.89663100	-1.77241600	-0.79757600
C	-1.05553700	-3.58892900	-4.09825700
H	0.71654600	-4.25527300	-3.10823000
C	-2.21699200	-2.82058700	-4.00440200
H	-3.43117900	-1.59131800	-2.73596100
H	-0.80313700	-4.10625600	-5.01630000
O	-3.10340600	-2.62750600	-5.02218000
C	-2.81111900	-3.25005300	-6.25401600
H	-2.77596800	-4.34225600	-6.15980300
H	-3.61720600	-2.97647700	-6.93286500
H	-1.85706100	-2.90044100	-6.66851100
H	1.39657400	0.06987100	0.09719100
H	2.10752800	-2.04941200	-1.64099100

III' (Quartet)

0 4

Fe	0.27014800	0.04263600	-0.22092500
N	0.13364400	0.44512800	1.68597300
C	1.21668400	0.83044100	2.59247200
C	-0.94073700	0.24331400	2.41312400
C	0.67861500	0.43421400	3.95694000
H	2.14344700	0.31529600	2.33362000
H	1.03798800	-0.54923200	4.28226600
N	-1.71922700	0.12066400	-0.38891100
C	-2.63902200	-0.04483600	0.58965600
C	-3.48472600	0.03780900	-2.06206400

C	-4.02648300	-0.25295400	0.27622300
C	-4.41262000	-0.19870800	-1.09763800
H	-3.77764100	0.08572300	-3.10539700
H	-5.45844200	-0.34620800	-1.34908800
C	-2.26962900	-0.03909000	1.97695800
C	-4.94799100	-0.50575800	1.29061900
C	-4.56061800	-0.54414300	2.63002900
H	-5.29030300	-0.74828400	3.40554400
C	-3.24569800	-0.30290100	2.96365100
H	-2.93457300	-0.30553200	4.00066900
H	-5.98506900	-0.67357900	1.01385600
O	-0.74334800	0.34021300	3.74979200
C	-2.11938900	0.18781800	-1.71787800
C	-1.08104300	0.36368000	-2.64552300
C	1.31761600	0.57089300	-2.88795900
C	1.59906100	-0.30617300	-3.94373600
C	2.28457000	1.51838900	-2.52875600
C	2.80531700	-0.22116400	-4.62904100
C	3.48526200	1.60057400	-3.21724200
C	3.75264900	0.73309300	-4.27405500
H	3.00952000	-0.91404200	-5.43950200
H	4.21973000	2.34536800	-2.92731300
H	4.69379800	0.79544500	-4.80953900
H	0.87475500	-1.07187000	-4.20519600
H	2.07044100	2.18195300	-1.69504200
H	1.39971200	1.90936500	2.50674100
H	0.85568000	1.15875200	4.75159500
N	0.15503800	0.47132300	-2.10477100
C	-1.34944200	0.48325000	-4.11226600
H	-0.56260400	1.04829900	-4.61385600
H	-1.41125100	-0.49206900	-4.61207200
H	-2.29485100	0.99673800	-4.29572300
C	2.06883500	-0.85724800	-0.11080600
H	2.42491800	-1.06033500	-1.12986400
H	2.84683900	-0.27129700	0.39457300
C	1.74037900	-2.16646400	0.61354700
H	1.65783300	-1.96597200	1.69460400
C	2.80865900	-3.25312100	0.42690400
H	2.89431900	-3.47389200	-0.64548500
H	3.77989200	-2.83652900	0.72139100
C	2.52447500	-4.52809300	1.20177400
H	3.31411700	-5.27154900	1.06732600
H	2.44039600	-4.32910000	2.27560000
H	1.58252700	-4.98516300	0.88422200
C	0.36389400	-2.62457800	0.15521800
C	-0.67426900	-2.89777400	1.05414300
C	0.07396900	-2.72254700	-1.21094500
C	-1.94724900	-3.22265200	0.61611400
H	-0.48138900	-2.82503500	2.12326500
C	-1.19627500	-3.05190400	-1.67220600
H	0.85849400	-2.51509900	-1.93521700

C	-2.22110500	-3.28717500	-0.75271600
H	-2.75887800	-3.39598000	1.31497300
H	-1.38149300	-3.09691900	-2.73936200
O	-3.50659800	-3.57532700	-1.08839700
C	-3.81817300	-3.61050500	-2.46437000
H	-3.26546100	-4.40254800	-2.98473000
H	-4.88544600	-3.81743500	-2.52881100
H	-3.60804500	-2.64809500	-2.94837400
H	-0.61587400	2.74042000	-0.05467100
H	-0.66521200	3.48626800	0.00356800

IV' (Quartet)

0 4

Fe	0.33144300	-0.14868400	-0.70650600
N	-0.34565700	-0.02464000	1.19128000
C	0.51074300	-0.03380400	2.37883400
C	-1.54648500	-0.38412200	1.56285700
C	-0.41701100	-0.46888300	3.51256400
H	1.34269000	-0.73134800	2.22847500
H	-0.14118800	-1.42979600	3.95529600
N	-1.63194600	0.06998100	-1.31591800
C	-2.75919100	-0.25630500	-0.64586500
C	-2.92522800	0.44874500	-3.32994400
C	-4.02429300	-0.33552900	-1.32213800
C	-4.05487600	0.01544800	-2.70448700
H	-2.95671400	0.74783700	-4.37146100
H	-5.00007100	-0.04268300	-3.23538400
C	-2.73182500	-0.53118400	0.76143100
C	-5.16912900	-0.73214500	-0.62750100
C	-5.11334800	-1.03666000	0.72860200
H	-6.00899300	-1.34464500	1.25766100
C	-3.91465000	-0.92956400	1.41051500
H	-3.86856500	-1.15546300	2.46818800
H	-6.11125600	-0.78403300	-1.16648600
O	-1.69894200	-0.62532600	2.88519900
C	-1.69920400	0.49749000	-2.62334900
C	-0.47688300	0.96273700	-3.17616800
C	1.85445900	1.35676600	-2.75048700
C	2.50721600	0.66571100	-3.77963600
C	2.55293500	2.35333800	-2.05985800
C	3.81907700	0.97571700	-4.11288100
C	3.86082900	2.66608300	-2.40392800
C	4.50120800	1.97976100	-3.43170100
H	4.31480100	0.42373100	-4.90535900
H	4.38510200	3.44840300	-1.86404200
H	5.52570500	2.21990700	-3.69502900
H	1.98320400	-0.13543200	-4.29212800
H	2.04683700	2.87472700	-1.25281500
H	0.94354800	0.95934800	2.53811200
H	-0.52129500	0.27112600	4.30938900
N	0.55530400	1.02219900	-2.32070700

C	-0.39133000	1.40707800	-4.60395800
H	0.45921100	2.07134000	-4.75969200
H	-0.27796500	0.56773400	-5.29963300
H	-1.29314700	1.94642300	-4.90042900
C	1.55928600	-1.70641600	-1.20263100
H	1.12434600	-2.09582500	-2.13744000
H	2.55460300	-1.32536500	-1.46893100
C	1.66106400	-2.80859600	-0.15343700
H	2.25023600	-2.42210900	0.69570200
C	2.42066600	-4.03769800	-0.69367200
H	1.84254300	-4.45385700	-1.52984200
H	3.36497200	-3.68769700	-1.12827400
C	2.69305400	-5.11680400	0.33970600
H	3.26836400	-5.94411700	-0.08379100
H	3.26541700	-4.72058400	1.18555700
H	1.76499400	-5.53251300	0.74236200
C	0.30854400	-3.20647500	0.40047600
C	0.12022100	-3.43940900	1.76677800
C	-0.79955700	-3.36586100	-0.43179000
C	-1.11408000	-3.80366500	2.28318200
H	0.96935100	-3.33543400	2.44096000
C	-2.04500700	-3.74477800	0.06206600
H	-0.69867800	-3.17947500	-1.49792700
C	-2.20832400	-3.96054300	1.43041900
H	-1.25923000	-3.97000400	3.34566500
H	-2.88426900	-3.83328100	-0.61834100
O	-3.38407000	-4.30644800	2.02460200
C	-4.47299400	-4.59339300	1.17116300
H	-4.23510000	-5.41094400	0.47947500
H	-5.29316200	-4.89922200	1.81940100
H	-4.77959100	-3.71310900	0.59380200
H	2.77756500	0.34238200	0.21254100
H	3.16837400	0.74205300	0.71245400

TS₄ (Quartet)

0 4

Fe	0.35938800	0.00789200	0.36529600
N	1.50436100	0.66844100	1.88347600
C	2.95883000	0.62677100	2.00034700
C	1.01140700	0.93926600	3.05803700
C	3.22392500	1.15186200	3.40830600
H	3.30631300	-0.40409600	1.85718400
H	3.88672000	0.52829800	4.00974200
N	-1.22746100	0.77281900	1.18147700
C	-1.44524400	1.01106800	2.49791500
C	-3.56940900	1.18856500	0.70362600
C	-2.77213500	1.26517900	2.98582600
C	-3.83317100	1.32275900	2.03577200
H	-4.36736700	1.27976400	-0.02455200
H	-4.84206800	1.50489800	2.39130300
C	-0.37113100	1.03507100	3.44855400

C	-2.99393900	1.45212900	4.35349800
C	-1.94434100	1.42975300	5.26653700
H	-2.13341000	1.57377900	6.32419200
C	-0.65287800	1.24208000	4.81294300
H	0.17627000	1.25660500	5.50895300
H	-4.01289400	1.62152300	4.69004000
O	1.92526100	1.15043400	4.03288900
C	-2.25506400	0.93506700	0.26237500
C	-1.87004300	0.84695300	-1.10070300
C	-0.02280700	0.65236800	-2.61365400
C	0.78779900	-0.38381600	-3.09550900
C	-0.20278000	1.79012300	-3.41452000
C	1.36657400	-0.30050900	-4.35257700
C	0.39445900	1.87465200	-4.66530200
C	1.17590500	0.82809900	-5.14606600
H	1.96840000	-1.12799700	-4.71718500
H	0.25253000	2.76746200	-5.26651300
H	1.63490500	0.89414900	-6.12676300
H	0.92126700	-1.26472300	-2.47674300
H	-0.79515000	2.61650100	-3.03427800
H	3.42704200	1.23445300	1.22203800
H	3.59891200	2.17978600	3.42145700
N	-0.58738200	0.53875600	-1.33511200
C	-2.88096500	1.03317000	-2.19146800
H	-3.10264500	2.08833900	-2.38403000
H	-2.53159100	0.59717600	-3.12837200
H	-3.82747400	0.55497900	-1.92782900
C	-0.10991500	-2.06074400	0.97763700
H	0.60930800	-2.88543600	1.08522000
H	-0.34133300	-1.73661200	2.00027100
C	-1.36141300	-2.54351100	0.25513700
H	-2.10164000	-1.72925300	0.26481000
C	-2.00232600	-3.73709800	0.98892100
H	-1.29165600	-4.57512700	0.98060100
H	-2.13027500	-3.46190500	2.04305000
C	-3.33314300	-4.17590100	0.40346600
H	-3.77634800	-4.99492200	0.97544700
H	-4.05287900	-3.35020400	0.40089700
H	-3.22456300	-4.51485600	-0.63082200
C	-1.09452400	-2.87299100	-1.19756100
C	-1.93322000	-2.39360100	-2.20909800
C	-0.02342800	-3.67555300	-1.58444700
C	-1.69813500	-2.66661600	-3.54517600
H	-2.78714300	-1.77970600	-1.93159700
C	0.23264900	-3.96859900	-2.92362200
H	0.64356300	-4.08188700	-0.82782400
C	-0.60168700	-3.44959900	-3.91328000
H	-2.33791300	-2.27115400	-4.32718700
H	1.08271800	-4.58927700	-3.18109400
O	-0.42648700	-3.63771200	-5.25108700
C	0.67770000	-4.41779200	-5.65015900

H	0.61522000	-5.44195900	-5.26174900
H	0.65343900	-4.44698200	-6.73837400
H	1.62738500	-3.97504600	-5.32366900
H	1.61328700	-0.73525500	-0.30248600
H	1.04408400	-1.40686100	0.10783800

Imaginary Frequency: -947.63

V' (Quartet)

0 4

Fe	-0.13658500	0.34132200	0.03906300
N	-0.33808100	-0.27170200	1.85966200
C	0.73769100	-0.78991300	2.70524100
C	-1.45359000	-0.32209100	2.53855000
C	-0.00157900	-1.37007400	3.90521900
H	1.32289200	-1.53066600	2.15470500
H	-0.06145600	-2.46332100	3.88694300
N	-2.08907900	0.71659700	-0.12468200
C	-3.05392900	0.61053800	0.82722600
C	-3.74837700	1.49504200	-1.72209100
C	-4.41306800	0.97097000	0.54230400
C	-4.72276300	1.42832700	-0.77124600
H	-3.98432300	1.81799100	-2.72950500
H	-5.74741400	1.70477700	-0.99852900
C	-2.76409200	0.10993800	2.13949000
C	-5.39905600	0.85866500	1.52809000
C	-5.09601400	0.38388800	2.79841400
H	-5.86921900	0.29972200	3.55345700
C	-3.79844600	0.00856900	3.09045400
H	-3.55102300	-0.37611500	4.07171100
H	-6.41554900	1.14529600	1.27373800
O	-1.34304500	-0.85575000	3.77618000
C	-2.42385400	1.12794200	-1.40453700
C	-1.36672800	1.09972200	-2.34757000
C	0.90130200	0.41349600	-2.71901300
C	0.72804200	-0.45418000	-3.80436700
C	2.18337800	0.90131200	-2.44021900
C	1.81139400	-0.81974900	-4.59273800
C	3.25758000	0.54497800	-3.24211200
C	3.08018700	-0.31857300	-4.32139900
H	1.66057600	-1.51361900	-5.41465400
H	4.24459500	0.93629400	-3.01674000
H	3.92613000	-0.60547400	-4.93718100
H	-0.25485300	-0.87371300	-3.99433800
H	2.31692100	1.54508000	-1.57830700
H	1.41916100	0.02609300	2.96679900
H	0.38575000	-1.05419500	4.87447500
N	-0.17349000	0.72854800	-1.86126600
C	-1.59963400	1.47912600	-3.77598000
H	-0.66333600	1.71785800	-4.27999700
H	-2.07941500	0.67166300	-4.34288300
H	-2.25182100	2.35255700	-3.84468300

C	1.88961100	-2.94673300	-1.01029100
H	2.22579300	-3.85726800	-1.51741500
H	2.51032600	-2.82594800	-0.11770500
C	0.41551400	-3.02049700	-0.63192000
H	0.19008800	-2.11578000	-0.04377700
C	0.13272000	-4.21552100	0.29027100
H	0.29497500	-5.14692100	-0.26948800
H	0.88444500	-4.21568900	1.09160700
C	-1.26019600	-4.20476500	0.89550900
H	-1.40472800	-5.03019100	1.59697700
H	-1.44805600	-3.27107800	1.43949300
H	-2.03389500	-4.28632300	0.12729300
C	-0.50282600	-2.99034300	-1.83433400
C	-1.69578400	-2.25899700	-1.79488700
C	-0.21008000	-3.67106400	-3.01411100
C	-2.53817900	-2.17314600	-2.89040200
H	-1.95826000	-1.72498000	-0.88422600
C	-1.04545500	-3.60678400	-4.12805900
H	0.70560800	-4.25123400	-3.08798800
C	-2.21026100	-2.84041300	-4.07340400
H	-3.45215300	-1.58858600	-2.85494700
H	-0.77226600	-4.14056000	-5.03063000
O	-3.07591900	-2.66984900	-5.11259800
C	-2.75705400	-3.31648500	-6.32519100
H	-2.72276700	-4.40654600	-6.20832000
H	-3.54883800	-3.05773600	-7.02631700
H	-1.79477000	-2.97401700	-6.72642500
H	1.40706000	0.17437100	0.16977800
H	2.08964500	-2.09752500	-1.66911200

III' (Sextet)

0 6

Fe	0.47640100	0.33867000	-0.15553200
N	0.05001500	0.72585500	1.87983100
C	1.07978400	1.06465100	2.85992200
C	-0.97627400	0.26566700	2.52906000
C	0.57087200	0.43204700	4.14908500
H	2.05006400	0.67152000	2.54446700
H	1.06103000	-0.52063600	4.37767300
N	-1.68712000	0.24989000	-0.33620800
C	-2.60318900	-0.05098200	0.61582500
C	-3.44443100	0.21316200	-2.01423300
C	-3.96995700	-0.33997500	0.27250400
C	-4.35996300	-0.17397000	-1.08407600
H	-3.73947900	0.34486800	-3.04874800
H	-5.39297100	-0.36640200	-1.35829400
C	-2.26403900	-0.11901000	2.01081300
C	-4.88229000	-0.76933000	1.24004600
C	-4.50781400	-0.90302100	2.56980400
H	-5.21752300	-1.24631400	3.31370500
C	-3.21887200	-0.56315700	2.94154200

H	-2.92270900	-0.62586600	3.98090100
H	-5.89624400	-0.99840400	0.92385400
O	-0.81633300	0.16091700	3.87357700
C	-2.08863100	0.38171900	-1.64754100
C	-1.08289100	0.60662800	-2.63442800
C	1.28002200	0.54093000	-3.06146200
C	1.33349600	-0.31388600	-4.17679500
C	2.44327300	1.25061900	-2.71686600
C	2.49590600	-0.42776100	-4.92599600
C	3.59808200	1.13701900	-3.47470300
C	3.63307700	0.30102500	-4.58799500
H	2.51721700	-1.10293100	-5.77597000
H	4.48131700	1.70029100	-3.19048000
H	4.53920100	0.20788100	-5.17641700
H	0.46591500	-0.91740700	-4.42391700
H	2.42280500	1.88926900	-1.83797900
H	1.17542300	2.15621500	2.93513100
H	0.62083000	1.07682300	5.02690100
N	0.17960400	0.60998400	-2.21203700
C	-1.47533400	0.86578800	-4.05991300
H	-0.64782400	1.30391300	-4.61797000
H	-1.77479300	-0.04714900	-4.58947200
H	-2.32066100	1.55576900	-4.11466000
C	2.15423400	-0.85612900	0.10802800
H	2.56941500	-1.07539700	-0.88688300
H	2.97162600	-0.40679500	0.68791500
C	1.65324200	-2.14327800	0.77097200
H	1.47997900	-1.93795300	1.84143500
C	2.66544300	-3.29787900	0.69037800
H	2.83474700	-3.53232000	-0.36929100
H	3.62826300	-2.93398800	1.07050900
C	2.24552900	-4.54977300	1.44137200
H	3.00582200	-5.33312600	1.38498200
H	2.07334000	-4.33662500	2.50218500
H	1.31519000	-4.96340900	1.04107400
C	0.30545600	-2.53828300	0.19245900
C	-0.77445600	-2.90081000	1.00460300
C	0.09330100	-2.52731300	-1.18953400
C	-2.01575000	-3.20923800	0.47206400
H	-0.64227900	-2.91652000	2.08538500
C	-1.14425100	-2.83492900	-1.74645100
H	0.91096300	-2.25307300	-1.85186700
C	-2.21278000	-3.16164900	-0.90966700
H	-2.85942200	-3.45509700	1.10861200
H	-1.26934200	-2.79680100	-2.82285700
O	-3.47548700	-3.43882300	-1.34196500
C	-3.70098500	-3.38206400	-2.73257100
H	-3.10101000	-4.12550900	-3.27220300
H	-4.75792900	-3.60110000	-2.87955600
H	-3.48032600	-2.38510800	-3.13658800
H	0.74938000	2.81406400	0.24028800

H	0.69614300	2.79219200	-0.50827800
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IV' (Sextet)

0 6

Fe	0.26472600	-0.30987300	-0.71797300
N	-0.46476300	-0.05706100	1.20342800
C	0.38636700	-0.02627600	2.39021500
C	-1.66546400	-0.40055900	1.57496700
C	-0.54082600	-0.45675400	3.52693300
H	1.23307100	-0.71030000	2.25771000
H	-0.26986800	-1.42033000	3.96737300
N	-1.76159700	0.06726800	-1.31035200
C	-2.88328400	-0.25373000	-0.63305100
C	-3.08219400	0.58988700	-3.26860500
C	-4.16463000	-0.27627800	-1.28600300
C	-4.21280700	0.14286500	-2.64610100
H	-3.12760900	0.95035400	-4.28975900
H	-5.16751000	0.13203200	-3.16299800
C	-2.85054700	-0.55920800	0.76903000
C	-5.30821000	-0.67740500	-0.59029400
C	-5.24227700	-1.03060100	0.75381100
H	-6.13390300	-1.34695400	1.28395800
C	-4.03178200	-0.95671400	1.42021600
H	-3.97591500	-1.20523600	2.47243000
H	-6.25650300	-0.69543300	-1.12068200
O	-1.82667000	-0.60439400	2.90210800
C	-1.84405400	0.56052100	-2.59208400
C	-0.62838800	1.04291200	-3.18060500
C	1.75573500	1.20273500	-2.90126700
C	2.24226600	0.77206800	-4.14609200
C	2.65198200	1.81094500	-2.00849800
C	3.57452700	0.96347700	-4.48474500
C	3.97911400	2.00610500	-2.35700000
C	4.44994100	1.58528000	-3.59849700
H	3.93650600	0.60924600	-5.44497500
H	4.65383500	2.48141900	-1.65173400
H	5.49083500	1.72816200	-3.86762700
H	1.57908200	0.24354700	-4.82297300
H	2.27614300	2.12290200	-1.03822500
H	0.79981400	0.97818800	2.53160300
H	-0.63924500	0.28268200	4.32439800
N	0.46722000	0.93179400	-2.44424500
C	-0.66446400	1.71272400	-4.52209500
H	0.23528600	2.30553700	-4.68548000
H	-0.73566700	0.99433700	-5.34641300
H	-1.52689100	2.37780100	-4.60346200
C	1.78593800	-1.65162500	-1.06927500
H	1.53948700	-2.07895200	-2.05580100
H	2.76654400	-1.17474000	-1.20244000
C	1.86381800	-2.76389600	-0.02061000
H	2.37990700	-2.36286900	0.86834800

C	2.68910100	-3.97022600	-0.50531800
H	2.18082400	-4.40274600	-1.37801700
H	3.64996700	-3.59403200	-0.87712400
C	2.92032000	-5.04131200	0.54652000
H	3.53904300	-5.85754200	0.16462800
H	3.42901100	-4.63035700	1.42547200
H	1.97777300	-5.47635000	0.89180700
C	0.48349800	-3.19019300	0.43911100
C	0.18704800	-3.40530600	1.78879800
C	-0.55753100	-3.35956300	-0.47595200
C	-1.08779900	-3.75211500	2.21115100
H	0.98066500	-3.29429000	2.52645000
C	-1.84113600	-3.72257300	-0.07764900
H	-0.36637800	-3.19801500	-1.53392400
C	-2.11387700	-3.91185900	1.27724500
H	-1.31823600	-3.90161800	3.26110000
H	-2.62207400	-3.82610800	-0.82195600
O	-3.33651800	-4.23428700	1.78126400
C	-4.36121800	-4.50983100	0.84737700
H	-4.09318800	-5.35155400	0.19707800
H	-5.24095300	-4.77371700	1.43287500
H	-4.59312300	-3.63520900	0.22842100
H	3.05251500	0.24636000	0.60861300
H	3.48984500	0.50903900	1.15661300

TS₄ (Sextet)

0 6

Fe	0.49031200	0.02404800	0.21291600
N	1.47394700	0.72813800	1.91733900
C	2.91667300	0.63054300	2.12503500
C	0.91629900	0.92169900	3.07464500
C	3.10555100	1.06896400	3.57316300
H	3.23667900	-0.40309200	1.94408000
H	3.72284500	0.40114200	4.17524100
N	-1.26147900	0.90333300	1.09842800
C	-1.53098200	1.03291500	2.41425000
C	-3.59076900	1.29769400	0.57035800
C	-2.87761700	1.23461600	2.87993700
C	-3.90041400	1.35798200	1.89887800
H	-4.36588400	1.42994800	-0.17503900
H	-4.92196000	1.52218400	2.22723800
C	-0.48845100	1.00141600	3.40443100
C	-3.15289400	1.32341900	4.24768600
C	-2.13486600	1.24899200	5.18913700
H	-2.35770500	1.31622100	6.24782800
C	-0.82454100	1.10847100	4.76492200
H	-0.02234700	1.08227200	5.49121900
H	-4.18485500	1.45968000	4.55910300
O	1.77137100	1.05169500	4.11752300
C	-2.25855300	1.06277900	0.16794600
C	-1.86674200	0.96613300	-1.20709400

C	-0.04966900	0.69493400	-2.74555800
C	0.75615500	-0.36534400	-3.18150200
C	-0.21947300	1.80343700	-3.58898200
C	1.33764600	-0.33337000	-4.44025800
C	0.37759300	1.83277300	-4.84174000
C	1.15231400	0.76205900	-5.27920600
H	1.94124000	-1.17496900	-4.76696300
H	0.24119300	2.70132000	-5.47854700
H	1.61239000	0.78581800	-6.26130000
H	0.89633800	-1.21793400	-2.52524600
H	-0.80323400	2.64999800	-3.24131800
H	3.45321500	1.25936100	1.41037900
H	3.49155200	2.08870400	3.66880500
N	-0.59985500	0.64421400	-1.45674200
C	-2.88714300	1.14513700	-2.29095300
H	-3.12623200	2.19809700	-2.47474800
H	-2.53675500	0.71962700	-3.23138000
H	-3.82360100	0.64990200	-2.02507100
C	0.20298900	-2.13728700	1.03925100
H	0.86435600	-3.00355200	1.17726100
H	0.02648600	-1.73451800	2.04544100
C	-1.11114200	-2.55311700	0.38195200
H	-1.81295500	-1.70661000	0.45474400
C	-1.76869900	-3.73122600	1.12674100
H	-1.10928100	-4.60602000	1.04277200
H	-1.80302400	-3.48131400	2.19435000
C	-3.16217900	-4.07591600	0.63116600
H	-3.60943200	-4.88560100	1.21325500
H	-3.83039500	-3.21075300	0.70499100
H	-3.15107600	-4.38917600	-0.41672400
C	-0.95322900	-2.85696000	-1.09358700
C	-1.87837000	-2.38054600	-2.02938100
C	0.09489000	-3.63987600	-1.57334800
C	-1.75392800	-2.64796300	-3.38139100
H	-2.71157300	-1.77457200	-1.67843200
C	0.23964000	-3.92642900	-2.92993700
H	0.83331800	-4.03084600	-0.87799100
C	-0.68465700	-3.41948900	-3.84301700
H	-2.46185100	-2.25868100	-4.10563800
H	1.07610300	-4.53027200	-3.26124600
O	-0.62418200	-3.60579600	-5.19063500
C	0.44182200	-4.38544000	-5.68430800
H	0.41644300	-5.40772800	-5.28700400
H	0.31937500	-4.41938900	-6.76572300
H	1.41602400	-3.93983600	-5.44718200
H	1.92785400	-0.94169700	-0.37652200
H	1.26962600	-1.53065600	0.16597500

Imaginary Frequency:-1575.54

V' (Sextet)

0 6

Fe	0.02689900	0.84509300	0.18527100
N	-0.44004800	-0.44338200	1.77635300
C	0.58923700	-1.09884800	2.57947000
C	-1.55175100	-0.46306500	2.44719900
C	-0.17041700	-1.62999000	3.79494200
H	1.07243000	-1.89346800	2.00091600
H	-0.24451900	-2.72099700	3.81984000
N	-2.10783300	0.83730600	-0.11600300
C	-3.08994100	0.67534900	0.79611000
C	-3.73348800	1.53859900	-1.76407400
C	-4.44703700	1.04086600	0.49381900
C	-4.72495100	1.50021600	-0.82431800
H	-3.95959200	1.82703300	-2.78369500
H	-5.74294000	1.78066600	-1.07610400
C	-2.83207200	0.09706500	2.08408600
C	-5.44597200	0.92394100	1.46435500
C	-5.16232000	0.42030100	2.72769800
H	-5.94293800	0.33764100	3.47506900
C	-3.87703800	-0.00398900	3.01819000
H	-3.65579700	-0.43884100	3.98469700
H	-6.45607400	1.22891100	1.20548000
O	-1.50338100	-1.10283000	3.63920600
C	-2.41452100	1.18709100	-1.40995800
C	-1.34979600	1.08859600	-2.36897400
C	0.92433600	0.37471200	-2.71018900
C	0.78370600	-0.48354600	-3.81171200
C	2.21313400	0.78622100	-2.33455200
C	1.89986200	-0.89606300	-4.52582100
C	3.32094500	0.37490600	-3.06126000
C	3.17283500	-0.46553600	-4.16259000
H	1.77151900	-1.57656000	-5.36259400
H	4.30895200	0.71036100	-2.76240000
H	4.04230800	-0.79164200	-4.72333300
H	-0.19993500	-0.86438700	-4.06737400
H	2.32387300	1.43251000	-1.46767200
H	1.36452700	-0.36801400	2.83483600
H	0.21780700	-1.28095300	4.75353600
N	-0.15663100	0.74210200	-1.90273400
C	-1.62099200	1.37524400	-3.81287300
H	-0.69542900	1.55168300	-4.36005700
H	-2.14171600	0.54226700	-4.30132600
H	-2.25262200	2.25920900	-3.92091700
C	2.03528200	-2.94579100	-1.19888200
H	2.30547100	-3.89534500	-1.67308600
H	2.71556400	-2.80770600	-0.35256400
C	0.58572300	-2.94436600	-0.72804300
H	0.41569600	-2.00992900	-0.17021300
C	0.32934900	-4.10629400	0.24527700
H	0.48216900	-5.05378500	-0.28986000
H	1.10421600	-4.08192100	1.02455200
C	-1.04741200	-4.08994300	0.88642100

H	-1.15366600	-4.87760900	1.63681700
H	-1.24606700	-3.13135000	1.37843700
H	-1.83773600	-4.23244500	0.14486100
C	-0.41165600	-2.92896700	-1.86421300
C	-1.57474500	-2.15913100	-1.75381200
C	-0.22909400	-3.65342600	-3.03930300
C	-2.49955900	-2.08395600	-2.78106200
H	-1.73646900	-1.58135400	-0.84580400
C	-1.14596200	-3.59399600	-4.08813100
H	0.66219700	-4.26239800	-3.16494000
C	-2.28296000	-2.79416900	-3.96510900
H	-3.39331500	-1.47357500	-2.69269000
H	-0.95963500	-4.16065700	-4.99273100
O	-3.22458600	-2.62916100	-4.93735600
C	-3.03188600	-3.33438800	-6.14413900
H	-3.01760900	-4.41911200	-5.98278000
H	-3.87506800	-3.07972800	-6.78414800
H	-2.10001500	-3.03928500	-6.64258400
H	1.28057300	1.64725300	0.87078600
H	2.22865500	-2.14666900	-1.91917700

TS_{5a}

0 2

Fe	0.44903600	-0.50129700	-0.07368500
N	0.63778100	-0.59048200	1.86755600
C	1.84868300	-0.78323100	2.66921200
C	-0.30615900	-0.20083100	2.68921500
C	1.53790100	-0.03890400	3.95560200
H	2.00711600	-1.85739300	2.82612400
H	1.85640000	-0.54030500	4.87013800
N	-1.46065600	-0.80656400	0.11263200
C	-2.25482400	-0.45702000	1.15601800
C	-3.42801900	-1.48289800	-1.14397800
C	-3.68530300	-0.49707700	1.04396400
C	-4.24413100	-1.02035700	-0.16006700
H	-3.84555500	-1.90599100	-2.05031900
H	-5.32402100	-1.06095300	-0.26004200
C	-1.69776000	-0.04591900	2.40978000
C	-4.48037200	-0.03804900	2.09589000
C	-3.91671100	0.43393700	3.27757400
H	-4.55121300	0.79205500	4.08065200
C	-2.54519500	0.41143100	3.43750900
H	-2.09420100	0.72338600	4.37122500
H	-5.55956700	-0.06347100	1.97394500
O	0.09734200	0.02963300	3.96399800
C	-2.02119100	-1.38439700	-1.01353500
C	-1.08866300	-1.81701700	-1.97040100
C	1.21310800	-1.96527100	-2.56160800
C	2.21527100	-2.86253000	-2.18475400
C	1.24384500	-1.41609900	-3.84868600
C	3.20404800	-3.23113500	-3.08909000

C	2.23947100	-1.77762900	-4.74466100
C	3.21779600	-2.69590700	-4.37342600
H	3.96837700	-3.94127800	-2.78837600
H	2.25931400	-1.33095400	-5.73427300
H	3.99455500	-2.97968800	-5.07648700
H	2.19178800	-3.26775000	-1.17790300
H	0.49025600	-0.68490900	-4.12699700
H	2.72281800	-0.39312000	2.15320300
H	1.93351400	0.98461400	3.94932000
N	0.20749200	-1.62430900	-1.62854000
C	-1.51536700	-2.50676800	-3.22888800
H	-2.44630100	-3.05436100	-3.07460900
H	-1.68187800	-1.81509100	-4.06241400
H	-0.76084700	-3.22211800	-3.56041300
C	0.36196200	1.35393700	-0.72583100
H	1.99144000	-0.46959600	-0.19677200
C	1.76605200	1.06264100	-0.63744800
H	-0.12925800	1.37409100	-1.69663600
C	2.47901300	1.76651900	0.51909600
H	-0.10284200	1.98003700	0.03563000
H	2.46956600	2.84285700	0.29449600
H	1.86509100	1.65404400	1.42102900
C	3.92170900	1.35413800	0.82271900
H	4.02305400	0.26554200	0.76495100
H	4.57843400	1.74355700	0.03345600
C	4.35033200	1.86533800	2.15956300
C	4.91452400	1.19004500	3.17029100
H	4.14208600	2.92353300	2.33079300
C	5.29285300	-0.25881800	3.12448600
C	5.22057700	1.86666000	4.47161500
H	6.28750700	1.80304300	4.71526400
H	4.93835100	2.92102300	4.46261800
H	4.69213300	1.38237800	5.30283200
H	6.36571800	-0.38160700	3.31172900
H	4.78508800	-0.82397500	3.91677800
H	5.07095400	-0.74099700	2.17206500
C	2.56822800	1.01742900	-1.90909600
C	3.66507600	0.17448500	-2.07442800
C	2.26085700	1.91531900	-2.93847000
C	4.42778200	0.22869600	-3.23415100
H	3.89780600	-0.55978000	-1.31029800
C	3.02239600	1.94936200	-4.10439300
H	1.41938100	2.58601900	-2.81010200
C	4.12827300	1.10180300	-4.27258500
H	5.26613900	-0.45243100	-3.35525800
O	2.76750200	2.78081800	-5.15776400
C	1.65803400	3.64470500	-5.04874000
H	1.76766600	4.34402600	-4.21101100
H	1.61712400	4.20714400	-5.98031300
H	0.72107900	3.08832000	-4.92195300
C	4.91179100	1.13396700	-5.54419200

H	4.27511300	0.92284700	-6.40961200
H	5.34822900	2.12082100	-5.72656600
H	5.71960800	0.39989600	-5.52634500

Imaginary Frequency:-602.46

VIIa

0 2

Fe	0.02017700	-1.39827200	0.04991400
N	0.62394000	-2.58417700	1.47962000
C	1.88150000	-3.34602400	1.53482500
C	-0.09262500	-2.95526600	2.51448300
C	1.89489700	-3.90523400	2.94367600
H	1.86322500	-4.12887200	0.76759900
H	2.21095100	-4.94570400	3.02031600
N	-1.82548800	-1.24535300	0.88191500
C	-2.26958700	-1.76447200	2.05745900
C	-3.99587500	-0.20190700	0.53985100
C	-3.60205700	-1.50701400	2.52871200
C	-4.45181700	-0.70239600	1.72294900
H	-4.63533700	0.41968300	-0.07492000
H	-5.46010500	-0.49696200	2.06821800
C	-1.43063000	-2.59022000	2.87591700
C	-4.04678100	-2.03496900	3.74657900
C	-3.21433300	-2.82372500	4.52845300
H	-3.56377100	-3.22740400	5.47198200
C	-1.93030000	-3.09393900	4.09409900
H	-1.27476300	-3.71056800	4.69470800
H	-5.06077400	-1.81130400	4.06502300
O	0.52120000	-3.82437500	3.35619800
C	-2.67749100	-0.47283800	0.12169500
C	-2.13601500	0.04861300	-1.08868200
C	-0.23875000	0.35124300	-2.46329000
C	0.26919400	-0.43779400	-3.49844700
C	-0.07980000	1.73966300	-2.53006400
C	0.92871100	0.14981400	-4.57123800
C	0.58121400	2.32278400	-3.60288800
C	1.09283900	1.53107400	-4.62737800
H	1.31653600	-0.47712700	-5.36824400
H	0.70089900	3.40142400	-3.63469900
H	1.61198000	1.98706100	-5.46451700
H	0.14587600	-1.51462100	-3.44469800
H	-0.44787000	2.35305900	-1.71224000
H	2.74096500	-2.70889000	1.32849600
H	2.49303500	-3.30032700	3.63474700
N	-0.86373900	-0.24885700	-1.34437000
C	-2.99323900	0.85189000	-2.01905700
H	-4.00337700	0.44251600	-2.07054800
H	-3.08423100	1.89586000	-1.69952500
H	-2.58151000	0.85977600	-3.02751900
C	1.87761700	-1.39185200	-0.75682600
H	2.86165000	-0.67415100	1.03785200

C	2.79064100	-0.39660300	-0.02699800
H	2.33509900	-2.38888200	-0.75233600
C	2.20296500	1.01598600	-0.09358600
H	1.82868600	-1.09744200	-1.81122300
H	2.11959100	1.30915300	-1.14732100
H	1.16705600	1.00067900	0.28130100
C	2.99621700	2.09379200	0.64556700
H	2.99498500	1.88034800	1.72129200
H	4.04613600	2.03494800	0.33377300
C	2.44145500	3.46150900	0.38584900
C	2.68205500	4.20667500	-0.70091900
H	1.73622300	3.85362400	1.11894100
C	3.60746000	3.78520600	-1.80150800
C	2.01874700	5.53339600	-0.90370300
H	1.42509700	5.54444900	-1.82690000
H	1.35616000	5.79146300	-0.07513500
H	2.75606500	6.33811000	-1.01092100
H	4.37559900	4.54640800	-1.98297700
H	4.11184100	2.83743500	-1.60337900
H	3.06015200	3.67353900	-2.74661900
C	4.19629000	-0.41982900	-0.58762500
C	5.28531300	-0.83347200	0.17083200
C	4.41966700	-0.01670900	-1.91120600
C	6.56742000	-0.84484000	-0.37932000
H	5.13394500	-1.13736600	1.20385200
C	5.70149000	-0.02162700	-2.44749800
H	3.57296000	0.29841300	-2.51398300
C	6.80794300	-0.44204500	-1.68536800
H	7.41080500	-1.16926900	0.22542800
O	5.99585500	0.36953700	-3.72236300
C	4.92117500	0.80427700	-4.52748900
H	4.41998100	1.68109000	-4.09879400
H	5.35242600	1.07135400	-5.49153500
H	4.17393900	0.01369400	-4.67039300
C	8.17459200	-0.43952400	-2.29060600
H	8.92096800	-0.79457800	-1.57774500
H	8.22090900	-1.07477400	-3.18058600
H	8.46567100	0.56250800	-2.62083300

TS_{6a}

0 2

Fe	-0.00058400	-0.80499700	0.60505200
N	0.68479800	-1.92526900	2.05527700
C	2.05916500	-1.92020900	2.56812000
C	0.00149300	-2.77081400	2.77320100
C	1.96863200	-2.72326900	3.85698500
H	2.73202100	-2.37012500	1.82807000
H	2.72546800	-3.50135800	3.96150300
N	-1.74337700	-1.73050400	0.66012700
C	-2.19279500	-2.67050100	1.54994800
C	-3.90322300	-1.82807800	-0.47613100

C	-3.51938400	-3.20672900	1.45837200
C	-4.35944100	-2.76264700	0.40054700
H	-4.53287300	-1.48323400	-1.28694500
H	-5.35819100	-3.17803500	0.31436700
C	-1.36937000	-3.16675500	2.60775600
C	-3.97787600	-4.14843100	2.38994700
C	-3.16991900	-4.59262500	3.42257600
H	-3.53717300	-5.31588900	4.14153800
C	-1.87842200	-4.10562600	3.52149300
H	-1.22529800	-4.45001500	4.31273900
H	-4.99274400	-4.52053300	2.28180500
O	0.68140400	-3.36377800	3.78073400
C	-2.60435100	-1.29715300	-0.33865300
C	-2.08413600	-0.27986200	-1.16963400
C	-0.24641700	1.12652300	-1.64488500
C	0.31159900	0.83683800	-2.89352800
C	-0.21060100	2.43754500	-1.17034300
C	0.90097500	1.84503700	-3.64896800
C	0.37699200	3.44201500	-1.93021300
C	0.93468600	3.15163900	-3.17092000
H	1.32729100	1.60942000	-4.61992200
H	0.40396300	4.45757200	-1.54707900
H	1.38832000	3.93919900	-3.76387500
H	0.27766600	-0.18517400	-3.26195800
H	-0.64529000	2.65605500	-0.20150000
H	2.39412600	-0.89481600	2.73100700
H	1.97911000	-2.09659900	4.75493800
N	-0.83423800	0.08978500	-0.86705500
C	-2.85881400	0.35286800	-2.28108500
H	-2.57466800	-0.05052500	-3.26006200
H	-3.93184900	0.20740500	-2.16577400
H	-2.67254800	1.42838000	-2.32393900
C	1.85795200	-0.67792600	-0.22339600
H	3.39364700	0.01803600	1.14518600
C	3.12202000	0.13309000	0.08603800
H	2.06720400	-1.75094200	-0.09362300
C	2.90807100	1.62337300	-0.18377000
H	1.61858900	-0.52636800	-1.27955000
H	2.62726600	1.76163600	-1.23671900
H	2.04156500	1.97851300	0.38877600
C	4.11501600	2.51016200	0.12088200
H	4.33071500	2.47741200	1.19649000
H	5.00166800	2.09204000	-0.37070800
C	3.88060700	3.92355400	-0.31762700
C	4.05661100	4.39490500	-1.55851400
H	3.47299000	4.60669300	0.42784500
C	4.57624000	3.56428900	-2.69187100
C	3.72484700	5.81102700	-1.91208300
H	2.96909300	5.85561900	-2.70683400
H	3.34363800	6.36887000	-1.05425100
H	4.60139400	6.34370400	-2.30005100

H	5.47719200	4.01148100	-3.12896700
H	4.81453700	2.53855900	-2.40353000
H	3.83710300	3.51522100	-3.50183400
C	4.27664700	-0.41049900	-0.72818100
C	5.36127600	-1.04187600	-0.13148500
C	4.25927500	-0.28394300	-2.12320500
C	6.40742500	-1.53451400	-0.91183400
H	5.39618500	-1.13969200	0.95064800
C	5.30893900	-0.77321900	-2.89175500
H	3.41371100	0.20735100	-2.59497000
C	6.41057700	-1.41398900	-2.29443500
H	7.25245200	-2.02325500	-0.43343400
O	5.36539400	-0.67790700	-4.25193500
C	4.28515800	-0.04171400	-4.89968200
H	4.17671100	1.00161500	-4.57797200
H	4.51066200	-0.06857300	-5.96480500
H	3.33744800	-0.56458700	-4.71707500
C	7.52473400	-1.93021600	-3.14629700
H	8.29999800	-2.39925400	-2.53805700
H	7.16631800	-2.66614000	-3.87252200
H	7.98616900	-1.12914500	-3.73182100
Si	-0.56379200	0.75973500	2.26848600
H	0.93175200	0.32618000	0.84183300
H	-1.10971900	2.03979600	1.76448500
H	-1.64572700	0.13537600	3.07113200
C	0.81914000	1.20403100	3.51751700
H	1.72936200	1.55502600	3.02267400
H	0.48622000	1.99464500	4.19524200
H	1.08223300	0.34279900	4.13703400

Imaginary Frequency: -462.81

VIIIa

0 2

Fe	-0.45457700	-1.06356700	0.55316300
N	0.32827500	-2.19207900	1.91001300
C	1.73598200	-2.26390900	2.32134200
C	-0.38016200	-2.82613800	2.81607000
C	1.68103300	-2.86495600	3.71969300
H	2.30040400	-2.88913400	1.61979700
H	2.34383100	-3.71866800	3.86736200
N	-2.18270300	-1.82902300	0.74355800
C	-2.64156000	-2.60448200	1.76818100
C	-4.43168400	-1.80227600	-0.21787700
C	-4.02290300	-2.99423000	1.83634900
C	-4.90302700	-2.56861200	0.79581700
H	-5.09115400	-1.47391300	-1.01259000
H	-5.94536100	-2.86618800	0.84144200
C	-1.78514200	-3.06459900	2.81840700
C	-4.48942800	-3.75594700	2.90732900
C	-3.64608500	-4.16369600	3.93713300
H	-4.03105100	-4.74645500	4.76614800

C	-2.31333900	-3.82216600	3.88735700
H	-1.63553000	-4.14024400	4.66874200
H	-5.54444100	-4.01451800	2.92645900
O	0.32655700	-3.32567300	3.85383500
C	-3.06988500	-1.42018000	-0.26191600
C	-2.49450900	-0.61708800	-1.23952700
C	-0.47350300	0.40123100	-1.99712500
C	-0.17295800	-0.15086100	-3.24858500
C	-0.01959900	1.68717400	-1.69733200
C	0.57666300	0.56634500	-4.17169400
C	0.72941200	2.40217700	-2.62609700
C	1.03566800	1.84637500	-3.86434800
H	0.80696300	0.12272200	-5.13589500
H	1.08086800	3.39875300	-2.37160400
H	1.61748600	2.40788900	-4.58905800
H	-0.51500400	-1.15662400	-3.47390300
H	-0.25361700	2.10967200	-0.72611800
H	2.18669200	-1.26925100	2.31550100
H	1.86881300	-2.13121600	4.51000500
N	-1.17164400	-0.36381500	-1.03233800
C	-3.23962500	-0.01528400	-2.38425100
H	-4.31742200	-0.06036300	-2.23287400
H	-2.96711100	1.03586800	-2.51773900
H	-3.02136400	-0.51322600	-3.33614900
C	2.07349200	-0.58726100	-0.32452800
H	3.55855700	-0.05729900	1.14672600
C	3.31841000	0.19368100	0.10263400
H	2.18438600	-1.66288900	-0.18540200
C	3.04100400	1.69702300	0.02092500
H	1.84567300	-0.40638400	-1.37563700
H	2.80607400	1.95133200	-1.01912300
H	2.12774600	1.93322900	0.58549800
C	4.18891700	2.58591500	0.49490800
H	4.36418500	2.42127000	1.56499900
H	5.11167200	2.26982900	-0.00839500
C	3.90960300	4.03572900	0.23096900
C	4.00984000	4.63969400	-0.96013200
H	3.54290900	4.62763800	1.06869200
C	4.47508000	3.93910200	-2.20083600
C	3.64063200	6.07824900	-1.14443000
H	2.84037400	6.19044300	-1.88661700
H	3.30168700	6.53664800	-0.21366500
H	4.48760000	6.66291100	-1.52259700
H	5.29312200	4.48954700	-2.67994600
H	4.81797800	2.91845000	-2.01853500
H	3.66844700	3.88864100	-2.94454700
C	4.50515500	-0.20593900	-0.74437200
C	5.61739000	-0.82733600	-0.19149100
C	4.49603400	0.06395700	-2.11891500
C	6.70371000	-1.17035600	-0.99644400
H	5.64153000	-1.03640100	0.87457800

C	5.58661400	-0.27732400	-2.91172100
H	3.62900000	0.54768000	-2.55968900
C	6.71814800	-0.90669200	-2.35859400
H	7.57071000	-1.65319800	-0.55327900
O	5.65835900	-0.03912800	-4.25109100
C	4.55705400	0.60883000	-4.85377000
H	4.39138400	1.60507300	-4.42536400
H	4.80403100	0.70722600	-5.90974400
H	3.63469700	0.02480300	-4.74832100
C	7.87492700	-1.26106000	-3.23557200
H	8.67357000	-1.73388800	-2.66180600
H	7.57575100	-1.94461800	-4.03587800
H	8.28537300	-0.37691100	-3.73244400
Si	-0.72425600	0.81742100	2.01683400
H	1.22891800	-0.17346400	0.27779800
H	-0.77331600	2.16629600	1.39829500
H	-2.00001100	0.66235200	2.75647500
C	0.66953200	0.88834900	3.34074700
H	1.66170100	0.98946200	2.88949700
H	0.53205700	1.73730700	4.01621400
H	0.66744100	-0.01813000	3.95247300

TS_{5b}

0 2

Fe	0.36397700	-0.33142300	0.13569000
N	0.70724400	-0.65623400	2.02222700
C	2.00489600	-0.75641400	2.69491200
C	-0.20976400	-0.52342600	2.94569600
C	1.69236600	-0.40709800	4.14669800
H	2.39391300	-1.77353900	2.57391800
H	2.08800300	-1.11354900	4.87759600
N	-1.48900400	-0.83438900	0.37338600
C	-2.23746300	-0.69982800	1.49555500
C	-3.46132900	-1.51777200	-0.86044400
C	-3.66570000	-0.83329500	1.44730200
C	-4.25313700	-1.22453700	0.20762800
H	-3.89922900	-1.86288700	-1.79005700
H	-5.33237300	-1.32191100	0.14901100
C	-1.62721600	-0.44780000	2.76730100
C	-4.42474700	-0.59920500	2.59611600
C	-3.81960900	-0.28110400	3.80831200
H	-4.42550500	-0.10485100	4.69025100
C	-2.44151900	-0.23176800	3.89713800
H	-1.95830600	-0.05168000	4.84993900
H	-5.50523700	-0.68740900	2.52791100
O	0.25148500	-0.46099200	4.21976000
C	-2.05932500	-1.34670600	-0.77732600
C	-1.13129900	-1.66392200	-1.78937200
C	1.18480700	-1.74904600	-2.37526800
C	2.18648900	-2.64388500	-1.98302900
C	1.25819000	-1.16836900	-3.64680000

C	3.22394200	-2.96529800	-2.84805600
C	2.30866800	-1.47916300	-4.50221100
C	3.29363700	-2.38123100	-4.11008300
H	3.98884800	-3.66729700	-2.53160600
H	2.36073900	-1.01053500	-5.48031800
H	4.11116700	-2.62247000	-4.78120000
H	2.12673200	-3.07654900	-0.98930300
H	0.49261000	-0.45959200	-3.94982800
H	2.72151300	-0.06929600	2.23679400
H	2.00515200	0.60560400	4.42066100
N	0.15824200	-1.44620400	-1.45673500
C	-1.55894700	-2.26546400	-3.09096700
H	-1.74879800	-1.51138000	-3.86339200
H	-0.79362400	-2.93613400	-3.48582600
H	-2.47707500	-2.84234500	-2.97298100
C	0.17345100	1.49104500	-0.60152400
H	1.88104400	-0.14107100	-0.04089700
C	1.58757500	1.35611900	-0.33788100
C	2.51114100	1.40240600	-1.55413100
H	-0.15348500	1.43529500	-1.63844700
H	1.91149600	1.14604500	-2.43221100
H	2.80426100	2.45111200	-1.69324100
C	3.77271300	0.50830900	-1.52342300
H	3.59440900	-0.36009900	-2.16526700
C	5.05177500	1.18417200	-1.93295600
H	5.80455200	1.32150900	-1.15614900
C	5.35125900	1.63094100	-3.15896200
C	6.65825400	2.29690500	-3.45530600
H	6.50954500	3.31175300	-3.84321200
H	7.29381500	2.36440900	-2.57032500
H	7.21340500	1.75514400	-4.23055000
C	4.41816800	1.50709500	-4.32295600
H	3.50480700	0.96479100	-4.07679400
H	4.13159800	2.49523100	-4.70315100
H	4.90163100	0.98737000	-5.15942100
C	2.11086400	2.05562500	0.88917600
C	1.26019600	2.35912000	1.96764900
C	3.44688200	2.44735400	0.99398700
C	1.73621100	3.00970700	3.09867800
C	3.91591400	3.08689000	2.14094000
H	4.13844300	2.27950200	0.17829500
C	3.09052700	3.37404100	3.21685800
H	4.96177600	3.37801500	2.19674900
C	3.57750700	4.04825300	4.45750200
H	3.03452200	4.97909400	4.64644800
H	3.41749600	3.42408600	5.34296200
H	4.64203600	4.27841400	4.38929500
H	-0.44569300	2.13485700	0.01785800
H	3.89598800	0.09354800	-0.51638300
O	0.96593900	3.32707300	4.17859000
C	-0.41701800	3.03665300	4.10685100

H	-0.60189300	1.95920900	4.03995800
H	-0.85322500	3.41630700	5.02954500
H	-0.88989100	3.53459700	3.25223600
H	0.21759100	2.07123800	1.92205100

Imaginary Frequency: -606.91

VIIb

0 2

Fe	0.64101400	-1.65300500	-0.36679800
N	0.38001300	-3.01013300	0.99735500
C	1.03787800	-4.31953800	1.06970100
C	-0.57419700	-3.00006100	1.89916100
C	0.50574900	-4.91490000	2.36284600
H	0.77450500	-4.91190700	0.18551600
H	0.19676200	-5.95822400	2.29219000
N	-0.92235700	-0.57415400	0.29639000
C	-1.64186800	-0.76227700	1.43136600
C	-1.93536600	1.61315000	0.01766400
C	-2.56158000	0.23639200	1.89971100
C	-2.67108700	1.44087100	1.15494200
H	-2.00342200	2.53707300	-0.54464000
H	-3.34446300	2.21500700	1.50903500
C	-1.51259000	-1.96416300	2.20802900
C	-3.31954000	0.02187500	3.05816000
C	-3.20425800	-1.16201000	3.77731700
H	-3.80198300	-1.32423200	4.66745100
C	-2.31663000	-2.13408800	3.35643500
H	-2.21101400	-3.05326700	3.91813500
H	-4.00467500	0.80150800	3.37821300
O	-0.65712100	-4.12426700	2.65752900
C	-1.06449400	0.59636400	-0.41704500
C	-0.28498300	0.69377700	-1.61220000
C	1.30787000	-0.41453200	-3.01884900
C	1.27601000	-1.61625600	-3.73593200
C	2.16465900	0.60400500	-3.44952600
C	2.05981200	-1.78522100	-4.86678700
C	2.95738100	0.42495700	-4.57747200
C	2.90645300	-0.76524900	-5.29431800
H	2.01750500	-2.72185700	-5.41328600
H	3.62407600	1.22142700	-4.89292800
H	3.52735200	-0.90143000	-6.17319500
H	0.63328900	-2.41579100	-3.37871700
H	2.22527200	1.52248000	-2.87617200
H	2.12336800	-4.20812400	1.07297800
H	1.20807100	-4.81041800	3.19780600
N	0.53490300	-0.32313000	-1.84474500
C	-0.47153700	1.84983100	-2.54320600
H	-1.51167800	2.17781300	-2.56092000
H	0.13702400	2.71129900	-2.24215200
H	-0.18119500	1.58987400	-3.56088300
C	2.54392800	-2.28826800	-0.72821500

H	3.08143100	-2.29837000	1.36247600
C	3.35541300	-1.73695200	0.45337700
C	4.86965700	-1.87878600	0.26889400
H	5.10307600	-2.93415300	0.07600400
H	5.18029600	-1.34394100	-0.63881900
C	5.69002800	-1.38798800	1.46451300
H	5.38129600	-1.93895300	2.36071000
C	7.16234800	-1.49987600	1.23967500
H	7.58586200	-0.75072100	0.56881300
C	8.00088000	-2.42541100	1.72273500
C	9.45775300	-2.40866400	1.37527400
H	9.76133600	-3.34048500	0.88292800
H	9.71088900	-1.57921200	0.71229800
H	10.08051200	-2.32476900	2.27424500
C	7.58935700	-3.54516600	2.62789900
H	6.52284500	-3.54770200	2.85387900
H	7.83647100	-4.51488800	2.17971700
H	8.13470500	-3.50479700	3.57838300
C	2.91469800	-0.30344600	0.68866300
C	2.04681200	0.00025400	1.74608200
C	3.25207100	0.71184400	-0.20477100
C	1.50183100	1.27695500	1.88096000
C	2.69553000	1.98007000	-0.06640400
H	3.92016900	0.50064700	-1.03476800
C	1.80433100	2.28993400	0.95536600
H	2.95702600	2.76329600	-0.77586400
C	1.17852100	3.63967300	1.09715100
H	1.52425400	4.31897000	0.31518000
H	0.08598500	3.57844900	1.04430500
H	1.40694300	4.08952300	2.06807200
H	5.42963300	-0.33903900	1.65919900
H	2.92417500	-1.83729100	-1.65483200
H	2.68348200	-3.37311800	-0.82621300
O	0.64578700	1.64247600	2.87525300
C	0.42043100	0.71717300	3.92118900
H	1.35791200	0.45019400	4.42394700
H	-0.24244900	1.21519800	4.62743000
H	-0.06806400	-0.19567200	3.56342700
H	1.78317600	-0.78752300	2.44566700

TS_{6b}

0 2

Fe	0.20771000	-1.18918000	0.64309300
N	0.62779000	-2.32198800	2.20191100
C	1.90166400	-2.32426800	2.92521900
C	-0.20970800	-3.04430500	2.88701500
C	1.68329400	-3.29663700	4.07795800
H	2.71105100	-2.63915300	2.26289300
H	2.24554100	-4.22892800	3.97207000
N	-1.65761100	-1.86175500	0.63680700
C	-2.27888700	-2.73124900	1.49568600

C	-3.74625100	-1.68100900	-0.61952100
C	-3.65422900	-3.09791500	1.32121200
C	-4.37009000	-2.54711400	0.22329600
H	-4.27529600	-1.25870000	-1.46497700
H	-5.40771400	-2.82953800	0.07835000
C	-1.59442900	-3.31169500	2.60623600
C	-4.28037200	-3.97717600	2.21556600
C	-3.59803200	-4.51640800	3.29219700
H	-4.09307200	-5.19234100	3.97990500
C	-2.26760900	-4.18342100	3.47864100
H	-1.71411200	-4.59822800	4.31069600
H	-5.32434500	-4.22266600	2.04242300
O	0.28233000	-3.61299200	4.01043700
C	-2.39559600	-1.33280100	-0.41224100
C	-1.69293000	-0.42980300	-1.23964300
C	0.36104900	0.62978100	-1.70177300
C	0.70358500	0.28728000	-3.01172200
C	0.76241700	1.86372400	-1.19140100
C	1.41721600	1.17749500	-3.80501400
C	1.45856600	2.75732800	-1.99492900
C	1.78755900	2.42052100	-3.30342700
H	1.68290500	0.89765200	-4.81964500
H	1.75431100	3.71965000	-1.58754300
H	2.34736000	3.11695700	-3.91990200
H	0.40189800	-0.68245700	-3.39718200
H	0.50756800	2.12644800	-0.16974900
H	2.13004700	-1.30598000	3.26239000
H	1.88611100	-2.87593600	5.06474300
N	-0.40602300	-0.26842800	-0.90982900
C	-2.34995400	0.32054100	-2.35556000
H	-3.41837200	0.44401900	-2.17887600
H	-1.91516000	1.31580000	-2.46413200
H	-2.23239500	-0.17981700	-3.32366400
C	2.10952300	-1.37566100	-0.06807800
H	3.34732700	-0.67882400	1.56301900
C	3.44776800	-0.85952700	0.48408700
C	4.55159200	-1.91353400	0.33125700
H	4.19775500	-2.85645000	0.77154800
H	4.71774800	-2.14443500	-0.72890200
C	5.87103300	-1.52238200	1.00141800
H	5.64930800	-1.17109400	2.01867300
C	6.86178900	-2.64474500	1.03587700
H	7.60279700	-2.66632200	0.23726800
C	6.88709500	-3.64450800	1.92644100
C	7.90064700	-4.74279600	1.84665600
H	7.41965100	-5.72402000	1.75388000
H	8.57319000	-4.61615100	0.99641500
H	8.51070700	-4.78910900	2.75676000
C	5.91148600	-3.76615300	3.05785600
H	5.25415500	-2.89916800	3.15045000
H	5.27769900	-4.65311400	2.92980700

H	6.42948000	-3.89973600	4.01456300
C	3.84349600	0.47121300	-0.11709500
C	3.65741000	1.64805000	0.61301300
C	4.40781900	0.55912100	-1.38730100
C	4.02785600	2.88098700	0.08109600
C	4.80986400	1.79114200	-1.89273000
H	4.54572300	-0.33737500	-1.98467100
C	4.63733500	2.97086200	-1.18011700
H	5.25584500	1.84617900	-2.88302900
C	5.01635100	4.30506000	-1.73635800
H	5.49830300	4.20171600	-2.71051300
H	4.13965900	4.95154200	-1.85742200
H	5.69687500	4.84518300	-1.07166100
H	6.29693700	-0.65690700	0.48268000
H	2.05338900	-1.15213600	-1.13821300
H	2.06338400	-2.47261700	0.04621200
Si	-0.27907900	0.63982100	2.05691800
H	-1.35507000	1.43435000	1.41562700
H	1.23818200	-0.14339300	0.88392100
H	0.79117500	1.62217800	2.37535400
C	-0.91970900	0.02197500	3.74860000
H	-0.13679300	-0.48226200	4.32141800
H	-1.27584700	0.86262800	4.35045000
H	-1.74883000	-0.67937500	3.63066800
O	3.81537500	4.07691300	0.70497000
C	3.10245500	4.05084100	1.92376200
H	3.64586100	3.50231500	2.70280400
H	2.98905900	5.08900500	2.23249500
H	2.11160100	3.59556300	1.80135200
H	3.20013200	1.58469600	1.59570100

Imaginary Frequency: -430.97

VIIIb

0 2

Fe	-0.71685400	-0.76124100	0.52927800
N	-0.36590800	-1.29187000	2.32395400
C	0.91138900	-1.25629000	3.04262700
C	-1.28030500	-1.70807800	3.16397500
C	0.47155200	-1.27449900	4.49464500
H	1.50226100	-2.14069500	2.76996500
H	1.08298400	-1.88883800	5.15509800
N	-2.46945900	-1.68715500	0.49131700
C	-3.19086500	-2.10191500	1.56624600
C	-4.33345900	-2.19855400	-0.97328800
C	-4.53244400	-2.57914700	1.40725300
C	-5.07634100	-2.61806700	0.09227400
H	-4.74601300	-2.21892200	-1.97560200
H	-6.09103000	-2.97950000	-0.04119800
C	-2.64151600	-2.07325200	2.89165600
C	-5.28000200	-2.97601900	2.52446400
C	-4.74021700	-2.92057700	3.80099400

H	-5.32962000	-3.22180800	4.65961100
C	-3.44001300	-2.47765700	3.97699100
H	-3.00717700	-2.44092200	4.96877900
H	-6.29953700	-3.31661200	2.36883200
O	-0.84670000	-1.85882600	4.44056800
C	-3.02004500	-1.73004700	-0.77082700
C	-2.16001000	-1.28423800	-1.81337200
C	0.05823900	-0.58037200	-2.34039900
C	0.53164900	-1.65847100	-3.10040000
C	0.69519900	0.65871700	-2.45186900
C	1.62694300	-1.50154900	-3.93908600
C	1.79025800	0.80847400	-3.29195000
C	2.26674200	-0.26885200	-4.03479900
H	1.99117200	-2.35021500	-4.50955000
H	2.27650300	1.77678800	-3.36152900
H	3.12751400	-0.14888400	-4.68431900
H	0.04944600	-2.62642500	-2.99747400
H	0.31687800	1.50034800	-1.88485600
H	1.48859900	-0.37187200	2.76369200
H	0.37708800	-0.26696500	4.91676200
N	-0.99275800	-0.77118500	-1.41532000
C	-2.57799900	-1.36162400	-3.24757300
H	-2.54783100	-2.38604500	-3.63404000
H	-3.60412600	-1.00616300	-3.37048500
H	-1.93260700	-0.75343200	-3.88062800
C	2.77724900	-1.64430500	-0.29292900
H	3.87883700	-1.69626900	1.54747400
C	3.99125300	-1.25143000	0.54642100
C	5.27910800	-1.81497500	-0.06252800
H	5.16738200	-2.89828900	-0.20043600
H	5.41160000	-1.40113400	-1.07198200
C	6.52818100	-1.53641500	0.77290000
H	6.38780600	-1.94820200	1.77894400
C	7.77273000	-2.06288400	0.13863900
H	8.05100400	-1.57207000	-0.79566900
C	8.55930900	-3.06305600	0.55536100
C	9.77318100	-3.46625300	-0.22453200
H	9.71907600	-4.51810400	-0.52988400
H	9.90321600	-2.86017100	-1.12298700
H	10.68317600	-3.37336700	0.38043400
C	8.32947400	-3.86244900	1.80049700
H	7.42779700	-3.57500700	2.34114400
H	8.25155300	-4.93047600	1.56579100
H	9.17733400	-3.76654100	2.48906100
C	4.04631100	0.24898500	0.72759700
C	3.90425500	0.81206000	1.99875100
C	4.20220200	1.09940400	-0.36313100
C	3.87982900	2.19483800	2.16723600
C	4.18850300	2.47937300	-0.18309400
H	4.30984400	0.68646100	-1.36251300
C	4.01445000	3.05804200	1.06827900

H	4.29545400	3.13492500	-1.04408200
C	3.94057700	4.53656700	1.26897200
H	4.10579700	5.06984000	0.33136800
H	2.96143600	4.83164900	1.66082500
H	4.67768100	4.88354600	1.99895900
H	6.61934600	-0.44976400	0.90810800
H	2.86439900	-1.25734100	-1.31321900
H	2.66592300	-2.73163900	-0.35772700
Si	0.14608800	1.50778800	0.78278800
H	-0.68808900	2.47544700	0.01560700
H	1.85150400	-1.22648400	0.12321100
H	1.52526900	1.74916700	0.29354300
C	0.12870900	2.15134100	2.60154500
H	0.89358700	1.65611700	3.20593700
H	0.34460100	3.22324900	2.64025400
H	-0.83695500	1.98605500	3.08738900
O	3.71837700	2.81372600	3.37363100
C	3.62446600	1.99526300	4.51558000
H	4.52506700	1.38391200	4.65289600
H	3.51141500	2.66662400	5.36547800
H	2.75066400	1.33063200	4.46935600
H	3.81658600	0.15056200	2.85506300

TS_{sc}

0 2

Fe	0.60917100	0.09276900	-0.07450700
N	1.85627000	0.17042000	1.41559000
C	3.32010800	0.24094000	1.40269600
C	1.46921300	0.45856100	2.63519900
C	3.63112500	1.04972700	2.64979000
H	3.72483300	-0.77736500	1.45266700
H	4.49561500	0.71034400	3.21982700
N	-0.78315800	-0.53335700	1.12863600
C	-0.90846300	-0.26706400	2.45259400
C	-2.91586000	-1.69962400	1.17630000
C	-2.11380000	-0.58374900	3.16291500
C	-3.12036500	-1.31794400	2.46552600
H	-3.66503300	-2.28124400	0.65114400
H	-4.03515500	-1.57541700	2.99077800
C	0.15753200	0.34568900	3.18886100
C	-2.26839000	-0.17389800	4.48806800
C	-1.25847600	0.51332500	5.15530900
H	-1.40657300	0.84497000	6.17752400
C	-0.05445300	0.74871400	4.52131500
H	0.75784200	1.23732300	5.04496300
H	-3.20533900	-0.40138200	4.98921900
O	2.45929600	0.86713900	3.46848500
C	-1.73649900	-1.31366600	0.49095500
C	-1.41668300	-1.66326700	-0.83076000
C	0.22959000	-1.45371500	-2.57483100
C	1.55994100	-1.85227600	-2.75587500

C	-0.56798400	-1.25884000	-3.71050800
C	2.07249700	-2.05716700	-4.02944900
C	-0.04844700	-1.45467300	-4.98350900
C	1.27259300	-1.85796200	-5.15131600
H	3.10439800	-2.37299600	-4.14720500
H	-0.67802800	-1.28089200	-5.85064900
H	1.67552500	-2.01196200	-6.14667200
H	2.17368700	-1.99277600	-1.87208700
H	-1.58853400	-0.91032500	-3.58951400
H	3.68287500	0.69334500	0.47941100
H	3.73608600	2.12199300	2.44217800
N	-0.21936000	-1.19358300	-1.26384300
C	-2.29114900	-2.58022400	-1.62813600
H	-2.81206000	-3.28138500	-0.97417600
H	-3.05738300	-2.05344800	-2.20872500
H	-1.70445500	-3.16618900	-2.33755300
C	-0.03999500	1.94745100	-0.39878500
H	1.76945900	0.30507100	-1.03810700
C	1.11795200	1.77998300	-1.23798600
C	0.87011600	1.69818200	-2.72696600
C	2.37806000	2.55349100	-0.91491400
H	3.24888800	2.12567000	-1.42160400
H	-1.00811300	1.84765600	-0.90042500
H	2.27731500	3.58876400	-1.26282500
H	1.63703200	1.11963100	-3.25159500
H	-0.09654800	1.24539200	-2.95007600
H	0.86810000	2.71024400	-3.15050100
H	2.59224200	2.59061300	0.15410500
C	-0.08152700	2.78373100	0.84855700
H	0.91167000	2.86409800	1.30523300
H	-0.70147100	2.29081500	1.60448600
C	-0.63360600	4.20014500	0.62968200
H	-0.00761600	4.74277900	-0.08661100
H	-1.62286200	4.12246900	0.15677800
C	-0.73093000	4.99273400	1.90767200
C	-0.07637700	6.15466200	2.03670700
C	-1.55372300	4.43440600	3.00388000
C	-1.28875900	4.72591400	4.34372700
C	-2.62247100	3.57060600	2.71792000
C	-2.08313100	4.19170000	5.35203400
H	-0.44164800	5.35287300	4.59994400
C	-3.39938200	3.02907700	3.73479500
C	-3.14850600	3.34126600	5.08167900
H	-1.86038700	4.42673800	6.38983000
C	-3.99537900	2.74510600	6.15722800
H	-5.04748900	3.02259300	6.04031800
H	-3.96789300	1.65103300	6.12529900
H	-3.66381900	3.06879200	7.14562100
H	-0.15107100	6.76430200	2.93045300
H	0.54104100	6.54174100	1.23300000
O	-4.43366200	2.16728200	3.51971500

C	-4.69182000	1.79491000	2.18135700
H	-3.81321900	1.33219200	1.71377800
H	-5.49831200	1.06381900	2.21869100
H	-5.00955300	2.65484600	1.57885000
H	-2.84554900	3.32907900	1.68658600

Imaginary Frequency: -528.68

VIIIc

0 2

Fe	0.06621900	-0.47209700	0.25054200
N	-0.44582300	0.45006000	1.88725500
C	-0.29117500	1.86960200	2.25215300
C	-1.05095700	-0.13231900	2.89585000
C	-1.23843400	2.03859800	3.42225000
H	0.74599300	2.06453000	2.54957200
H	-0.85166500	2.66068300	4.22965200
N	-0.98153600	-2.11023000	0.74121300
C	-1.41965200	-2.45717700	1.98107700
C	-1.57228000	-4.31442500	-0.08557100
C	-1.92770300	-3.77152500	2.24283600
C	-1.98225900	-4.69291400	1.16033600
H	-1.60946600	-5.01272800	-0.91406400
H	-2.35970900	-5.69366100	1.34550300
C	-1.42633500	-1.50992300	3.05790600
C	-2.36185800	-4.12378700	3.52862600
C	-2.34252600	-3.20018400	4.56265800
H	-2.68176700	-3.47826200	5.55425000
C	-1.89759400	-1.91089100	4.32214900
H	-1.90284000	-1.17867200	5.11944100
H	-2.71821300	-5.13627800	3.69464000
O	-1.39753000	0.69813300	3.91686900
C	-1.06705200	-3.01550500	-0.29283000
C	-0.58751000	-2.54910600	-1.55226900
C	0.55461100	-0.75367300	-2.66725000
C	1.50096400	-1.40489500	-3.46697300
C	0.26259800	0.58969100	-2.93058600
C	2.13114700	-0.72708000	-4.50368600
C	0.89100400	1.26087900	-3.96901000
C	1.83072100	0.60614200	-4.76184300
H	2.87462700	-1.24215500	-5.10382000
H	0.65177700	2.30310900	-4.15615200
H	2.33031200	1.13354400	-5.56722200
H	1.77074300	-2.43158500	-3.24093700
H	-0.45754200	1.09758900	-2.29399200
H	-0.51466200	2.52263600	1.40531000
H	-2.22606000	2.41162600	3.12469600
N	-0.01083900	-1.34902400	-1.52544300
C	-0.78707000	-3.35515500	-2.79681200
H	-1.74717100	-3.87416000	-2.77602600
H	-0.76374200	-2.72089400	-3.68328300
H	-0.01148900	-4.11871300	-2.92713400

C	1.97396100	0.14379000	-0.06634100
H	2.34737000	-1.56737600	1.17038400
C	2.83607800	-0.59508100	0.97460400
C	4.22651600	-0.93413500	0.42969800
C	2.94950800	0.11061400	2.32109500
H	3.53893700	-0.48401000	3.02568500
H	2.26493200	-0.22096600	-1.05874300
H	3.44141200	1.08602800	2.23061000
H	4.79845300	-1.54631000	1.13577400
H	4.15670700	-1.48657500	-0.51205400
H	4.81104200	-0.02984500	0.23185400
H	1.96968500	0.27594300	2.77693100
C	2.01558500	1.65535300	-0.06115600
H	1.76676200	2.02300300	0.93415900
H	1.22447900	2.04596400	-0.72114100
C	3.31672400	2.37289200	-0.47353100
H	4.13741500	2.03677900	0.17352800
H	3.59407500	2.11595400	-1.50211200
C	3.11854700	3.85650400	-0.32448800
C	3.11041200	4.70048700	-1.36037500
C	2.77850300	4.30015600	1.05133400
C	3.57471000	3.95238700	2.14228400
C	1.57686300	4.98051000	1.28923400
C	3.18295800	4.29135700	3.43403700
H	4.50816900	3.42183300	1.98265700
C	1.18162300	5.28625500	2.58886100
C	1.98745100	4.95226900	3.69144400
H	3.81968900	4.02738600	4.27441200
C	1.54599100	5.30458600	5.07537500
H	2.27331400	4.97066500	5.81696500
H	1.41172900	6.38461300	5.18909500
H	0.57797900	4.85635800	5.31964100
H	2.92196200	5.76165600	-1.22959000
H	3.31521700	4.35549000	-2.36910000
O	-0.00178500	5.89065300	2.90482100
C	-0.85402900	6.24727900	1.83770800
H	-1.17994000	5.36810500	1.26712700
H	-1.72329200	6.72356000	2.28839500
H	-0.37157600	6.95222400	1.15067800
H	0.94205900	5.21567600	0.44216800

TS_{6c}

0 2

Fe	-0.42704200	-0.63247800	0.08440400
N	-1.08751400	0.12154500	1.76095500
C	-1.36271500	1.54284400	2.01499100
C	-1.66939800	-0.54177600	2.72037400
C	-1.69885800	1.55888300	3.49082900
H	-0.51452700	2.17357700	1.75839900
H	-0.81932900	1.74603200	4.11988900
N	-1.19673600	-2.41939300	0.52289400

C	-1.72372900	-2.84343100	1.70546200
C	-1.45547800	-4.66127000	-0.38321300
C	-2.11800700	-4.21144200	1.89117600
C	-1.97905900	-5.10507000	0.79343000
H	-1.32718700	-5.33769500	-1.22011600
H	-2.28725800	-6.13829500	0.91782500
C	-1.91006600	-1.95383000	2.81329200
C	-2.62676800	-4.64772300	3.12109700
C	-2.77602100	-3.77356200	4.18738500
H	-3.16887400	-4.12180000	5.13586400
C	-2.42824100	-2.44416000	4.02537200
H	-2.55930100	-1.74347200	4.84014000
H	-2.90590400	-5.69300500	3.21809500
O	-2.15458400	0.21611100	3.73849900
C	-1.03910700	-3.31988900	-0.51200400
C	-0.42927600	-2.81312800	-1.68983400
C	0.65588700	-0.95677400	-2.70936400
C	1.79084200	-1.54921900	-3.28009900
C	0.24389000	0.29301100	-3.19030900
C	2.49372400	-0.90954800	-4.29293700
C	0.94596400	0.92380400	-4.20798500
C	2.07705200	0.33159400	-4.76304000
H	3.37718500	-1.38214100	-4.71056600
H	0.60549900	1.88907800	-4.56932100
H	2.62811600	0.83213000	-5.55187900
H	2.13009700	-2.50943800	-2.90310800
H	-0.62761700	0.76721900	-2.75263100
H	-2.21106300	1.85296300	1.38923700
H	-2.49583200	2.24451300	3.77680400
N	-0.00436100	-1.54980900	-1.61180600
C	-0.40556900	-3.63194900	-2.94472600
H	-0.29254000	-3.00030200	-3.82570600
H	0.41203700	-4.36167600	-2.96310400
H	-1.33781000	-4.19084400	-3.05557400
C	1.27822900	0.44761100	-0.01341600
H	0.97562900	-1.43235000	1.03880500
C	1.78625600	-0.65266800	0.92335800
C	2.94588800	-1.43255000	0.30702800
C	2.09294400	-0.22168500	2.35227800
H	2.28223600	-1.09428900	2.98387800
H	1.69024600	0.28645100	-1.01227100
H	2.98799200	0.40641300	2.39156000
H	3.23769400	-2.28204300	0.93227100
H	2.67584100	-1.81270900	-0.68085100
H	3.82339000	-0.78902000	0.18613100
H	1.26888600	0.33693500	2.80102400
C	1.57801900	1.88766500	0.36283700
H	1.35558600	2.09267300	1.41335900
H	0.93706300	2.56192000	-0.22091500
C	3.03773500	2.27561800	0.09130700
H	3.70286600	1.67451300	0.72690500

H	3.29695800	2.01302200	-0.94091900
C	3.30224200	3.74276600	0.30702300
C	3.74206400	4.50945900	-0.69913300
C	3.03448600	4.30250100	1.65029100
C	3.18945000	3.53100400	2.80380200
C	2.60493800	5.63071800	1.79700300
C	2.94288100	4.07784800	4.05974700
H	3.52563800	2.50274700	2.72768700
C	2.36080200	6.16575000	3.05626400
C	2.52603600	5.39255900	4.22047800
H	3.08009400	3.46519700	4.94702300
C	2.24714300	5.99261800	5.55947800
H	2.41422500	5.26874300	6.35863500
H	2.88214700	6.86391200	5.74623600
H	1.21615200	6.35246600	5.63003000
H	3.96583500	5.56262000	-0.56654400
H	3.91572400	4.09422200	-1.68609100
Si	-2.48335500	0.04550800	-0.84289200
H	-2.54241600	1.42878700	-1.38810100
H	-3.50095100	0.02593000	0.24213600
H	-0.28194700	0.72500900	-0.50455700
C	-3.11994000	-1.09175500	-2.24097900
H	-4.11831000	-0.78390800	-2.56366100
H	-2.46051100	-1.05902000	-3.11240300
H	-3.18261300	-2.13078300	-1.90822500
O	1.93626300	7.44236500	3.27383500
C	1.75822200	8.27106900	2.14484000
H	0.98872100	7.87726600	1.47023300
H	1.43798500	9.23913800	2.52632200
H	2.69183500	8.39511200	1.58334800
H	2.43868800	6.22523100	0.90690400

Imaginary Frequency:-422.37

VIIIc

0 2

Fe	-0.39289400	-0.31356100	0.54001000
N	-0.12546600	0.31603800	2.31336500
C	0.55077800	1.55315600	2.71531400
C	-0.56289500	-0.26631300	3.40200100
C	0.03551600	1.77239200	4.12176100
H	1.63771100	1.39791400	2.68696100
H	0.77708700	2.13652200	4.83282300
N	-1.08822300	-2.06665000	1.15079600
C	-1.44237500	-2.41495800	2.41736300
C	-2.13405800	-4.08537200	0.29665100
C	-2.10923700	-3.65736700	2.67554300
C	-2.44174200	-4.48247500	1.56358200
H	-2.40781800	-4.69643500	-0.55586400
H	-2.95911000	-5.41895300	1.74672000
C	-1.18531800	-1.55142600	3.53424100
C	-2.44722400	-4.02363300	3.98439000

C	-2.16712000	-3.18660900	5.05523800
H	-2.43721900	-3.47644800	6.06441400
C	-1.55752400	-1.96550400	4.82673600
H	-1.35545000	-1.29496600	5.65238200
H	-2.95332400	-4.97195000	4.14023800
O	-0.37635700	0.45043900	4.53784200
C	-1.43603600	-2.87563500	0.08918000
C	-1.01849800	-2.41887900	-1.18721800
C	0.40397600	-0.86498300	-2.30411500
C	1.25778000	-1.80287000	-2.91434100
C	0.43966900	0.45990400	-2.76160300
C	2.08391400	-1.43767500	-3.96645300
C	1.26471400	0.81362700	-3.82117000
C	2.08764600	-0.12670700	-4.43471300
H	2.73866800	-2.17886100	-4.41403800
H	1.26034500	1.84003800	-4.17483500
H	2.73143700	0.16065500	-5.25891100
H	1.28322800	-2.81793900	-2.52998000
H	-0.18299600	1.20666100	-2.28129000
H	0.31201100	2.36527800	2.02929000
H	-0.84447900	2.42758700	4.14693100
N	-0.39325000	-1.23164200	-1.20707200
C	-1.36799400	-3.19044100	-2.42331300
H	-2.42522600	-3.47023000	-2.40285200
H	-1.19818500	-2.59706700	-3.32105400
H	-0.79612700	-4.11861800	-2.52740900
C	3.67568700	0.33686600	-0.74795200
H	4.54526400	-1.55473800	-0.32130100
C	3.93852100	-0.81871200	0.22535700
C	4.74839000	-0.36921400	1.43689600
C	2.65606200	-1.51416300	0.66520700
H	2.86457900	-2.40680400	1.26257100
H	4.63971200	0.80480900	-0.99362400
H	2.04362100	-0.85442300	1.29311400
H	4.99176800	-1.21320200	2.08841700
H	5.68909700	0.10453100	1.14127000
H	4.19370600	0.35326100	2.04607500
H	2.04597800	-1.82346800	-0.18933700
C	2.71841800	1.41637100	-0.25353800
H	2.90138600	1.64275600	0.80301100
H	1.67816200	1.05491100	-0.30306100
C	2.84080600	2.69923900	-1.07850900
H	3.81765100	3.15748000	-0.86348400
H	2.86924600	2.43784900	-2.14235700
C	1.74193000	3.70845000	-0.86716400
C	1.02555800	4.15356300	-1.90792600
C	1.48134300	4.18433400	0.50789500
C	2.48715000	4.19379100	1.47809800
C	0.19737400	4.61558400	0.88281600
C	2.21496000	4.62343100	2.77412900
H	3.49216000	3.87543100	1.22177100

C	-0.06430100	5.03553800	2.18210100
C	0.94893300	5.04615100	3.16053500
H	3.01156400	4.63131300	3.51414100
C	0.64065400	5.50093500	4.55007900
H	1.51358100	5.40796300	5.19881400
H	0.31469300	6.54555500	4.56355900
H	-0.18149200	4.92856700	4.99084100
H	0.24801600	4.90177200	-1.80117400
H	1.21390400	3.79155200	-2.91284400
Si	-1.85711000	1.47717300	-0.17596600
H	-1.34295700	2.63497900	-0.95969600
H	-2.48443900	2.10819000	1.02593500
H	3.28941500	-0.06219400	-1.69533200
C	-3.27476700	0.71719400	-1.22534800
H	-2.88331000	0.35264100	-2.17931100
H	-3.72132700	-0.13803500	-0.71138700
H	-4.07214000	1.43389600	-1.43975400
O	-1.28956700	5.42865400	2.62404300
C	-2.35161500	5.42760100	1.68583000
H	-2.53918100	4.42217800	1.29191800
H	-3.23016500	5.77462000	2.22692000
H	-2.14795300	6.10925500	0.85181100
H	-0.60349600	4.56288000	0.15628300

TS_{1a}

0 2

Fe	-0.24219700	0.14567100	-0.11030200
N	-0.06379200	-0.12013400	1.81202800
C	1.15293100	-0.06671400	2.62301000
C	-1.08717100	-0.10768400	2.62997700
C	0.64394600	0.24442900	4.02770800
H	1.67231800	-1.02937800	2.56014300
H	1.03827600	-0.40912300	4.80697300
N	-2.01572900	-0.61978500	-0.05460900
C	-2.89366600	-0.59289000	0.97803100
C	-3.72587400	-1.58164700	-1.48051200
C	-4.27225600	-0.93945000	0.78276300
C	-4.65994800	-1.41582500	-0.50475100
H	-4.00807700	-1.98222100	-2.44729700
H	-5.70040000	-1.67322100	-0.67482000
C	-2.47104600	-0.24082700	2.30100200
C	-5.17695600	-0.81347700	1.83925100
C	-4.76188000	-0.39386000	3.09950100
H	-5.48001100	-0.29844500	3.90636600
C	-3.42504300	-0.13363100	3.33149600
H	-3.08124300	0.13830800	4.32163900
H	-6.21880200	-1.06226100	1.65858000
O	-0.77675100	0.02530300	3.94387000
C	-2.38048700	-1.20299600	-1.25473600
C	-1.32014200	-1.37402000	-2.16722100
C	1.04018800	-1.11166700	-2.50885900

C	2.16378300	-1.70218200	-1.91876900
C	1.12818300	-0.68033400	-3.83797800
C	3.32679500	-1.89779700	-2.65168000
C	2.29799300	-0.86523300	-4.56301800
C	3.39817600	-1.48636300	-3.97932900
H	4.18244500	-2.37457100	-2.18330500
H	2.35729200	-0.50472500	-5.58581000
H	4.30897600	-1.63256500	-4.55067900
H	2.09151100	-2.01209200	-0.88048500
H	0.28144300	-0.17216900	-4.28808600
H	1.83432500	0.69453200	2.23462100
H	0.80993800	1.28587900	4.32237900
N	-0.11722500	-0.95139800	-1.71837700
C	-1.52685700	-2.06974800	-3.47624100
H	-0.62885700	-2.60852400	-3.78268200
H	-2.34006900	-2.79346000	-3.40649000
H	-1.77706900	-1.38106400	-4.29117200
C	-0.69971100	1.97869400	-0.68150200
H	1.23663000	0.58418400	-0.16524900
C	0.73430900	1.97567100	-0.57980000
C	1.54023700	2.06026000	-1.84905500
C	2.86024600	1.59774300	-1.88027900
C	1.04128700	2.69578300	-2.98615000
C	3.65448300	1.74560900	-3.00575200
H	3.26154800	1.08151000	-1.01141500
C	1.81795700	2.84559400	-4.13157300
H	0.03040700	3.09015800	-2.97685200
C	3.11252000	2.36200500	-4.12215400
H	4.66784700	1.36321300	-3.04412500
H	1.43261900	3.32980100	-5.02163100
C	1.39074500	2.81791100	0.52629100
H	2.30770200	2.31810400	0.86447200
C	0.52170300	3.19129500	1.71483900
H	1.12330300	3.65310200	2.50229400
H	-0.24925900	3.91283400	1.43455900
H	0.00862200	2.32990700	2.14562100
H	-1.30214600	2.46972200	0.07867500
H	-1.17344200	1.91513000	-1.65829100
H	1.74132400	3.74119000	0.04726100
F	3.86446200	2.47030600	-5.23624400

Imaginary Frequency: -613.87

IIa

0 2

Fe	0.01356200	-0.19014900	0.12832800
N	-0.11377900	-0.18354500	2.05023100
C	0.99058900	-0.22763100	3.01722100
C	-1.23016600	-0.15059000	2.73151000
C	0.32172400	0.19032700	4.31399700
H	1.39590000	-1.24587400	3.05730700
H	0.62345900	-0.37943200	5.19247200

N	-1.93809100	-0.58039200	-0.08258200
C	-2.90401700	-0.49455900	0.87299800
C	-3.63856500	-1.00900100	-1.76308000
C	-4.28871900	-0.65379500	0.53644600
C	-4.62129900	-0.92220600	-0.82016000
H	-3.88647000	-1.19587100	-2.80151400
H	-5.66598700	-1.04701500	-1.08670500
C	-2.57945600	-0.24509100	2.24794000
C	-5.27977800	-0.53831300	1.52092300
C	-4.94688500	-0.27593500	2.84100800
H	-5.71982600	-0.18286400	3.59546700
C	-3.61550500	-0.13625900	3.19411200
H	-3.34465400	0.05742500	4.22407800
H	-6.31787400	-0.65306100	1.22287900
O	-1.07603200	-0.06388200	4.07696400
C	-2.29221900	-0.82704900	-1.39141800
C	-1.21212000	-0.85075400	-2.32240100
C	1.12370400	-0.46692300	-2.64233300
C	2.26102600	-1.21552100	-2.32650400
C	1.18063800	0.43760400	-3.70716100
C	3.42246400	-1.07705300	-3.07249900
C	2.34993300	0.58028200	-4.44459500
C	3.47403700	-0.17793000	-4.13475600
H	4.29650100	-1.66785000	-2.81790000
H	2.38398000	1.29496900	-5.26082100
H	4.38624700	-0.06320200	-4.71020200
H	2.21994200	-1.89181100	-1.47758000
H	0.31052700	1.04789300	-3.93046100
H	1.80127500	0.44044700	2.72076000
H	0.44095000	1.26009700	4.52222800
N	-0.01466400	-0.56396200	-1.81545900
C	-1.44189700	-1.21322200	-3.75600900
H	-0.52016300	-1.55197300	-4.22859700
H	-2.18183500	-2.01103500	-3.84322300
H	-1.81262300	-0.36515900	-4.34270200
C	1.68397500	0.92618400	0.08902800
H	0.87970000	2.16722400	1.67627000
C	1.54561900	2.27664000	0.80350900
C	2.86143300	2.80331100	1.33598600
C	2.96870500	3.28494800	2.64210600
C	4.00552800	2.83651100	0.53130500
C	4.16866600	3.78153200	3.14356000
H	2.08834300	3.27723200	3.28162900
C	5.21163500	3.33283900	1.00757200
H	3.94965900	2.45555900	-0.48494800
C	5.27371700	3.79731400	2.31196600
H	4.25650500	4.15309600	4.15819000
H	6.10166500	3.36161900	0.38913300
C	0.88520500	3.32806900	-0.10285900
H	0.84099600	4.28150500	0.43852800
C	-0.50577400	2.94365100	-0.57861800

H	-0.99935600	3.77451100	-1.09040100
H	-0.47705300	2.09798800	-1.27221400
H	-1.14748700	2.65092900	0.26222400
H	2.06768500	1.09016700	-0.92546100
H	2.43167700	0.29441800	0.59683700
H	1.53916500	3.50544600	-0.96818100
F	6.44440500	4.27357800	2.78340400

IIIa

0 2

Fe	0.16445700	0.52586700	0.08004500
N	0.27813900	0.45084600	1.99583200
C	1.49385800	0.35834600	2.81013700
C	-0.74465800	0.45252200	2.81228100
C	0.96297200	-0.08371100	4.16264700
H	2.19805800	-0.35159900	2.37200500
H	1.01995000	-1.17055900	4.29943500
N	-1.77909000	0.99573400	0.12159900
C	-2.62204400	0.89945700	1.18564900
C	-3.66917600	1.41667300	-1.34169600
C	-4.03701600	1.05515600	1.01783900
C	-4.53061900	1.32332300	-0.28780000
H	-4.04228100	1.59416300	-2.34371000
H	-5.60129300	1.43072700	-0.42885800
C	-2.13594400	0.62063300	2.50675400
C	-4.90488400	0.92154600	2.11146900
C	-4.41609500	0.64605400	3.37927600
H	-5.09334900	0.54205600	4.21958600
C	-3.05189600	0.50059000	3.56872800
H	-2.66116700	0.28469400	4.55496100
H	-5.97162900	1.03020200	1.93898200
O	-0.42608900	0.28814100	4.12412400
C	-2.28684700	1.24352500	-1.13330200
C	-1.33034500	1.25680000	-2.19150000
C	0.94585500	0.81539100	-2.78835800
C	0.81454600	0.02303700	-3.93504100
C	2.18285400	1.41300600	-2.52205300
C	1.88954100	-0.14908300	-4.79940100
C	3.24833500	1.24786400	-3.39334800
C	3.10856600	0.46597000	-4.53803200
H	1.77386500	-0.77620900	-5.67777000
H	4.19840200	1.72459600	-3.17425100
H	3.94648500	0.32892800	-5.21286900
H	-0.12859400	-0.47932200	-4.12853000
H	2.29095000	1.99670000	-1.61203600
H	1.98703800	1.33749300	2.84659200
H	1.42129600	0.40771000	5.02065300
N	-0.08474300	0.94067200	-1.83944800
C	-1.74046600	1.64623700	-3.57705600
H	-0.88384400	1.96623000	-4.16967000
H	-2.21722800	0.81851000	-4.11575300

H	-2.46091300	2.46624600	-3.55139200
C	1.56099200	-0.89881000	-0.22402400
H	1.77900600	-1.05440900	-1.28887100
H	2.51988800	-0.64762400	0.25398900
C	0.97179400	-2.18337900	0.37656000
H	1.02842400	-2.12467000	1.47602200
C	1.73884800	-3.44429900	-0.05053700
H	1.68063200	-3.53322200	-1.14372800
H	2.80142900	-3.29173400	0.17589200
C	1.23887700	-4.72045400	0.60438100
H	1.82624100	-5.59124300	0.30223500
H	1.29115100	-4.65239500	1.69648700
H	0.19504400	-4.91985700	0.34418300
C	-0.50376000	-2.27944400	0.03087100
C	-1.48539200	-2.41186700	1.01294000
C	-0.92044000	-2.16576000	-1.30188800
C	-2.84167700	-2.40559900	0.69553700
H	-1.18464700	-2.49599200	2.05567800
C	-2.26518200	-2.15618000	-1.64253600
H	-0.17160200	-2.04706800	-2.08139200
C	-3.20815100	-2.26719900	-0.63042100
H	-3.60771900	-2.47984400	1.45953900
H	-2.59559800	-2.04728000	-2.67062900
F	-4.51789000	-2.22962800	-0.95116500

TS_{2a}

0 2

Fe	0.06807700	0.13460100	-0.06893300
N	0.14366300	0.12279200	1.86830900
C	1.37188700	0.20658100	2.66428100
C	-0.85692700	0.27239900	2.68684500
C	0.87261800	-0.00224400	4.08205200
H	2.09810400	-0.54381100	2.34828100
H	0.95416800	-1.04704500	4.40587900
N	-1.87221800	0.49213800	-0.05043700
C	-2.72226500	0.52228100	1.01922600
C	-3.76869900	0.81376100	-1.54265300
C	-4.13629100	0.66807900	0.83443700
C	-4.63215000	0.81780300	-0.48894900
H	-4.13498700	0.91360800	-2.55766900
H	-5.70170800	0.92455500	-0.63798500
C	-2.25064300	0.39710200	2.36503400
C	-5.00626000	0.65854000	1.93479000
C	-4.52749800	0.52404400	3.22735300
H	-5.20813000	0.51954800	4.07110000
C	-3.16298400	0.40238000	3.43339400
H	-2.77004300	0.30616300	4.43760900
H	-6.07082000	0.76294200	1.74605000
O	-0.52609100	0.33092000	4.00271100
C	-2.38791700	0.63745300	-1.32325800
C	-1.44324300	0.55234000	-2.37934500

C	0.80957700	0.05947800	-2.95741600
C	0.65709100	-0.91344200	-3.95406900
C	2.01630500	0.76406000	-2.88944900
C	1.68482600	-1.17831600	-4.85051300
C	3.03539800	0.50277000	-3.79477900
C	2.88041700	-0.47197400	-4.77622500
H	1.54944800	-1.94348900	-5.60837500
H	3.96081400	1.06621000	-3.73068300
H	3.68314100	-0.67856300	-5.47576500
H	-0.27481100	-1.46840900	-4.01181300
H	2.14578900	1.52163600	-2.12487700
H	1.83130500	1.19328400	2.51352400
H	1.33110000	0.64062600	4.83315700
N	-0.19964100	0.26600000	-1.99101200
C	-1.84352200	0.83221900	-3.79461100
H	-0.98156800	1.10441600	-4.40343500
H	-2.32043200	-0.03020600	-4.27658400
H	-2.55703700	1.65770000	-3.83959400
C	1.60787500	-1.20852900	-0.18238000
H	1.79538500	-1.42798300	-1.23972800
H	2.59623000	-1.03820600	0.26369800
C	0.97262400	-2.43230200	0.50470900
H	1.03555900	-2.29898200	1.59464800
C	1.74535000	-3.71580700	0.15729200
H	1.68367400	-3.88011600	-0.92661100
H	2.80802600	-3.54743000	0.37162000
C	1.24839100	-4.94341900	0.90095200
H	1.83859500	-5.83008400	0.65725900
H	1.30320800	-4.79974400	1.98527600
H	0.20524400	-5.16378100	0.65659500
C	-0.50097000	-2.56091300	0.17119100
C	-1.47678800	-2.66453600	1.16521400
C	-0.91675100	-2.58862700	-1.16481500
C	-2.82834000	-2.74582800	0.84912300
H	-1.17349400	-2.65429900	2.20990100
C	-2.25967700	-2.66777000	-1.50473000
H	-0.16847000	-2.52453700	-1.95005200
C	-3.19730300	-2.73015900	-0.48472000
H	-3.59329400	-2.79238200	1.61632200
H	-2.59175800	-2.66533500	-2.53771900
Si	0.62052100	2.41510200	0.00160800
H	1.50454500	0.48570700	-0.16858800
H	0.13526000	3.05537300	-1.24495200
C	-0.25178400	3.26639400	1.47484800
H	0.15055300	2.94185600	2.43827100
H	-0.12778500	4.35143900	1.41803500
H	-1.32292500	3.05112400	1.47652700
H	2.05426200	2.79394600	0.10331200
F	-4.50551600	-2.77547000	-0.80289700

Imaginary Frequency; -471.31

IVa

0 2

Fe	-0.41693200	0.92933300	-0.22121700
N	-0.68550700	0.16069000	1.51519200
C	0.29048100	0.05136700	2.60691500
C	-1.80392900	-0.37536400	1.92909500
C	-0.56962600	-0.30661000	3.80888900
H	1.01525100	-0.73131000	2.35535800
H	-0.17979900	-1.11846200	4.42289600
N	-2.08660200	0.10116200	-0.95093300
C	-3.07369600	-0.51421200	-0.24959400
C	-3.30992800	-0.26117700	-3.01272200
C	-4.24030800	-1.01911300	-0.91321900
C	-4.31812400	-0.87547900	-2.32690500
H	-3.37218800	-0.13651200	-4.08762600
H	-5.19505100	-1.25459000	-2.84212100
C	-2.98574900	-0.68896600	1.17051600
C	-5.27005600	-1.62376200	-0.17977900
C	-5.18428900	-1.74886800	1.19887900
H	-5.99081800	-2.20591000	1.76096500
C	-4.05607400	-1.28859300	1.85801800
H	-3.97151700	-1.40054500	2.93182200
H	-6.14438500	-1.98178800	-0.71559400
O	-1.81091500	-0.75625800	3.22717600
C	-2.18954300	0.23412800	-2.31666400
C	-1.09105200	0.88720000	-2.95039200
C	0.98103300	2.03806100	-2.62423100
C	2.25236700	1.63065200	-2.20760900
C	0.86460700	3.16141900	-3.44718100
C	3.38189300	2.32245900	-2.61876200
C	1.99886200	3.85731000	-3.84728100
C	3.26119200	3.44044900	-3.44037400
H	4.36147300	1.99407100	-2.28695100
H	1.89229900	4.73897200	-4.47119300
H	4.14405600	3.98939100	-3.74944600
H	2.33371300	0.77470500	-1.54247100
H	-0.12253200	3.50712500	-3.73674100
H	0.83985900	0.98573500	2.73406200
H	-0.79205500	0.55549900	4.44654300
N	-0.14767900	1.34896500	-2.13005800
C	-1.00434400	0.95032100	-4.44287000
H	0.02482600	1.09240700	-4.77197700
H	-1.37913200	0.02701500	-4.88973600
H	-1.59373500	1.77358400	-4.86169200
C	0.17335500	-2.24547600	-2.15543000
H	-0.91473200	-2.36139400	-2.20817700
H	0.54391400	-2.16323900	-3.18234400
C	0.82307100	-3.41503100	-1.42492000
H	1.91391500	-3.28222100	-1.46832100
C	0.49522400	-4.74351200	-2.12170800
H	-0.59306500	-4.89206100	-2.09938500

H	0.76046900	-4.65120700	-3.18222800
C	1.19491100	-5.94571600	-1.51423000
H	0.97225800	-6.86249500	-2.06465600
H	2.28211700	-5.81579500	-1.51877000
H	0.89201600	-6.10288400	-0.47510200
C	0.44226900	-3.45192400	0.03832700
C	1.42147100	-3.51750300	1.03077100
C	-0.89869400	-3.46750700	0.43686500
C	1.08891400	-3.59375100	2.38036200
H	2.46914100	-3.51414300	0.74087200
C	-1.25421100	-3.54855800	1.77693800
H	-1.68857800	-3.41191800	-0.30890900
C	-0.24984500	-3.60748300	2.72827600
H	1.84690900	-3.64523000	3.15411400
H	-2.29135100	-3.54707400	2.09247100
Si	0.81190700	2.84850200	0.62569800
H	0.37072600	-1.29633100	-1.64790300
H	1.10430200	3.94366600	-0.33280200
C	-0.12331400	3.66116300	2.10447200
H	-0.37170600	2.93497000	2.88409300
H	0.46296200	4.45837000	2.56986100
H	-1.06647000	4.09949300	1.76944200
H	2.14754600	2.45357200	1.16884900
F	-0.58756700	-3.66259900	4.03459500

TS_{1b}

0 2

Fe	-0.23549600	0.15862300	-0.10460000
N	-0.05609500	-0.14220100	1.81028000
C	1.16138700	-0.09591200	2.62036700
C	-1.07853700	-0.15668300	2.63009400
C	0.65213400	0.18482600	4.03115400
H	1.68699100	-1.05387300	2.53876300
H	1.05608100	-0.47729700	4.79830300
N	-2.00756100	-0.61563100	-0.06327000
C	-2.88369000	-0.61897400	0.97065500
C	-3.71537100	-1.55013700	-1.51045600
C	-4.26090500	-0.96973700	0.77002200
C	-4.64823800	-1.41567900	-0.52870800
H	-3.99787700	-1.92685300	-2.48677600
H	-5.68749800	-1.67522400	-0.70318000
C	-2.46107200	-0.29475500	2.30119300
C	-5.16393500	-0.87613000	1.83084400
C	-4.74910700	-0.48398300	3.10059400
H	-5.46641200	-0.41333700	3.91084500
C	-3.41431600	-0.21882700	3.33604900
H	-3.07044300	0.03332600	4.33140900
H	-6.20448500	-1.12770000	1.64619500
O	-0.76575900	-0.04924500	3.94678700
C	-2.37140600	-1.17035500	-1.27786700
C	-1.31189800	-1.31283600	-2.19524700

C	1.04712700	-1.03462000	-2.53405600
C	2.17255800	-1.63992000	-1.96269000
C	1.13128200	-0.56976500	-3.85192800
C	3.33175300	-1.82081300	-2.70505800
C	2.29732200	-0.73913600	-4.58615900
C	3.39792700	-1.37820500	-4.02292700
H	4.18833100	-2.31041000	-2.25172900
H	2.35377200	-0.34964700	-5.59858400
H	4.30471300	-1.51818100	-4.60306200
H	2.10427000	-1.97387800	-0.93166300
H	0.28559700	-0.04521000	-4.28442700
H	1.83694600	0.67693600	2.24520200
H	0.80731700	1.22309100	4.34294400
N	-0.10902600	-0.89760600	-1.73749700
C	-1.51758500	-1.97429300	-3.52225400
H	-2.33205200	-2.69828100	-3.47267700
H	-1.76476900	-1.26435000	-4.31974500
H	-0.61968500	-2.50628700	-3.84092300
C	-0.70449100	2.00061600	-0.63686200
H	1.24005200	0.60279900	-0.15224800
C	0.72918800	2.01162100	-0.54192300
C	1.52765000	2.12199300	-1.80966400
C	2.85484400	1.68657500	-1.86050500
C	1.03172100	2.76441100	-2.94252800
C	3.64244900	1.85464200	-2.98359100
H	3.27614600	1.17285700	-0.99848400
C	1.80166200	2.93662600	-4.08588300
H	0.01922900	3.15723300	-2.93183000
C	3.12312500	2.46215400	-4.14349000
H	4.65685500	1.47562200	-2.97199100
H	1.36541900	3.44495600	-4.93724900
C	1.38033600	2.82730800	0.58602600
H	2.29962000	2.32369700	0.91186200
C	0.51028200	3.16953600	1.78357000
H	1.10984800	3.61435300	2.58255800
H	-0.26302900	3.89513300	1.52020000
H	-0.00104000	2.29703300	2.19374200
C	5.28916700	2.26713000	-5.24844600
H	5.83906200	2.92910400	-4.56140900
H	5.46990300	1.23526100	-4.92984500
H	5.71625500	2.38127700	-6.24455700
H	-1.31047200	2.46779600	0.13577200
H	-1.17988100	1.95395200	-1.61390000
H	1.72737900	3.76268200	0.12858500
N	3.87525400	2.55230700	-5.30466600
C	3.39171000	3.37395800	-6.38769500
H	3.26620400	4.43171600	-6.10822500
H	4.09572200	3.32271300	-7.21794000
H	2.42509900	3.01244000	-6.75429800

Imaginary Frequency: -597.69

Иб

0 2

Fe	0.02072100	-0.22351900	0.10891800
N	-0.08104900	-0.21740300	2.03316900
C	1.03673500	-0.27026300	2.98470400
C	-1.18669400	-0.15517800	2.72874600
C	0.39275800	0.16474200	4.28850700
H	1.42913300	-1.29356100	3.02452000
H	0.69523100	-0.40769200	5.16512200
N	-1.94430400	-0.56542400	-0.07581900
C	-2.89472800	-0.45923600	0.89303600
C	-3.67699900	-0.94705500	-1.73416500
C	-4.28732400	-0.58442500	0.57533600
C	-4.64450600	-0.83987300	-0.77766200
H	-3.94372600	-1.12385300	-2.76972900
H	-5.69549600	-0.93815800	-1.03042200
C	-2.54492200	-0.22054800	2.26379600
C	-5.26179400	-0.44884500	1.57383800
C	-4.90417000	-0.19827800	2.88968500
H	-5.66399600	-0.08929900	3.65534800
C	-3.56487400	-0.09018200	3.22430000
H	-3.27508800	0.09505100	4.25068600
H	-6.30639900	-0.53816700	1.28999500
O	-1.01321600	-0.06312100	4.07173400
C	-2.32152300	-0.79944000	-1.38022300
C	-1.25485600	-0.84870200	-2.32563300
C	1.08547500	-0.52382200	-2.67630700
C	2.21248400	-1.29129600	-2.36818400
C	1.14600700	0.36817100	-3.75167300
C	3.36515000	-1.18529900	-3.13260900
C	2.30683700	0.47844200	-4.50762100
C	3.41934200	-0.29989500	-4.20626300
H	4.23074000	-1.79071200	-2.88335900
H	2.34373500	1.18402700	-5.33165100
H	4.32512300	-0.21040800	-4.79622800
H	2.17025600	-1.95627800	-1.51041100
H	0.28598200	0.99477900	-3.96840400
H	1.85098400	0.38690600	2.67320000
H	0.53624900	1.23256600	4.49024700
N	-0.04341900	-0.59253200	-1.83473400
C	-1.51401500	-1.20614700	-3.75569100
H	-0.60866300	-1.57122100	-4.24026400
H	-2.27691700	-1.98329700	-3.83141700
H	-1.86891800	-0.34913300	-4.33926200
C	1.70759500	0.86179100	0.05360900
H	0.88537100	2.10762700	1.62711300
C	1.58745600	2.20790000	0.78129100
C	2.89341700	2.69053600	1.37511900
C	2.95397100	3.21632000	2.66555500
C	4.08920900	2.65954600	0.65341800
C	4.13764600	3.68185000	3.22434500

H	2.03809400	3.27771400	3.25200400
C	5.28155400	3.12341400	1.18712100
H	4.08650000	2.25771800	-0.35711200
C	5.34055400	3.63409200	2.49833000
H	4.12108000	4.08440500	4.22987900
H	6.17678600	3.08352500	0.57843100
C	0.98255900	3.28369600	-0.13494000
H	0.94014000	4.23135900	0.41667500
C	-0.39957800	2.93356400	-0.66139700
H	-0.85841900	3.77722900	-1.18489900
H	-0.36555000	2.09013200	-1.35759200
H	-1.07533000	2.64944900	0.15582100
C	6.50056300	4.82697000	4.27677400
H	5.92711400	5.76326600	4.18265400
H	6.05669500	4.24784500	5.09228900
H	7.51830000	5.07908900	4.57465900
H	2.08568800	1.02573100	-0.96328000
H	2.44818300	0.21473800	0.55228300
H	1.66993000	3.45648600	-0.97487900
N	6.54211700	4.05676700	3.05660500
C	7.67281800	4.26646900	2.18327300
H	7.96652500	3.33559800	1.68904800
H	7.48421100	5.01590400	1.39798500
H	8.52383200	4.60119400	2.77642500

IIIb

0 2

Fe	0.24348000	-0.10919300	-0.12771600
N	0.10377200	-0.03480400	1.80305600
C	1.16649700	0.25808200	2.76980200
C	-1.01539400	-0.14892700	2.47800100
C	0.53912200	-0.13905400	4.09192700
H	2.07140300	-0.30400900	2.53758600
H	0.78516000	-1.16983800	4.37716300
N	-1.74965000	-0.05250800	-0.35542200
C	-2.68810000	-0.29274900	0.59519600
C	-3.45572200	-0.18194200	-2.07655200
C	-4.06146200	-0.50844300	0.23914200
C	-4.40999000	-0.44774200	-1.13751200
H	-3.71454100	-0.14420600	-3.12872400
H	-5.44423500	-0.61932300	-1.42242800
C	-2.34540200	-0.34818300	1.98994600
C	-5.02228400	-0.77433400	1.22470100
C	-4.66995600	-0.82708400	2.56798800
H	-5.41906000	-1.03165300	3.32494900
C	-3.35527100	-0.61214100	2.93822800
H	-3.07269200	-0.64899500	3.98258400
H	-6.05071000	-0.93530800	0.91275500
O	-0.87341300	-0.07249000	3.82961400
C	-2.11625100	0.00098900	-1.68163000
C	-1.05270600	0.20408700	-2.61177300

C	1.31895800	0.35500500	-2.88845800
C	1.57547600	-0.49819200	-3.96786600
C	2.28779300	1.29858200	-2.52939600
C	2.76585800	-0.39564400	-4.67824100
C	3.46810600	1.40465100	-3.24894200
C	3.71458700	0.55852700	-4.32773800
H	2.95468900	-1.07222200	-5.50579100
H	4.20666500	2.14560700	-2.96020200
H	4.64326400	0.63563200	-4.88273800
H	0.84548000	-1.25945900	-4.22697700
H	2.09939300	1.93278300	-1.66811100
H	1.41886700	1.32516300	2.72504600
H	0.75986000	0.52450000	4.92792600
N	0.16842000	0.22739000	-2.08878900
C	-1.34597300	0.41420800	-4.06476000
H	-0.52145700	0.92097800	-4.56574500
H	-1.51247400	-0.53208500	-4.59379800
H	-2.24565400	1.01810000	-4.19722900
C	2.12130100	-0.89320900	-0.04134300
H	2.53985000	-0.97864800	-1.05416200
H	2.86258800	-0.34466100	0.55481100
C	1.86320200	-2.29817100	0.52435800
H	1.76721500	-2.23219600	1.62058300
C	2.99373000	-3.29233000	0.22588000
H	3.09670400	-3.38688700	-0.86374600
H	3.93870400	-2.85552100	0.57280900
C	2.78514600	-4.66160700	0.84984100
H	3.61572700	-5.34003500	0.63780300
H	2.68948400	-4.59014900	1.93882700
H	1.86997300	-5.13178100	0.47729500
C	0.51608700	-2.78608100	0.01644000
C	-0.53339800	-3.12719900	0.87400800
C	0.24995100	-2.84731500	-1.35742500
C	-1.79542500	-3.45963200	0.40549700
H	-0.36254500	-3.10279200	1.94933500
C	-1.00229700	-3.17569900	-1.85182500
H	1.04422900	-2.59990100	-2.05921300
C	-2.07134000	-3.45733900	-0.97597400
H	-2.58055500	-3.68114900	1.11912200
H	-1.15677100	-3.19332800	-2.92514200
C	-3.58605100	-3.71141600	-2.87051900
H	-3.04880000	-4.51720500	-3.39246600
H	-4.65238500	-3.84442000	-3.05157200
H	-3.28637700	-2.76058900	-3.33149800
N	-3.34260300	-3.70245200	-1.45221900
C	-4.39327900	-4.08772700	-0.54229700
H	-5.31932000	-4.21907400	-1.10157100
H	-4.17423100	-5.03182800	-0.02333000
H	-4.56959600	-3.31969700	0.22155400

0 2

Fe	0.23044500	-0.28061100	-0.21039100
N	0.09292200	-0.21482200	1.72197100
C	1.19269100	0.11348500	2.63353700
C	-1.00174000	-0.21886500	2.42563500
C	0.58735700	-0.14455400	4.00051200
H	2.07136200	-0.49929400	2.42779900
H	0.81179700	-1.15151800	4.37351500
N	-1.73985400	-0.25606900	-0.40578900
C	-2.69159100	-0.34677700	0.56794200
C	-3.48843600	-0.30954800	-2.09660600
C	-4.08260100	-0.45436100	0.23490700
C	-4.44964500	-0.43441100	-1.13792500
H	-3.75494600	-0.29362600	-3.14734000
H	-5.50030900	-0.51867500	-1.40051700
C	-2.35295700	-0.34852400	1.96010100
C	-5.05197100	-0.57977000	1.24153800
C	-4.69825400	-0.59297400	2.58161100
H	-5.45505100	-0.68816800	3.35213300
C	-3.36291100	-0.47136400	2.92917100
H	-3.06902100	-0.47011600	3.97116100
H	-6.09343200	-0.66176700	0.94163700
O	-0.83048900	-0.06190600	3.76541100
C	-2.13023700	-0.23869700	-1.72967700
C	-1.07627400	-0.19163100	-2.68175500
C	1.27424700	-0.30349200	-3.01398200
C	1.40192700	-1.31923900	-3.97030700
C	2.32297900	0.61056100	-2.86494400
C	2.54789800	-1.42047000	-4.74921600
C	3.46050800	0.51121900	-3.65383200
C	3.58412600	-0.50578300	-4.59607400
H	2.63093100	-2.22181600	-5.47672600
H	4.25931600	1.23527400	-3.52855200
H	4.47915700	-0.58494900	-5.20364900
H	0.59552400	-2.03735700	-4.08735600
H	2.23621400	1.40230900	-2.12943100
H	1.48151500	1.16369400	2.48521200
H	0.84639000	0.58596800	4.76672400
N	0.14892100	-0.24901600	-2.16339500
C	-1.37057800	-0.03793400	-4.14191900
H	-0.50449100	0.34132400	-4.68366400
H	-1.65708200	-0.98651700	-4.61386300
H	-2.19517300	0.66045900	-4.30065200
C	1.99966500	-1.30135600	-0.10021900
H	2.33960200	-1.50889400	-1.12156400
H	2.87724400	-0.91717900	0.43518900
C	1.52548100	-2.59952700	0.57262700
H	1.45502000	-2.43149100	1.65800500
C	2.53282600	-3.74009000	0.35366600
H	2.61023000	-3.93672100	-0.72397500
H	3.52630500	-3.39173800	0.66357100

C	2.17003900	-5.01712300	1.09161700
H	2.91507400	-5.80143500	0.93607800
H	2.09480500	-4.84403300	2.17055400
H	1.20357700	-5.40726400	0.75944000
C	0.13219400	-2.97589800	0.10729300
C	-0.91465500	-3.22532500	0.99857600
C	-0.14730900	-3.12983400	-1.25512900
C	-2.19228800	-3.53844300	0.56469200
H	-0.72809600	-3.14280700	2.06813200
C	-1.41422200	-3.44137000	-1.71604300
H	0.65487700	-2.98170400	-1.97394400
C	-2.48367900	-3.61505700	-0.81223500
H	-2.97752100	-3.68213500	1.29778300
H	-1.58108900	-3.53166700	-2.78357600
C	-4.03776800	-3.87740000	-2.67349100
H	-3.54554000	-4.72152300	-3.17720000
H	-5.11155300	-3.97226000	-2.83167800
H	-3.70561200	-2.95486000	-3.16917100
Si	0.34560600	2.06377200	-0.19993000
H	1.55210600	0.38578000	-0.18611000
H	-0.12667700	2.55370700	-1.51766000
C	-0.80730300	2.78649000	1.14310300
H	-0.44779200	2.57670600	2.15402000
H	-0.87818500	3.87294600	1.04024700
H	-1.81562900	2.37437300	1.06048600
H	1.66327800	2.72016300	0.00697300
N	-3.76683600	-3.84011600	-1.25963000
C	-4.83362400	-4.06692300	-0.31547500
H	-4.95676200	-3.22008100	0.37230400
H	-5.76934700	-4.19767300	-0.85802700
H	-4.66720800	-4.96768100	0.29115500

Imaginary Frequency; -328.69

IVb

0 2

Fe	-0.08106900	0.08783200	-0.07542000
N	-0.00398500	-0.11329700	1.82132900
C	1.19459800	-0.08490500	2.66665700
C	-1.03655000	-0.31798300	2.59194200
C	0.63020100	-0.02200200	4.08039500
H	1.77587000	-0.99643900	2.48619300
H	1.05833900	-0.75657600	4.76459800
N	-1.93853400	-0.58857300	-0.18633400
C	-2.81107200	-0.74717200	0.84672800
C	-3.72625800	-1.01212100	-1.77191000
C	-4.18412200	-1.07698800	0.60089200
C	-4.60899600	-1.21038500	-0.75138500
H	-4.04894200	-1.09489300	-2.80332800
H	-5.64715800	-1.45755000	-0.94919600
C	-2.39686800	-0.58651900	2.21002500
C	-5.07872800	-1.23736000	1.66740000

C	-4.66167200	-1.07256400	2.97955200
H	-5.36354900	-1.18601800	3.79807900
C	-3.34066000	-0.74858200	3.24079100
H	-3.00891000	-0.60294500	4.26148800
H	-6.11363900	-1.47668100	1.44085900
O	-0.76770100	-0.34444500	3.91814500
C	-2.37962600	-0.70385700	-1.48729100
C	-1.38688200	-0.50676000	-2.48515300
C	0.94970000	-0.25467200	-2.88925000
C	1.16031100	-1.39862400	-3.67455200
C	1.92269900	0.75160700	-2.90630200
C	2.30777000	-1.53258800	-4.44324400
C	3.06527800	0.61462500	-3.68236400
C	3.27013100	-0.52744000	-4.45121600
H	2.45552300	-2.43470700	-5.02917500
H	3.80220700	1.41136500	-3.68550700
H	4.16907400	-0.63383400	-5.04893300
H	0.42919000	-2.20015800	-3.64509800
H	1.76134200	1.64936500	-2.32448600
H	1.82320500	0.77291100	2.41268000
H	0.69135300	0.97513000	4.52830900
N	-0.17246700	-0.16095500	-2.03890600
C	-1.74195000	-0.60677800	-3.93712500
H	-0.96607700	-0.17147100	-4.56548100
H	-1.89169000	-1.64033800	-4.26695700
H	-2.67441600	-0.07228000	-4.13606400
C	2.89314600	-1.87072400	-0.31675700
H	2.05635300	-1.15783500	-0.27869200
H	3.35686400	-1.76889800	-1.30336300
C	2.39959200	-3.29727000	-0.06523900
H	3.27902300	-3.95979000	-0.08527100
C	1.46554000	-3.74418600	-1.18933300
H	0.60128900	-3.06258500	-1.23078900
H	1.98971100	-3.59239800	-2.13977200
C	1.00362500	-5.18695200	-1.08475600
H	0.36851200	-5.46897200	-1.92835400
H	1.85787200	-5.87133500	-1.07484600
H	0.43584700	-5.36875200	-0.16861700
C	1.79288600	-3.40774100	1.31716900
C	2.61285000	-3.58457700	2.43404200
C	0.42450700	-3.27633100	1.55902000
C	2.11307900	-3.59354600	3.72832800
H	3.68320100	-3.71473800	2.28631900
C	-0.10130000	-3.30104400	2.84356800
H	-0.26497000	-3.14160300	0.72881800
C	0.73483300	-3.42562500	3.96744900
H	2.79876800	-3.73906500	4.55423800
H	-1.17331100	-3.20387500	2.96759900
C	-1.20431100	-3.43481800	5.44695500
H	-1.63476500	-4.38514800	5.09498700
H	-1.42758700	-3.33128200	6.50881600

H	-1.70845900	-2.61867700	4.92263000
Si	0.98016900	2.26485200	0.08921700
H	3.61756400	-1.55191600	0.43862600
H	0.87827800	3.19802800	-1.06249100
C	0.18381100	3.18854800	1.58142000
H	0.38787100	2.67625500	2.52570600
H	0.55614800	4.21236300	1.67390900
H	-0.90296900	3.23864400	1.47454400
H	2.44340100	2.20270900	0.38329500
N	0.22759700	-3.35417800	5.25774900
C	1.06959300	-3.76593800	6.35676500
H	1.96404300	-3.13763600	6.42438900
H	0.51946200	-3.64923400	7.29013600
H	1.40315600	-4.81265800	6.28209100

TS_{1c}

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Fe	-0.03438000	0.02168800	0.00568800
N	-0.02722000	0.01233100	1.95407700
C	1.12449900	0.10459700	2.85189500
C	-1.10699100	0.19609500	2.67319200
C	0.53226300	0.63310800	4.15529700
H	1.57943000	-0.88622700	2.95991500
H	0.81968600	0.06970200	5.04409800
N	-1.86040900	-0.61946900	0.00975700
C	-2.81083300	-0.40099400	0.95127900
C	-3.52014000	-1.66580000	-1.41730100
C	-4.19152000	-0.68954300	0.68699500
C	-4.51229300	-1.31391700	-0.55490300
H	-3.75441800	-2.17797600	-2.34337000
H	-5.55208300	-1.53124100	-0.77707400
C	-2.46723100	0.10188300	2.24814600
C	-5.16307300	-0.36839600	1.63726800
C	-4.81727000	0.19348800	2.86281000
H	-5.58660400	0.43921200	3.58644800
C	-3.48737100	0.40392800	3.17137100
H	-3.20160900	0.78699000	4.14306500
H	-6.20281100	-0.57837700	1.40298800
O	-0.88944900	0.48806700	3.98035800
C	-2.17307300	-1.33893300	-1.12980000
C	-1.06152000	-1.69289000	-1.91940600
C	1.32601400	-1.60968100	-2.10601900
C	2.36045200	-2.20638400	-1.37652800
C	1.53309000	-1.33045600	-3.46181900
C	3.55310700	-2.55371900	-1.99700500
C	2.73168100	-1.66773300	-4.07504200
C	3.74301800	-2.29176900	-3.35067300
H	4.33926800	-3.03092500	-1.41993500
H	2.88102100	-1.42783400	-5.12369700
H	4.67752000	-2.55782200	-3.83466900
H	2.19709600	-2.39770500	-0.32021400

H	0.75718000	-0.81878100	-4.02219800
H	1.88431400	0.76490400	2.42636800
H	0.74719300	1.69345000	4.32425900
N	0.13091300	-1.28695500	-1.42898600
C	-1.21571500	-2.54042200	-3.14358200
H	-0.33673300	-3.16709500	-3.30275100
H	-2.08050400	-3.19910700	-3.05268200
H	-1.35388000	-1.95054400	-4.05679100
C	-0.30889100	1.77656800	-0.85720400
H	1.47174700	0.34666100	0.02706300
C	1.10480900	1.71018000	-0.61087400
C	2.03453800	1.58083000	-1.78790700
C	3.31365900	1.03728400	-1.62645400
C	1.70757500	2.10651800	-3.03606300
C	4.22069100	1.01191300	-2.67101500
H	3.58545000	0.60246000	-0.66682600
C	2.61809600	2.07305700	-4.08951100
H	0.73232800	2.56015400	-3.18486400
C	3.88847000	1.52620400	-3.92889200
H	5.19947500	0.56236900	-2.52141100
H	2.33448500	2.48484000	-5.05507900
C	1.71079400	2.65597900	0.43817700
H	2.55708000	2.15704100	0.92772300
C	0.76420100	3.23696300	1.47450100
H	1.32146500	3.77201100	2.24822700
H	0.07106600	3.95219600	1.02537600
H	0.15844600	2.47312000	1.96472100
H	-0.94637000	2.39998200	-0.23490600
H	-0.69001100	1.60443000	-1.86119300
H	2.16677100	3.48422500	-0.11953200
C	4.86593700	1.45909300	-5.06209700
H	5.14186400	0.42293100	-5.28696200
H	4.45847500	1.89913700	-5.97441300
H	5.79627000	1.98516300	-4.82660800

Imaginary Frequency- -686.33

He

0 2

Fe	0.01289900	-0.18592800	0.13254000
N	-0.11850900	-0.16090700	2.05436100
C	0.98457200	-0.18927500	3.02366900
C	-1.23616700	-0.12389800	2.73309200
C	0.31143100	0.23787700	4.31516400
H	1.39548500	-1.20482400	3.07411700
H	0.61353200	-0.32274300	5.19944500
N	-1.93946100	-0.57942600	-0.07826900
C	-2.90698600	-0.48729900	0.87503400
C	-3.63669000	-1.02350900	-1.75792100
C	-4.29096600	-0.65146100	0.53781500
C	-4.62102700	-0.93082600	-0.81720600
H	-3.88275800	-1.21868600	-2.79528400

H	-5.66516300	-1.05909300	-1.08440100
C	-2.58465600	-0.22607200	2.24834100
C	-5.28370400	-0.53014600	1.51993600
C	-4.95299200	-0.25682500	2.83835400
H	-5.72709800	-0.15921600	3.59108900
C	-3.62231400	-0.11170600	3.19208000
H	-3.35324700	0.09100700	4.22077000
H	-6.32119700	-0.64903900	1.22131700
O	-1.08507200	-0.02344300	4.07808100
C	-2.29112500	-0.83693300	-1.38554300
C	-1.20953100	-0.86697700	-2.31464400
C	1.12543900	-0.48267200	-2.63574500
C	2.26325900	-1.22871100	-2.31584400
C	1.18122100	0.41451400	-3.70685200
C	3.42373500	-1.09546400	-3.06423400
C	2.34961500	0.55217100	-4.44657900
C	3.47402900	-0.20400200	-4.13294100
H	4.29829300	-1.68393400	-2.80602000
H	2.38280800	1.26145300	-5.26756600
H	4.38567500	-0.09302300	-4.71003800
H	2.22340500	-1.89849500	-1.46174000
H	0.31082400	1.02331500	-3.93306800
H	1.79177500	0.48110400	2.72254300
H	0.42658200	1.30988500	4.51350300
N	-0.01292600	-0.57506300	-1.80846500
C	-1.43718000	-1.24119600	-3.74566600
H	-0.51445500	-1.58258700	-4.21442000
H	-2.17602000	-2.04065800	-3.82729600
H	-1.80828300	-0.39843600	-4.33975800
C	1.68240900	0.92894500	0.08845400
H	0.86308500	2.18751400	1.65513900
C	1.53780900	2.28776000	0.78797100
C	2.85064800	2.81103600	1.32834700
C	2.97038100	3.23937800	2.64987100
C	3.98976900	2.88883100	0.51858100
C	4.17657000	3.72394200	3.14984200
H	2.09625700	3.20059300	3.29799100
C	5.18921300	3.37666300	1.01393000
H	3.92993500	2.55092700	-0.51321200
C	5.30860400	3.80219900	2.34175300
H	4.23939100	4.04944500	4.18552400
H	6.05786100	3.42833800	0.36133300
C	0.88724100	3.32944700	-0.13570800
H	0.84048900	4.28893700	0.39451100
C	-0.50097600	2.94151000	-0.61725800
H	-0.99043200	3.76706200	-1.14162400
H	-0.46849200	2.08816600	-1.30130400
H	-1.14882400	2.65835300	0.22226500
H	2.07659600	1.08226700	-0.92369100
H	2.42527800	0.30287700	0.61025700
H	1.54722600	3.49603300	-0.99846900

C	6.61418000	4.31615200	2.86961200
H	6.99302900	5.14806300	2.26809700
H	6.52127900	4.66769800	3.89909500
H	7.38802600	3.54179300	2.85500300

IIIc

0 2

Fe	0.28304400	0.09930900	-0.11151000
N	0.15816500	0.10224800	1.80395500
C	1.24217800	0.32991400	2.76418900
C	-0.93371400	-0.12708600	2.48792800
C	0.65953600	-0.19781600	4.06371200
H	2.14772600	-0.19513000	2.45413900
H	0.95675200	-1.23437400	4.26472300
N	-1.70449000	0.08250200	-0.33455700
C	-2.63181000	-0.19401700	0.62193500
C	-3.42887400	-0.00976600	-2.03905200
C	-4.00783800	-0.39534400	0.27433700
C	-4.37457800	-0.28567800	-1.09452100
H	-3.69820700	0.04915100	-3.08753800
H	-5.41282000	-0.44325800	-1.37075900
C	-2.27185400	-0.31286600	2.00613900
C	-4.95386200	-0.71722900	1.25871400
C	-4.58440600	-0.83533500	2.58988800
H	-5.32076200	-1.08561100	3.34543300
C	-3.26315300	-0.63252900	2.95252300
H	-2.96502300	-0.72315000	3.98929500
H	-5.98345800	-0.87782400	0.95136200
O	-0.76057400	-0.17725100	3.83618800
C	-2.08571700	0.16567400	-1.65388400
C	-1.02873500	0.38623600	-2.58640100
C	1.34546900	0.51486000	-2.86968400
C	1.57459000	-0.31280700	-3.97500300
C	2.34467000	1.41562700	-2.48452100
C	2.76644400	-0.22447600	-4.68508500
C	3.52620200	1.50847500	-3.20338900
C	3.74455600	0.68908200	-4.30892600
H	2.93339100	-0.88202100	-5.53243600
H	4.28725200	2.21793600	-2.89452900
H	4.67416200	0.75461100	-4.86380100
H	0.82338200	-1.04543300	-4.25486300
H	2.17721200	2.02901600	-1.60345600
H	1.47596800	1.40084900	2.80752600
H	0.87022300	0.41011000	4.94342200
N	0.19707400	0.39739000	-2.06629600
C	-1.33108700	0.62240700	-4.03285800
H	-0.50713700	1.13098700	-4.53281400
H	-1.51133700	-0.31367100	-4.57506300
H	-2.22744900	1.23527800	-4.14703900
C	2.00651100	-0.94884000	-0.17007500
H	2.38321900	-1.07350700	-1.19378000

H	2.80966800	-0.45493100	0.39767500
C	1.67582100	-2.32224900	0.43201600
H	1.59949700	-2.22541900	1.52765300
C	2.76260200	-3.36969800	0.14378300
H	2.84160500	-3.49703300	-0.94427200
H	3.72855000	-2.95904400	0.46342400
C	2.51503500	-4.71251700	0.80939800
H	3.32045000	-5.42313100	0.60657800
H	2.43617600	-4.60740800	1.89697700
H	1.58077000	-5.16310700	0.46149300
C	0.31199400	-2.78290200	-0.05011800
C	-0.70654300	-3.13078000	0.83626400
C	0.01477100	-2.80279700	-1.41827100
C	-1.98041300	-3.45847500	0.38174100
H	-0.50514000	-3.11353000	1.90664000
C	-1.25496100	-3.12713700	-1.87247200
H	0.78698600	-2.51783800	-2.12976700
C	-2.28206500	-3.45363300	-0.97985200
H	-2.76277600	-3.69414000	1.09976200
H	-1.46666400	-3.10558400	-2.94055700
C	-3.65591700	-3.79936800	-1.46994100
H	-3.75454200	-4.87330300	-1.66502600
H	-4.42123600	-3.53444400	-0.73566400
H	-3.89244000	-3.28073800	-2.40262700

TS_{2c}

0 2

Fe	0.23525100	-0.25227000	-0.21323400
N	0.10046100	-0.19805300	1.72001100
C	1.20204700	0.12024400	2.63322300
C	-0.99378100	-0.20586900	2.42410900
C	0.59539400	-0.13941600	3.99967500
H	2.07690700	-0.49752900	2.42534100
H	0.81887400	-1.14634700	4.37288300
N	-1.72954100	-0.23716100	-0.40838500
C	-2.68226900	-0.33258700	0.56561400
C	-3.47814600	-0.29706900	-2.10019700
C	-4.07185900	-0.44528800	0.23105100
C	-4.43911100	-0.41887400	-1.14164800
H	-3.74335000	-0.28757300	-3.15117000
H	-5.48923600	-0.50316600	-1.40418900
C	-2.34510400	-0.33684800	1.95692600
C	-5.04095100	-0.58415700	1.23580500
C	-4.68897100	-0.59812600	2.57550500
H	-5.44560100	-0.70284000	3.34480000
C	-3.35463800	-0.46776700	2.92494400
H	-3.06174600	-0.46757500	3.96723700
H	-6.08107700	-0.67401200	0.93479400
O	-0.82273700	-0.05719000	3.76339200
C	-2.12039800	-0.22109500	-1.73232900
C	-1.06630400	-0.16893900	-2.68174700

C	1.28553900	-0.27301400	-3.00574000
C	1.41380900	-1.28913300	-3.96156500
C	2.33439800	0.64022700	-2.85453100
C	2.56147100	-1.39193800	-4.73767000
C	3.47384100	0.53909900	-3.64072400
C	3.59843100	-0.47840900	-4.58214700
H	2.64504700	-2.19328200	-5.46505700
H	4.27296100	1.26256700	-3.51424700
H	4.49460500	-0.55858600	-5.18787200
H	0.60647000	-2.00583100	-4.08104100
H	2.24621200	1.43285300	-2.12018200
H	1.49756800	1.16883100	2.48866200
H	0.85317500	0.59080300	4.76651000
N	0.15805000	-0.22045900	-2.15665300
C	-1.35306000	-0.00801700	-4.14244500
H	-0.48995700	0.39288100	-4.67356900
H	-1.61781300	-0.95645500	-4.62623800
H	-2.18908700	0.67647500	-4.30097100
C	1.99050900	-1.29925300	-0.11227000
H	2.32357100	-1.50729800	-1.13537000
H	2.88018800	-0.94207500	0.42234700
C	1.51046200	-2.59960700	0.56006000
H	1.44564200	-2.43349200	1.64569900
C	2.52258300	-3.73498300	0.33200300
H	2.59232700	-3.93045600	-0.74621300
H	3.51550500	-3.37920500	0.63420400
C	2.17543000	-5.01450200	1.07324200
H	2.92809800	-5.79061500	0.91429900
H	2.10421400	-4.84120300	2.15228100
H	1.21188900	-5.41595500	0.74647200
C	0.11978300	-2.99374000	0.10220900
C	-0.91418400	-3.23610100	1.00888500
C	-0.16410000	-3.13560400	-1.25991400
C	-2.19252800	-3.55898800	0.57208600
H	-0.71689200	-3.13756600	2.07492100
C	-1.44150400	-3.45503700	-1.69747400
H	0.62979100	-2.96380700	-1.98229400
C	-2.48500600	-3.65957900	-0.78944700
H	-2.98780100	-3.70585200	1.29940400
H	-1.64329500	-3.52804200	-2.76480500
Si	0.37339100	2.09099300	-0.18801500
H	1.58749600	0.35103800	-0.18252800
H	-0.08306400	2.60373300	-1.50277000
C	-0.78149800	2.81177300	1.15467600
H	-0.42597600	2.59500900	2.16561900
H	-0.84980500	3.89896700	1.05849300
H	-1.79076800	2.40278700	1.06648400
H	1.70069500	2.72137000	0.03686500
C	-3.86863700	-3.99338300	-1.25860100
H	-4.01859600	-5.07693300	-1.32518300
H	-4.62743100	-3.60552300	-0.57389700

H -4.06770800 -3.57875100 -2.24983800
Imaginary Frequency: -493.76

IVc

0 2

Fe	-0.44948100	0.40045300	-0.10056600
N	-0.50914100	-0.16437500	1.71301300
C	0.63148900	-0.34093500	2.61540300
C	-1.60601000	-0.36188100	2.40249500
C	0.00448900	-0.96635700	3.85314000
H	1.38874100	-0.98145900	2.15473200
H	0.15884500	-2.04954100	3.90337000
N	-2.43025300	0.31950000	-0.32962200
C	-3.35556100	0.10373200	0.63944300
C	-4.19099000	0.77939900	-1.93218800
C	-4.75703300	0.18967600	0.34530500
C	-5.13946100	0.54692600	-0.97868500
H	-4.47868300	1.05481700	-2.94058500
H	-6.19674200	0.62919200	-1.21060900
C	-2.97019100	-0.24461700	1.97846300
C	-5.70945300	-0.07919500	1.33631100
C	-5.31874300	-0.43435500	2.62093700
H	-6.06215100	-0.64224600	3.38248100
C	-3.97281000	-0.51252900	2.93226800
H	-3.66268400	-0.77982200	3.93442300
H	-6.76147700	0.00097800	1.07850800
O	-1.40472700	-0.72727300	3.69391100
C	-2.82474600	0.64862500	-1.60747800
C	-1.76751700	0.79627600	-2.54831000
C	0.57191200	0.49451900	-2.90684000
C	0.53521600	-0.49881400	-3.89919600
C	1.75901400	1.21458800	-2.72669200
C	1.65077200	-0.76281300	-4.68196000
C	2.86590100	0.95581500	-3.52374300
C	2.82344500	-0.03519600	-4.50067400
H	1.60530100	-1.54635300	-5.43187300
H	3.77293100	1.53316600	-3.37544000
H	3.69554700	-0.24126200	-5.11181300
H	-0.37205300	-1.08396500	-4.02282000
H	1.79375000	1.98702400	-1.96864800
H	1.09690700	0.63219800	2.81494600
H	0.31795500	-0.51731400	4.79632800
N	-0.53095400	0.69054500	-2.05176400
C	-2.05969400	1.11630700	-3.98184200
H	-1.16301400	1.44639600	-4.50515400
H	-2.46569500	0.25992600	-4.53116300
H	-2.80188200	1.91605000	-4.04975900
C	2.86353900	-1.43990700	-0.43770100
H	2.63108700	-1.32391900	-1.50103600
H	3.94858400	-1.34754500	-0.33663500
C	2.37815900	-2.78661400	0.09370800

H	2.74262800	-2.90752900	1.12609900
C	2.97977200	-3.92922900	-0.74024100
H	2.62706400	-3.82120400	-1.77539000
H	4.06729400	-3.78996200	-0.78053000
C	2.65401400	-5.31746600	-0.22138700
H	3.13222100	-6.09357800	-0.82326200
H	2.99630900	-5.44617100	0.81085500
H	1.57717300	-5.50764400	-0.23199000
C	0.86942900	-2.87817700	0.14083300
C	0.20200300	-3.40941600	1.24608800
C	0.09067600	-2.45510700	-0.93871600
C	-1.18510700	-3.50635700	1.27705800
H	0.78569200	-3.75245300	2.09901100
C	-1.29696300	-2.55408300	-0.90914600
H	0.57426400	-2.04790100	-1.82222000
C	-1.96444900	-3.08286800	0.19718900
H	-1.67643100	-3.90917400	2.16060700
H	-1.87537800	-2.20186100	-1.76108800
Si	0.75370900	2.41264400	0.48040100
H	2.40430100	-0.59313700	0.08407100
H	0.89839800	3.47566700	-0.54677600
C	-0.25607400	3.18998600	1.92396800
H	-0.27182100	2.53523400	2.79999500
H	0.14876000	4.15598600	2.23766700
H	-1.29634100	3.34659400	1.62605200
H	2.13756400	2.20642700	1.00136300
C	-3.45731200	-3.21396300	0.21166800
H	-3.88306300	-2.92338300	1.17625300
H	-3.92002500	-2.59150900	-0.55803300
H	-3.76538800	-4.24837900	0.02337700

I'''(2a)

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Fe	0.09586900	0.02684400	-0.09563300
N	0.26029700	0.08854100	1.89498600
C	1.42126600	0.05409800	2.83964200
C	-0.75924500	0.50935000	2.60076900
C	0.96356700	1.02000500	3.91306100
H	1.28002200	0.76404000	4.92405100
N	-1.83542800	-0.45373300	0.08424600
C	-2.67274700	-0.06443900	1.07517600
C	-3.70555800	-1.47620300	-1.07533200
C	-4.09055400	-0.24847400	0.96656000
C	-4.57890400	-0.98205200	-0.15284400
H	-4.06161300	-2.05894200	-1.91770300
H	-5.64735500	-1.14953700	-0.24394100
C	-2.15959900	0.54192800	2.26324400
C	-4.93913500	0.28667000	1.94162500
C	-4.42785600	0.96882200	3.03760000
H	-5.09655300	1.39271200	3.77844600

C	-3.05669000	1.07367900	3.20562200
H	-2.64979100	1.54570700	4.09079700
H	-6.01110100	0.15771600	1.82226400
O	-0.46978000	0.92694100	3.85685300
C	-2.32471400	-1.19740700	-0.96243200
C	-1.35512400	-1.61361400	-1.90940500
C	0.93257100	-1.43545500	-2.62395800
C	1.99988900	-2.28577700	-2.24391500
C	0.95232200	-0.78635500	-3.88107800
C	3.10012700	-2.40326200	-3.08756500
C	2.09143500	-0.92923400	-4.68011800
C	3.16350600	-1.71110400	-4.29045500
H	3.92459200	-3.04714800	-2.80137000
H	2.12388200	-0.41899800	-5.63912600
H	4.03620800	-1.80185300	-4.92905900
H	1.24200500	2.05707600	3.68913200
N	-0.10423000	-1.21217000	-1.67436800
C	-1.74641600	-2.49710500	-3.05285900
H	-0.86877000	-2.85510800	-3.59192000
H	-2.29717400	-3.37120900	-2.69196500
H	-2.39700600	-1.98595500	-3.77009500
C	-0.30164100	1.75480000	-1.16172300
H	1.57484900	-0.16215500	-0.14733600
C	0.98261900	2.07357800	-0.69319600
C	2.15356500	1.95664500	-1.65383600
H	-1.19336500	2.21568800	-0.74689200
H	-0.41691400	1.39450600	-2.17720900
C	1.90044200	-3.11073300	-0.97721200
H	1.47693400	-2.45448700	-0.20523500
C	3.24101600	-3.63981200	-0.48269800
H	3.99733300	-2.85323300	-0.41790400
H	3.13118800	-4.07887600	0.51268900
H	3.63219500	-4.42595000	-1.13714800
C	0.92377100	-4.27477900	-1.16755700
H	-0.08004100	-3.92891500	-1.42060700
H	1.26339500	-4.93892900	-1.96969000
H	0.84641400	-4.87014400	-0.25289600
C	-0.20912100	0.00781500	-4.46448000
H	-1.01736300	0.04687100	-3.72532300
C	0.15497900	1.44693200	-4.83821300
H	0.96978700	1.46948700	-5.56820100
H	-0.70374900	1.94551200	-5.29729500
H	0.46416500	2.04806300	-3.98258200
C	-0.74456700	-0.68787900	-5.72322300
H	-0.94569600	-1.74873400	-5.56750300
H	-1.66814200	-0.21245600	-6.06698300
H	-0.01844500	-0.61418600	-6.53887700
C	1.11195200	2.96054100	0.48178100
C	0.01528400	3.25017400	1.32144000
C	2.31360300	3.60870400	0.79769400
C	0.11785500	4.09821900	2.40514100

H	-0.94920100	2.79442400	1.12675400
C	2.43902700	4.46171400	1.89167500
H	3.18613600	3.46163800	0.17222400
C	1.33992500	4.70510100	2.71294200
H	-0.73744700	4.29484100	3.04368300
H	3.39565000	4.93163800	2.08725900
O	1.35434300	5.49759100	3.81981900
C	2.58521200	6.09674500	4.16100500
H	2.40465600	6.66940200	5.06916600
H	3.36045500	5.34481000	4.35672400
H	2.94052900	6.77299000	3.37395200
H	1.78999800	1.45284500	-2.55267800
H	2.40478300	2.98121500	-1.97301800
C	3.43861600	1.24360700	-1.24404500
H	4.19843300	1.37785300	-2.02018300
H	3.86560200	1.60425300	-0.30478800
H	3.26679100	0.17021500	-1.13339100
H	1.43537000	-0.96514800	3.26092500
C	2.79361400	0.34747700	2.22834200
H	2.61508600	1.01901900	1.38363000
C	3.43403800	-0.93086400	1.71238400
H	4.34876700	-0.72041000	1.15027700
H	3.70119200	-1.59637100	2.54228900
H	2.75311600	-1.46797100	1.05335300
C	3.73693900	1.04003100	3.20835500
H	4.71172000	1.19722900	2.73745000
H	3.37558400	2.02136200	3.52745900
H	3.90893900	0.43132000	4.10406100

I'''(2b)

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Fe	0.08924500	-0.11882900	-0.03577400
N	0.30247200	-0.15564400	1.93632700
C	1.48312900	-0.02545800	2.84469700
C	-0.75369100	-0.04045600	2.70472500
C	0.87517400	0.75746300	3.99180300
H	1.70022200	-1.04743400	3.20104200
H	1.29144600	0.53613100	4.97403900
N	-1.69060200	-1.01407200	0.14282400
C	-2.55809500	-0.88208300	1.17179100
C	-3.35575600	-2.26379200	-1.09638700
C	-3.91521300	-1.33356800	1.06099000
C	-4.28577300	-2.02573400	-0.12730500
H	-3.61798600	-2.81975500	-1.98971100
H	-5.30756700	-2.37642500	-0.23186700
C	-2.13675900	-0.29553800	2.40729800
C	-4.81824800	-1.08570200	2.10018800
C	-4.41356000	-0.43442600	3.25868500
H	-5.12636200	-0.23879600	4.05204700
C	-3.08907100	-0.06297900	3.41623100
H	-2.75719800	0.39509500	4.33913200

H	-5.84671600	-1.41481300	1.98267100
O	-0.49891200	0.34228800	3.98334300
C	-2.04424200	-1.75917700	-0.95429700
C	-0.99835900	-1.97246400	-1.89114400
C	1.30436200	-1.56464600	-2.43492200
C	2.38325500	-2.33253600	-1.93100000
C	1.39749400	-0.93959500	-3.69583900
C	3.56331100	-2.38949100	-2.66762500
C	2.60755500	-1.02726800	-4.39064600
C	3.68772300	-1.72645100	-3.88361300
H	4.39965100	-2.96884200	-2.29169400
H	2.69485300	-0.53053600	-5.35377800
H	4.61924800	-1.77526700	-4.43929200
H	0.90588400	1.84277000	3.81905400
N	0.16960900	-1.40340700	-1.59177200
C	-1.21975900	-2.84912800	-3.08412700
H	-0.27531600	-3.10209700	-3.56702700
H	-1.71076200	-3.78317400	-2.79655400
H	-1.85950000	-2.36881300	-3.83258700
C	-0.73826400	1.49702200	-1.01810900
H	1.55961900	0.05995300	-0.07670300
C	0.43472400	2.03585400	-0.47058800
C	1.56871700	2.40710600	-1.38592000
C	2.64150900	1.60025000	-1.75354800
C	1.50498400	3.68339300	-1.97665900
C	3.58718100	2.00988800	-2.69305500
H	2.72962200	0.60796100	-1.32538400
C	2.42957600	4.10754100	-2.91243400
H	0.67901000	4.34272600	-1.71951900
C	3.47587600	3.26065300	-3.29103900
H	4.38676900	1.32898200	-2.95867400
H	2.35266500	5.08228500	-3.38199700
C	0.35313400	2.89635000	0.78711900
H	1.02519900	2.50023300	1.55627700
C	-1.02805100	3.10752300	1.38205000
H	-0.96603100	3.69368600	2.30314300
H	-1.68207100	3.64815900	0.69202000
H	-1.53025500	2.16910800	1.62887900
O	4.31657800	3.73863500	-4.25047300
C	5.31963600	2.85937800	-4.70973100
H	6.02900300	2.59839200	-3.91470100
H	4.88998000	1.93337100	-5.11435600
H	5.84941900	3.38688200	-5.50146600
H	-1.70847900	1.66724400	-0.55862000
H	-0.76806200	1.21727200	-2.06763400
H	0.78159900	3.87662300	0.53804400
C	2.77815800	0.54815600	2.25539600
H	2.50477000	1.28187300	1.48954900
C	3.61074800	1.24129600	3.33175300
H	3.10812600	2.10787400	3.76963600
H	3.86266400	0.55229800	4.14634200

H	4.55397200	1.59645700	2.91025400
C	3.60679200	-0.53727200	1.58657800
H	3.02955900	-1.04923600	0.81855900
H	4.49567000	-0.11460200	1.10880800
H	3.94345100	-1.28133200	2.31834700
C	0.24869800	-0.20574000	-4.36648500
H	-0.62113500	-0.24179900	-3.70068100
C	-0.13221900	-0.88822800	-5.68489300
H	-1.03659400	-0.43891200	-6.10602400
H	0.66367100	-0.76790900	-6.42657100
H	-0.30749700	-1.95980000	-5.57075000
C	0.56651500	1.26399400	-4.64026800
H	-0.27591600	1.74973700	-5.14232800
H	0.78161000	1.81825800	-3.72750900
H	1.43819000	1.36401100	-5.29600000
C	2.22123300	-3.13748100	-0.65480500
H	1.71220000	-2.48940800	0.07368400
C	1.31707700	-4.35237600	-0.88783700
H	1.74435900	-5.00883800	-1.65350200
H	1.21291000	-4.93761800	0.03066700
H	0.31482600	-4.06791200	-1.20999300
C	3.53967500	-3.60920700	-0.05164900
H	3.99719600	-4.39835600	-0.65768200
H	4.27011500	-2.80330000	0.04841700
H	3.36936800	-4.02964100	0.94322800

I'''(2c)

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Fe	0.96337300	-0.49533700	0.28169500
N	0.39027500	1.04774900	1.42510500
C	-0.59446900	0.97001000	2.27491800
H	1.11503900	2.77805800	3.82597600
N	-0.96200900	-1.05151600	0.25181900
C	-1.87787500	-0.90499300	1.24036900
C	-2.56600400	-2.36740500	-1.01114400
C	-3.12288500	-1.61699500	1.21187700
C	-3.42923800	-2.37290600	0.04343500
H	-2.80492600	-2.89665400	-1.92720100
H	-4.36777100	-2.91620400	0.00118600
C	-1.65053200	-0.00365200	2.32680800
C	-3.99587100	-1.53691000	2.30205600
C	-3.70802100	-0.73217000	3.39710600
H	-4.39252800	-0.68519000	4.23659500
C	-2.56499800	0.04949100	3.39129600
H	-2.36827800	0.73886800	4.20298000
H	-4.91751200	-2.11101100	2.26825600
O	-0.66727900	1.96814600	3.18482500
C	-1.32480000	-1.70056300	-0.90462300
C	-0.35453000	-1.66277400	-1.93425200
C	1.86167100	-1.02782700	-2.55981800
C	2.61161500	-2.16353500	-2.92688700

C	2.16240900	0.24492100	-3.10795900
C	3.69209100	-1.96760400	-3.79984200
C	3.23572900	0.37054600	-3.98173400
C	4.01275900	-0.73045600	-4.32069400
H	4.31518100	-2.82505600	-4.04312500
H	3.47202100	1.34142500	-4.40396300
H	4.86306500	-0.61965600	-4.98606400
H	0.07526600	3.85866700	2.87380500
N	0.80311100	-1.08331300	-1.60646600
C	-0.66520800	-2.21202900	-3.29253300
H	0.11576300	-1.96589700	-4.01228000
H	-0.77303700	-3.30222400	-3.28255900
H	-1.61053600	-1.80628800	-3.66580200
C	1.38541900	-1.87257900	1.76076200
C	2.62104000	-1.27650400	1.45117300
H	0.83485200	-1.54908300	2.64293900
H	1.12657300	-2.86642600	1.40677600
C	1.27751500	1.43708100	-2.80489000
H	0.92481300	1.31513300	-1.77389800
C	2.00479600	2.77286800	-2.89915500
H	1.35698600	3.58446500	-2.55463600
H	2.91407100	2.78445300	-2.28930200
H	2.29024900	3.01608000	-3.92744100
C	0.04363400	1.43969800	-3.70996900
H	-0.54119400	0.52372300	-3.59962700
H	-0.61400200	2.28213500	-3.47263300
H	0.33134500	1.52650500	-4.76342300
C	1.10442000	2.30895300	1.66964800
C	0.45744700	2.83718900	2.95359300
H	2.16016900	2.08629800	1.83711200
C	1.02014000	3.23208300	0.45067800
H	1.51841500	2.67226600	-0.34793700
C	-0.41414100	3.50427300	0.02153300
C	1.80602900	4.51293000	0.69128700
H	-0.98594200	4.01454700	0.80578000
H	-0.44279600	4.14719700	-0.86255400
H	-0.93911700	2.57636000	-0.22456600
H	1.35237000	5.13087800	1.47473100
H	2.83748900	4.30133700	0.99111400
H	1.84491300	5.12491400	-0.21355900
H	2.21837600	0.27986700	-0.07899800
C	2.45207900	-3.61643200	-2.46965800
H	3.46015700	-3.88918900	-2.12338400
C	2.13738500	-4.52503400	-3.66463000
C	1.51528400	-3.96967000	-1.32020700
H	2.85923100	-4.41582800	-4.47637600
H	2.13803100	-5.57471500	-3.35531400
H	1.14753900	-4.30609100	-4.07636200
H	1.57791700	-3.26112200	-0.49985800
H	0.46923600	-4.03910600	-1.62958500
H	1.79446600	-4.95312700	-0.92916900

C	3.19327300	-0.28494300	2.45277800
C	3.64354300	-2.03587400	0.67133000
C	3.91912400	-3.36458100	1.00461900
C	4.43342600	-1.45122300	-0.33009100
C	4.91994800	-4.09668900	0.37046200
H	3.33076700	-3.84266900	1.78359000
C	5.44474400	-2.15441700	-0.95782700
H	4.21709600	-0.43435800	-0.64414400
C	5.69139300	-3.48698500	-0.61901600
H	5.08872500	-5.12831800	0.65577100
H	6.03472700	-1.70203200	-1.74747900
H	2.36198500	0.25262700	2.92317300
H	3.64064500	-0.88211400	3.26310100
C	4.24795300	0.68797300	1.95028000
H	5.17093900	0.17261000	1.67396500
H	3.90734400	1.23339000	1.06377400
H	4.50319100	1.41797000	2.72440600
O	6.67809500	-4.10750800	-1.32493000
C	6.91580200	-5.46703100	-1.03438600
H	7.71736800	-5.78565800	-1.69888500
H	7.23249500	-5.61225400	0.00574500
H	6.02658200	-6.08246700	-1.22152300

I'''(2d)

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Fe	0.35576400	-0.79852400	0.41235400
N	0.11358100	0.73009600	1.66826400
C	-0.86762900	0.77921900	2.52223200
H	1.12161000	2.29363700	4.17326300
N	-1.64205600	-0.92441200	0.32218900
C	-2.51850900	-0.66669300	1.32327300
C	-3.47528400	-1.71480600	-1.05919300
C	-3.89089800	-1.07080200	1.22967200
C	-4.33889300	-1.61544200	-0.00934300
H	-3.81114100	-2.08533900	-2.02190900
H	-5.37721500	-1.91675400	-0.10420300
C	-2.10977900	0.04953400	2.49165400
C	-4.74080000	-0.90590500	2.32881400
C	-4.29461900	-0.30414000	3.49813800
H	-4.96321600	-0.18962000	4.34391400
C	-3.00468500	0.19814300	3.56237000
H	-2.67229600	0.74359800	4.43702800
H	-5.76784700	-1.24966300	2.24395000
O	-0.73597500	1.67633900	3.52217200
C	-2.11411800	-1.37409400	-0.88812100
C	-1.12983100	-1.49912500	-1.89720200
C	1.21693600	-1.41576300	-2.40083300
C	1.69056800	-2.68382300	-2.79959900
C	1.87385200	-0.23404800	-2.83127900
C	2.87771700	-2.72278200	-3.54689400
C	3.02847200	-0.34005900	-3.59636200

C	3.54850900	-1.58205100	-3.93822500
H	3.28168800	-3.69563900	-3.81593000
H	3.53748800	0.55992900	-3.92379700
H	4.46729900	-1.65549800	-4.51097700
H	0.22554200	3.45752100	3.16859600
N	0.12326700	-1.25538500	-1.50080100
C	-1.51142700	-1.83745800	-3.30531000
H	-0.65264000	-1.77882000	-3.97491100
H	-1.93377800	-2.84407600	-3.39524100
H	-2.27457900	-1.14487200	-3.67464800
C	0.46159300	-2.39900500	1.73104900
C	1.79662700	-1.99662500	1.56686400
C	2.67469400	-2.78125100	0.61504300
H	-0.12446700	-2.09977700	2.59553700
H	0.09833100	-3.29910000	1.24634900
C	1.28770700	1.12718500	-2.51384900
H	0.85007300	1.05665000	-1.51118100
C	2.32228400	2.24580100	-2.49536200
H	1.87097300	3.17430400	-2.13373800
H	3.16812300	2.00611700	-1.84350000
H	2.71894600	2.45794900	-3.49344300
C	0.15463600	1.46957600	-3.48342700
H	-0.64272100	0.72383700	-3.45377500
H	-0.29033800	2.43897500	-3.23708600
H	0.52288700	1.52320200	-4.51378500
C	2.47838000	-1.16801400	2.58593400
C	1.90182600	-0.89335100	3.83844900
C	3.73355000	-0.59913400	2.33711300
C	2.51419800	-0.06211000	4.75852200
H	0.94681000	-1.33652800	4.10123100
C	4.36666400	0.23718500	3.25102700
H	4.21859100	-0.77703600	1.38299200
C	3.74756300	0.52671200	4.46764700
H	2.05492200	0.14645800	5.71941800
H	5.33134900	0.66308700	3.00141500
O	4.25462400	1.35608500	5.42202000
C	5.49482100	1.96942000	5.14431800
H	5.72732700	2.59147800	6.00705200
H	6.29300900	1.22953700	5.00909000
H	5.44295200	2.60104200	4.24838900
H	3.37588000	-2.11869700	0.09665900
C	1.08963500	1.76931800	2.02836700
C	0.48941400	2.40154200	3.28936900
H	2.04057800	1.28235100	2.25882100
C	1.33400900	2.73069600	0.86272700
H	1.76517300	2.10336100	0.07460200
C	0.04804000	3.34811300	0.33270700
C	2.36479100	3.78089400	1.25263700
H	-0.46640400	3.94305900	1.09669000
H	0.25037100	4.01820700	-0.50754700
H	-0.64838200	2.57800000	-0.01300200

H	1.98343200	4.46008900	2.02404200
H	3.27814500	3.31795400	1.64097600
H	2.64359800	4.39776000	0.39412600
H	1.75196700	-0.28617700	0.10469200
H	2.04818900	-3.19245500	-0.17837500
C	3.42817600	-3.91055200	1.30863300
H	4.09334000	-3.52847100	2.08863800
H	2.73596700	-4.61120400	1.78528700
H	4.03916500	-4.47477600	0.59838500
C	1.10458200	-4.07704900	-2.52977600
H	1.96438600	-4.65594800	-2.15917100
C	0.67826100	-4.73107100	-3.85054700
C	-0.00880700	-4.28491800	-1.50654900
H	0.36372000	-5.76529500	-3.68152000
H	-0.16867500	-4.19849900	-4.29343300
H	1.48089400	-4.74072000	-4.59024200
H	0.12407800	-3.70431800	-0.59800100
H	-0.99642800	-4.04326500	-1.90403100
H	-0.03676300	-5.34256200	-1.22832900

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Fe	0.63259700	-0.56705900	-0.04269800
N	0.68755100	-0.64613200	1.91414000
C	1.85765100	-0.88246600	2.76341800
C	-0.26597000	-0.19603400	2.68613500
C	1.52024600	-0.13656200	4.04308000
H	1.98048500	-1.96194000	2.91283400
H	1.75419400	-0.66835400	4.96588700
N	-1.34883300	-0.75562600	0.06750300
C	-2.16585100	-0.34747300	1.06854700
C	-3.29160100	-1.27016900	-1.29448900
C	-3.58848500	-0.29248200	0.89148300
C	-4.12262100	-0.76820700	-0.34132600
H	-3.69113600	-1.64928100	-2.22799500
H	-5.19668500	-0.73435600	-0.49373300
C	-1.63847000	0.03605900	2.34349500
C	-4.40078800	0.21743700	1.90840000
C	-3.86123300	0.65155300	3.11289300
H	-4.50499300	1.05048000	3.88874600
C	-2.49914700	0.54421900	3.33130300
H	-2.07203400	0.83154700	4.28394100
H	-5.47236500	0.26588800	1.73640100
O	0.08585000	0.02327700	3.97495400
C	-1.89008100	-1.26807800	-1.09035300
C	-0.94545900	-1.74656300	-2.02383600
C	1.37039300	-1.99401500	-2.54248800
C	2.39027400	-2.84314100	-2.10334600
C	1.41434500	-1.50367900	-3.85233800
C	3.40719200	-3.22260700	-2.96892500
C	2.43782600	-1.87907200	-4.71096900

C	3.43404300	-2.74787900	-4.27760900
H	4.18582600	-3.89316300	-2.61853200
H	2.46613200	-1.47599700	-5.71872600
H	4.23431300	-3.04042800	-4.94991700
H	2.36062300	-3.19381700	-1.07721500
H	0.65485600	-0.80009400	-4.17992000
H	2.75852200	-0.51094100	2.28124700
H	1.97456500	0.86113900	4.07579200
N	0.34241700	-1.62384400	-1.64544900
C	-1.38624700	-2.42168300	-3.28643200
H	-2.30960300	-2.97985400	-3.12081600
H	-1.57729000	-1.71823200	-4.10442500
H	-0.63154100	-3.12354400	-3.64197300
C	0.34470100	1.37124800	-0.58431100
H	2.10303000	-0.93634400	-0.02955400
C	1.74330100	1.20339300	-0.57225400
H	-0.21264700	1.35366400	-1.51820400
C	2.47942700	1.79048900	0.62198500
H	-0.15910100	1.86610100	0.24454700
H	2.51765200	2.88293400	0.48126000
H	1.85970100	1.64261400	1.51563600
C	3.90335900	1.31286100	0.91555400
H	3.95392100	0.22344300	0.82872500
H	4.57912300	1.69885600	0.14067100
C	4.34716000	1.77271700	2.26653300
C	4.94028000	1.06244900	3.23601700
H	4.13191400	2.82071400	2.48651700
C	5.33528500	-0.37782100	3.11710300
C	5.26733000	1.68599000	4.55859200
H	6.34026800	1.62639600	4.77589200
H	4.97212600	2.73605200	4.60167800
H	4.76423600	1.15917800	5.37978300
H	6.41660400	-0.49243900	3.25524900
H	4.86827100	-0.98166800	3.90616200
H	5.07998600	-0.82359000	2.15520200
C	2.48554100	1.12842100	-1.86329700
C	3.63998200	0.36056200	-2.03455500
C	2.04918700	1.90393600	-2.94869500
C	4.33554700	0.38709600	-3.23599700
H	3.96377900	-0.30212400	-1.24115200
C	2.74357400	1.90441700	-4.15577200
H	1.16805800	2.52227200	-2.82450800
C	3.91306600	1.14765900	-4.32004800
H	5.22017300	-0.23374500	-3.35343300
O	2.36108700	2.62205700	-5.25538000
C	1.17737700	3.38055700	-5.15436000
H	1.25536400	4.15819900	-4.38472800
H	1.03375400	3.85293000	-6.12514200
H	0.30842600	2.74954500	-4.92823800
C	4.63291800	1.14850700	-5.62915000
H	3.96713400	0.86739100	-6.45137400

H	5.01697900	2.14225800	-5.88099100
H	5.47355500	0.45176100	-5.61434500

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Fe	0.55092300	-0.48667800	0.12354100
N	0.80516200	-0.68088700	2.04438100
C	2.09812300	-0.71591600	2.73187900
C	-0.12020200	-0.45932000	2.93585000
C	1.75966700	-0.37198700	4.18175400
H	2.54154600	-1.70944200	2.61552400
H	2.06328900	-1.13147300	4.90491600
N	-1.38990600	-0.86312400	0.36141300
C	-2.14616600	-0.65594800	1.46643500
C	-3.38642800	-1.42869300	-0.89583000
C	-3.57838700	-0.72930600	1.40675900
C	-4.17294100	-1.10250100	0.16675700
H	-3.83072900	-1.74711100	-1.83182900
H	-5.25511900	-1.14892800	0.09914600
C	-1.54125200	-0.37933600	2.73504200
C	-4.34230100	-0.44824600	2.54345900
C	-3.73903600	-0.13473400	3.75440300
H	-4.34427200	0.07355600	4.62958800
C	-2.35826500	-0.12195100	3.85046700
H	-1.87886700	0.06589900	4.80343000
H	-5.42461500	-0.49275300	2.46239700
O	0.31567500	-0.30200600	4.20577700
C	-1.97887800	-1.33015500	-0.79271000
C	-1.06778700	-1.69264600	-1.81228100
C	1.23993700	-1.84112500	-2.42596800
C	2.25491400	-2.72825400	-2.05323800
C	1.29064300	-1.24560500	-3.69071800
C	3.28775800	-3.02291700	-2.93149400
C	2.33607000	-1.53300600	-4.56097500
C	3.33777100	-2.42286200	-4.18756600
H	4.06711800	-3.71515700	-2.62938400
H	2.37293200	-1.04950300	-5.53237400
H	4.15409500	-2.64252200	-4.86744800
H	2.21650400	-3.16388600	-1.06059400
H	0.51689400	-0.53795900	-3.97530000
H	2.77669000	0.00544000	2.26818500
H	2.14354400	0.60028300	4.50125200
N	0.22698100	-1.53427400	-1.49097400
C	-1.53716300	-2.28084500	-3.10613500
H	-1.77210300	-1.51659700	-3.85564100
H	-0.77667400	-2.92986900	-3.54202100
H	-2.44021600	-2.87560700	-2.96004500
C	0.12782100	1.39064000	-0.56291800
H	2.02315800	-0.76925400	0.01351300
C	1.51539500	1.47335000	-0.33548700
C	2.44245100	1.44587500	-1.53403300

H	-0.22872600	1.25592800	-1.58203300
H	1.84645200	1.16136600	-2.40714400
H	2.75538000	2.48386000	-1.72332800
C	3.70830700	0.55480700	-1.47338200
H	3.52429100	-0.34387500	-2.07177000
C	4.97963400	1.21892900	-1.92540200
H	5.74641400	1.37153100	-1.16478100
C	5.26142300	1.64093400	-3.16436300
C	6.56465200	2.29908900	-3.49398800
H	6.41143600	3.30594100	-3.90090300
H	7.21299200	2.38454200	-2.61981900
H	7.10844000	1.74072200	-4.26567400
C	4.31107500	1.49641600	-4.31193600
H	3.40700700	0.94912400	-4.04399300
H	4.00981400	2.47772500	-4.69894700
H	4.78516400	0.97051500	-5.15003600
C	2.02789300	2.10110000	0.90384000
C	1.18001800	2.38734600	1.99436300
C	3.37304500	2.47286300	1.02930100
C	1.66714900	2.98201500	3.15031900
C	3.85109300	3.05160200	2.20217400
H	4.06125100	2.33278800	0.20573400
C	3.02952700	3.30767000	3.29011800
H	4.90168500	3.32287400	2.27041000
C	3.52702500	3.91887700	4.55887400
H	3.00342200	4.85233300	4.78654200
H	3.35317200	3.26261000	5.41860000
H	4.59637800	4.12944200	4.50177400
H	-0.59497700	1.85314400	0.10366500
H	3.83750300	0.18663600	-0.45247500
O	0.89915200	3.28299000	4.23791300
C	-0.49869700	3.10807700	4.11983800
H	-0.76713400	2.05517400	3.98684400
H	-0.92877400	3.47000400	5.05277500
H	-0.90609000	3.68892900	3.28370600
H	0.12885000	2.13498600	1.93372200

Ic

02

Fe	0.77783700	-0.04990400	-0.12295900
N	1.94938600	0.08638000	1.42870200
C	3.41179300	0.18551300	1.43898700
C	1.53379100	0.36376800	2.63783000
C	3.69249400	0.96398000	2.71295500
H	3.83718000	-0.82495900	1.45728600
H	4.54003800	0.60753800	3.29785600
N	-0.68642700	-0.63864900	1.08677000
C	-0.84846900	-0.35406200	2.40222300
C	-2.86067600	-1.72323000	1.06954700
C	-2.08220900	-0.63327000	3.07850900
C	-3.09204900	-1.33058500	2.35185400

H	-3.61404900	-2.27651800	0.52060200
H	-4.03229400	-1.55267000	2.84774300
C	0.20697300	0.24505800	3.16376300
C	-2.26465600	-0.21873300	4.40064800
C	-1.25580800	0.43808700	5.09475500
H	-1.41943600	0.77089500	6.11396000
C	-0.03020300	0.64811800	4.48883600
H	0.77702700	1.12183200	5.03347300
H	-3.22312900	-0.41489200	4.87366300
O	2.49829200	0.76966100	3.49876500
C	-1.64253100	-1.38691400	0.42862600
C	-1.29336200	-1.77097600	-0.88252800
C	0.38695200	-1.64703400	-2.59189600
C	1.69209100	-2.12717400	-2.74759800
C	-0.38295500	-1.41798700	-3.73912000
C	2.20630800	-2.37849300	-4.01165500
C	0.13983200	-1.65855500	-5.00327300
C	1.43554900	-2.14313300	-5.14722200
H	3.21882200	-2.75676800	-4.11154000
H	-0.46678500	-1.45686700	-5.88058200
H	1.84276700	-2.33138600	-6.13493500
H	2.28668100	-2.28816100	-1.85534300
H	-1.38341800	-1.01015100	-3.63430800
H	3.76868700	0.67587700	0.53321500
H	3.80621700	2.04010400	2.53499100
N	-0.07810200	-1.34719100	-1.29221500
C	-2.17686700	-2.67879600	-1.68172100
H	-2.70953700	-3.37169800	-1.02824200
H	-2.93330000	-2.14026200	-2.26397500
H	-1.59565900	-3.27179300	-2.38885500
C	-0.08354600	1.79936600	-0.40202300
H	2.02602100	-0.11323200	-0.96214200
C	1.06540300	1.75685500	-1.22376100
C	0.89251300	1.57686300	-2.70654200
C	2.31041300	2.51885500	-0.85592400
H	3.19511000	2.06934700	-1.31683600
H	-1.03786400	1.57884500	-0.89021500
H	2.24874400	3.55314000	-1.22358500
H	1.68921900	0.97154400	-3.15030100
H	-0.05940200	1.10201300	-2.94938300
H	0.90690800	2.55660700	-3.20520000
H	2.47941300	2.57036800	0.22160200
C	-0.20333000	2.60075800	0.86065000
H	0.76205000	2.67341300	1.37521600
H	-0.87061700	2.09797700	1.56591500
C	-0.73118500	4.02490900	0.62877600
H	-0.10993800	4.53816600	-0.11253100
H	-1.73386800	3.96248700	0.18244900
C	-0.77002400	4.84370300	1.89311100
C	-0.09234500	5.99657400	1.97454800
C	-1.55391600	4.32158600	3.03438200

C	-1.20679300	4.61457500	4.35513900
C	-2.66831300	3.49735000	2.81329200
C	-1.96517900	4.11983300	5.41012700
H	-0.32403000	5.21121300	4.55791600
C	-3.41127100	2.99851400	3.87650100
C	-3.07588800	3.31031600	5.20477800
H	-1.67794100	4.35399700	6.43215500
C	-3.88599100	2.75408700	6.32918400
H	-4.93014100	3.07629400	6.26984600
H	-3.90872000	1.65961000	6.30224600
H	-3.48621600	3.06595600	7.29583800
H	-0.12263900	6.62286600	2.85943400
H	0.49883600	6.35888500	1.14012000
O	-4.49081800	2.17817800	3.72965100
C	-4.83993200	1.80132100	2.41386000
H	-4.01237600	1.28902600	1.90682800
H	-5.67995900	1.11396900	2.50723400
H	-5.14752900	2.66707400	1.81464600
H	-2.95444300	3.25692900	1.79698900