

Supporting Information for

Selective Activation of C-F and C-H Bonds with Iron Complexes, the Relevant Mechanism Study by DFT Calculations and Study on the Chemical Properties of Hydrido Iron Complexes

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Cartesian coordinates and free energies for all structures given in Figure 3, as well as the imaginary frequencies for transition states.

R^{C-H}

C	-1.08135700	0.24655400	0.22069400
C	-2.08231200	0.87292300	-0.53127400
C	-3.30030300	0.27152300	-0.82619900
H	-4.02723500	0.81142100	-1.42202100
C	-3.54625800	-1.01384200	-0.34319500
H	-4.49343400	-1.49744800	-0.55940900
C	-2.58644300	-1.68179600	0.41814100
H	-2.75468200	-2.67760000	0.81189300
C	-1.38106900	-1.04156700	0.67884700
C	0.20565100	0.94274500	0.56635900
C	1.49051800	0.34086600	0.11094800
C	1.53044000	-0.68454400	-0.84473000
H	0.60705900	-1.06588000	-1.26855900
C	2.75063200	-1.20892400	-1.27229200
H	2.76569100	-1.99941500	-2.01702600
C	3.94559400	-0.71937400	-0.74515100
H	4.89572400	-1.13071900	-1.07415000
C	3.91554100	0.30273000	0.20933700
H	4.84338400	0.68627500	0.62422700
C	2.70019300	0.83057500	0.63233600
F	-1.85133500	2.11628500	-0.99708200
F	-0.45655200	-1.68320200	1.41880600
H	2.65990600	1.62561400	1.36854200

N	0.23198600	2.03815200	1.23132400
H	-0.71429800	2.33572100	1.47879500

G= -755.067255 au

IM1

C	-3.22094400	-0.31723200	-0.24208000
C	-3.60629300	-1.40259800	0.56831900
C	-4.88253400	-1.94373200	0.59974900
H	-5.08766800	-2.77391000	1.26640100
C	-5.86787000	-1.38881300	-0.21892700
H	-6.87466200	-1.79319200	-0.20825900
C	-5.55294000	-0.31685100	-1.05429300
H	-6.28557000	0.12855800	-1.71812200
C	-4.25668200	0.18241100	-1.05577200
C	-1.84512200	0.21113900	-0.25895800
C	-1.49127100	1.58313300	-0.23903500
C	-2.36982000	2.64681400	0.10208500
H	-3.41776500	2.43140600	0.28560700
C	-1.90107900	3.93337200	0.24104900
H	-2.58175800	4.73388900	0.51770700
C	-0.52945200	4.21785400	0.01450400
H	-0.16497000	5.23647900	0.11964800
C	0.33507300	3.20960800	-0.35591200
H	1.36728400	3.46285200	-0.56143200
C	-0.09084000	1.85290500	-0.46959600
C	0.55700900	-3.40155400	0.78994400
H	0.61728000	-4.45483300	0.49636100
H	-0.49323800	-3.11588700	0.87422200
H	1.00224300	-3.29445300	1.78272200
C	3.16383000	-3.08774000	-0.18645800
H	3.55676600	-2.83310000	0.80193600
H	3.86999500	-2.72878200	-0.93871400
H	3.10210200	-4.17812100	-0.26666900
C	0.98025900	-3.12444000	-2.01370800
H	1.54029700	-2.67951400	-2.83967700
H	-0.07926700	-2.92482100	-2.19465700
H	1.14913600	-4.20758300	-2.00380800
C	-0.20013000	0.33028900	2.92187800
H	-0.00635400	0.55233200	3.97682600
H	-0.67105800	-0.65135600	2.83094200
H	-0.89840100	1.06757100	2.51785600
C	2.46001700	-0.70454900	2.95457300
H	3.47293200	-0.70186500	2.54216900
H	2.09255200	-1.73377100	2.94833200

H	2.50163800	-0.35810800	3.99320200
C	2.01974800	2.03307300	2.44008500
H	1.40956900	2.82492500	1.99976300
H	3.04819500	2.15608200	2.08691400
H	2.01220200	2.13424500	3.53097300
C	3.38726800	2.30556200	-1.60023300
H	4.35067600	2.37506300	-2.11581700
H	3.41887000	2.94927100	-0.71782900
H	2.60385900	2.67148900	-2.26805500
C	4.63673300	0.24459600	-0.16960500
H	4.72339000	-0.80258600	0.12568900
H	4.63856700	0.85239600	0.73987400
H	5.51141800	0.51510400	-0.77101200
C	3.48987300	-0.25017600	-2.73431500
H	2.71821900	0.00244800	-3.46709400
H	3.52012300	-1.33803800	-2.64459600
H	4.46139000	0.09785800	-3.10295300
F	-2.67278300	-1.96098900	1.38860100
F	-3.97797000	1.19244800	-1.90538800
Fe	1.01514200	-0.07396500	-0.21491500
H	0.39139300	1.23552900	-1.29865100
N	-0.78874600	-0.62867900	-0.27949000
H	-1.09274500	-1.59488900	-0.26962900
P	1.48283300	-2.31412900	-0.41238400
P	1.35396500	0.37815100	1.91176200
P	3.04778000	0.54261800	-1.10301800

G= -2261.532981 au

TS1

C	-3.24816500	-0.20681400	-0.12710900
C	-3.74203600	-1.12986800	0.80799800
C	-5.05588200	-1.57708100	0.83614000
H	-5.35872300	-2.28198900	1.60200400
C	-5.94577800	-1.09866000	-0.12594700
H	-6.97762000	-1.43470600	-0.12258100
C	-5.51026700	-0.19943900	-1.09838000
H	-6.17008500	0.17471700	-1.87288200
C	-4.18421100	0.21771000	-1.08390500
C	-1.83099500	0.24076000	-0.12566100
C	-1.38417800	1.59942800	-0.19196800
C	-2.23521500	2.72513400	-0.13232500
H	-3.30818600	2.58446400	-0.03788700
C	-1.70981700	4.00146400	-0.17067800
H	-2.35850000	4.87085000	-0.11811800

C	-0.31263400	4.15335500	-0.27864500
H	0.11599500	5.15377300	-0.29685600
C	0.52715200	3.05367900	-0.34499600
H	1.58934800	3.24186700	-0.41224000
C	0.05421100	1.70744500	-0.29144000
C	0.60793400	-3.53783000	0.24729400
H	0.54099600	-4.50187100	-0.26853600
H	-0.38997000	-3.26028900	0.59546900
H	1.23680000	-3.66181600	1.13378600
C	2.97311500	-3.14635200	-1.14595100
H	3.52074000	-3.25337300	-0.20531200
H	3.61545700	-2.62177300	-1.85640100
H	2.76933500	-4.14781900	-1.53940000
C	0.52233000	-2.60407900	-2.45930200
H	1.00043900	-2.02592500	-3.25463500
H	-0.51680700	-2.27210100	-2.40085900
H	0.55437500	-3.66953700	-2.71488700
C	-0.23916200	0.06316800	3.03420900
H	-0.03120000	0.23455400	4.09560800
H	-0.77667700	-0.87963200	2.91666000
H	-0.88481000	0.86101700	2.65820300
C	2.29748200	-1.21546000	3.01118200
H	3.30917600	-1.30297200	2.60427900
H	1.81468300	-2.19371800	2.93051400
H	2.36472700	-0.94734000	4.07182500
C	2.10917300	1.59783200	2.67617100
H	1.58208000	2.45607600	2.25150300
H	3.15658000	1.65138200	2.36584600
H	2.06830100	1.64935700	3.76958400
C	3.82191900	2.35612300	-0.74850300
H	4.88559600	2.34115800	-1.00852100
H	3.70891500	2.79023000	0.24766100
H	3.30253900	2.99476100	-1.46593200
C	4.58322800	-0.20795300	0.02339900
H	4.43984800	-1.28619700	0.08686600
H	4.67931400	0.17871000	1.04255700
H	5.51743900	-0.00332000	-0.51041700
C	3.49332700	0.29436000	-2.59888000
H	2.83625600	0.93391200	-3.19495800
H	3.26426900	-0.74026000	-2.85885500
H	4.53664800	0.50838600	-2.85593600
F	-2.89102200	-1.62425600	1.74066200
F	-3.77778800	1.05374100	-2.05741300
Fe	1.00167400	-0.03169000	-0.17214000

H	0.55376700	0.80375900	-1.42803800
N	-0.84908700	-0.63600000	-0.08937300
H	-1.17757800	-1.59376000	-0.03095400
P	1.37367600	-2.22573000	-0.84639200
P	1.32114000	0.04104400	2.03211700
P	3.12896600	0.62058400	-0.80188400

G= -2261.52706 au

Imaginary frequency: -823.7651 cm⁻¹

IM2

C	-3.26090500	-0.27826700	-0.22825400
C	-3.77607300	-1.25699800	0.63396900
C	-5.08658700	-1.71345100	0.58434900
H	-5.41412100	-2.46487800	1.29364600
C	-5.94171600	-1.18336700	-0.38227900
H	-6.96940300	-1.52727400	-0.43995400
C	-5.48132100	-0.22066800	-1.28010400
H	-6.11738300	0.19741100	-2.05193500
C	-4.16152200	0.20636500	-1.18780000
C	-1.84699800	0.17753100	-0.14126300
C	-1.42178900	1.55753300	-0.02258500
C	-2.31707800	2.62958900	0.15504600
H	-3.38881600	2.45104700	0.17546300
C	-1.83015200	3.91794300	0.32172100
H	-2.51020900	4.75384500	0.45895200
C	-0.44349400	4.11400900	0.32558900
H	-0.04295100	5.11578400	0.47138300
C	0.43162900	3.03928300	0.15670700
H	1.49266000	3.25862700	0.20387400
C	0.00357700	1.70648200	-0.04120100
C	0.66617600	-3.51381200	0.48596600
H	0.86245700	-4.53461400	0.14166800
H	-0.41397200	-3.34869600	0.47356500
H	0.99390300	-3.42890500	1.52480100
C	3.28332600	-2.97288000	-0.36342200
H	3.62750700	-2.79865200	0.65968200
H	3.98914500	-2.48824800	-1.04149700
H	3.29709700	-4.05009200	-0.56098900
C	1.12940800	-2.94981700	-2.24578900
H	1.69813000	-2.43115300	-3.01989200
H	0.07093500	-2.75182600	-2.43604400
H	1.31680000	-4.02698400	-2.31557800
C	-0.11586100	-0.10430900	3.06766000
H	0.12165000	-0.05804600	4.13566800

H	-0.61973200	-1.04743200	2.84450300
H	-0.80590200	0.70577700	2.81751400
C	2.54490600	-1.12245900	2.88044400
H	3.54690600	-1.04694900	2.44706900
H	2.19861700	-2.15145300	2.75727900
H	2.61125700	-0.90683500	3.95238100
C	2.09206400	1.63911700	2.72974200
H	1.44344600	2.47716200	2.47070400
H	3.08609700	1.83574500	2.31827600
H	2.17309100	1.56504300	3.81936500
C	2.99580300	2.53691900	-1.76378900
H	3.81538800	2.64152500	-2.48194100
H	3.17217500	3.23164900	-0.94031300
H	2.05136800	2.80488800	-2.24116100
C	4.56320100	0.70962900	-0.27797200
H	4.78492300	-0.31913100	0.02011900
H	4.52917400	1.32109300	0.62855200
H	5.37870500	1.07478200	-0.91197000
C	3.39552200	-0.03187300	-2.75346400
H	2.58435700	0.11319900	-3.47087600
H	3.54971500	-1.10483500	-2.62979900
H	4.31637400	0.40714400	-3.15136800
F	-2.95477900	-1.79007800	1.56953900
F	-3.72412800	1.11342500	-2.07913000
Fe	0.98360200	-0.04338600	-0.24912000
H	0.68780100	0.05976400	-1.74910600
N	-0.86872000	-0.68295800	-0.15403300
H	-1.18576900	-1.64114900	-0.26582800
P	1.56971800	-2.26554600	-0.57434600
P	1.39928600	0.07041100	2.01075600
P	2.90789100	0.78128800	-1.14868800

G= -2261.539664 au

IM3

C	-2.63721900	-0.66984900	0.10507800
C	-2.89400500	-1.27954400	1.34044400
C	-4.10343200	-1.87986300	1.66484500
H	-4.23083600	-2.32251000	2.64606800
C	-5.12040000	-1.88812600	0.70956100
H	-6.07313200	-2.35324900	0.94123900
C	-4.91923700	-1.30735200	-0.54245000
H	-5.68674200	-1.30982300	-1.30791300
C	-3.69148100	-0.71608200	-0.81754100
C	-1.32460700	-0.03916800	-0.20221900

C	-1.14757800	1.34439700	-0.60293400
C	-2.18659200	2.28559400	-0.73156700
H	-3.21717000	2.00330000	-0.53282900
C	-1.88835000	3.58771500	-1.10989500
H	-2.67983600	4.32449500	-1.21310400
C	-0.55261600	3.94199700	-1.36135300
H	-0.31928000	4.96079400	-1.66531400
C	0.47337900	3.00747700	-1.22316600
H	1.49447500	3.32730300	-1.43413500
C	0.22373200	1.67494100	-0.82895000
C	3.70887400	-2.66924100	0.24491500
H	4.22103900	-3.50658100	-0.24202700
H	3.05406300	-3.06579900	1.02674900
H	4.45781600	-2.03386300	0.72702100
C	4.01976400	-1.31852200	-2.23689200
H	4.75320000	-0.61326200	-1.83317900
H	3.55168800	-0.86032500	-3.11116800
H	4.54231800	-2.23281000	-2.53805300
C	1.76592500	-3.02708400	-1.79581400
H	1.20784600	-2.60744800	-2.63515200
H	1.04799500	-3.46509100	-1.09519600
H	2.43289600	-3.82031500	-2.14979700
C	2.80868900	-0.13428400	2.83923500
H	2.94603600	0.40499000	3.78283400
H	3.78865800	-0.42121000	2.44901000
H	2.24294700	-1.04962000	3.03619700
C	2.94987600	2.42784900	1.57887500
H	2.44858400	3.19313800	0.98059700
H	3.92423200	2.21977800	1.12577400
H	3.10847600	2.81058800	2.59249300
C	0.45460400	1.44488700	2.58726100
H	-0.23303100	0.60664400	2.72405300
H	-0.07736900	2.22891600	2.04440700
H	0.76627500	1.82169000	3.56687200
F	-1.91277700	-1.28195700	2.27453200
F	-3.49999300	-0.17976300	-2.03570800
Fe	1.42503300	0.17305300	-0.55172400
H	1.19510300	-0.03522100	-2.05910700
N	-0.21402500	-0.72262300	-0.09915500
H	-0.33376500	-1.69149500	0.18396700
P	2.70753200	-1.66019400	-0.96723200
P	1.90538800	0.89266000	1.57887100

G= -2261.540266 au

PMe₃

P	0.00015100	-0.00050700	-0.60408600
C	-1.38535300	-0.88415600	0.28031700
H	-2.34537900	-0.45883900	-0.02793000
H	-1.38532300	-1.94095600	-0.00386400
H	-1.30336200	-0.81311300	1.37110300
C	1.45894800	-0.75648700	0.28049300
H	1.56933700	-1.80178800	-0.02400400
H	2.37363500	-0.22957400	-0.00811200
H	1.35951200	-0.71636100	1.37139600
C	-0.07383700	1.64130100	0.27990100
H	0.77892600	2.25762000	-0.02088600
H	-0.98519500	2.17244200	-0.01148400
H	-0.06296700	1.53423100	1.37080700

G= -461.023744 au

TS2

C	-2.63807800	-0.67909000	0.07439700
C	-2.91605100	-1.33602500	1.28105900
C	-4.12244100	-1.96791100	1.55168100
H	-4.26795100	-2.44648500	2.51330300
C	-5.11364300	-1.96014200	0.56957700
H	-6.06344300	-2.44953100	0.75940300
C	-4.89066300	-1.33239800	-0.65587100
H	-5.63776700	-1.32138500	-1.44116400
C	-3.66729300	-0.71069600	-0.87709600
C	-1.32998000	-0.01704200	-0.17614200
C	-1.17040900	1.38275600	-0.52863700
C	-2.23244800	2.30547100	-0.61383700
H	-3.25918800	1.98515600	-0.45876000
C	-1.95992400	3.63893600	-0.88338500
H	-2.76896000	4.36107600	-0.94824800
C	-0.62934700	4.04612300	-1.07413700
H	-0.41753600	5.09036700	-1.29567000
C	0.41652200	3.12622800	-0.99990800
H	1.43069600	3.47304300	-1.18798700
C	0.19483200	1.76180400	-0.72172600
C	4.53090800	-1.24770900	-1.21044400
H	5.06340000	-2.13403900	-1.57175100
H	4.96264700	-0.94304800	-0.25239800
H	4.66367800	-0.42671900	-1.91895200
C	2.30250500	-2.30775400	-2.66239900
H	2.41068500	-1.53705700	-3.42837700
H	1.25831400	-2.63455800	-2.66248900
H	2.94587600	-3.16246200	-2.89818100

C	2.74897300	-3.11290600	0.02820000
H	1.73251800	-3.50620700	0.13469600
H	3.12682900	-2.88578200	1.02862500
H	3.37535100	-3.89408700	-0.41584900
C	2.77011900	-0.42868200	2.68167400
H	2.98816200	0.03770600	3.64837500
H	3.71113800	-0.75304800	2.22881700
H	2.14912400	-1.31298900	2.85165100
C	3.03295600	2.19757500	1.56147200
H	2.54538800	3.03312800	1.05403800
H	3.94774400	1.95463100	1.01360400
H	3.29228500	2.49424300	2.58324700
C	0.51648200	1.30982900	2.64097000
H	-0.21453300	0.50560400	2.75388400
H	0.01390700	2.16063000	2.17655900
H	0.89269000	1.59915600	3.62738800
F	-1.95978800	-1.35318500	2.24041100
F	-3.45302400	-0.12893900	-2.07039800
Fe	1.40174700	0.23469900	-0.58070000
H	2.03581600	0.70162300	-1.99499900
N	-0.20733600	-0.68319400	-0.04496000
H	-0.32032800	-1.65765400	0.22094500
P	2.71524100	-1.56444500	-1.01457100
P	1.88919700	0.74296400	1.53793100

G= -2261.530336 au

Imaginary frequency: -480.2647 cm⁻¹

IM4

C	-2.73309800	-0.64866800	0.12281500
C	-3.07582900	-1.17742100	1.37389200
C	-4.31493400	-1.73973300	1.65262900
H	-4.51393000	-2.11946200	2.64815300
C	-5.26736800	-1.79380400	0.63441000
H	-6.24087800	-2.23114500	0.83106700
C	-4.97637800	-1.29558100	-0.63561700
H	-5.69290100	-1.33570100	-1.44796100
C	-3.72424400	-0.73694300	-0.86292100
C	-1.38901200	-0.05732200	-0.13846100
C	-1.18362300	1.33014700	-0.55577300
C	-2.23038000	2.24790800	-0.74709400
H	-3.26562300	1.94984300	-0.60428600
C	-1.93458700	3.55536700	-1.12113100
H	-2.73381300	4.27574900	-1.27120300

C	-0.59828000	3.92849300	-1.30799800
H	-0.36525900	4.94762800	-1.61077800
C	0.43605800	3.00667600	-1.11052000
H	1.46198300	3.32683400	-1.27635500
C	0.19334300	1.67762500	-0.71756500
C	4.58124500	-1.48020200	-0.82183300
H	5.09364800	-2.30914000	-1.32197000
H	4.88556900	-1.46517100	0.22832900
H	4.87984900	-0.53339100	-1.27707900
C	2.55316500	-1.95141100	-2.77582400
H	2.79573000	-1.03429200	-3.31895000
H	1.51609100	-2.21784000	-3.00218300
H	3.20802200	-2.75908100	-3.12011600
C	2.50619100	-3.36557900	-0.29048200
H	1.46789400	-3.67854500	-0.43938300
H	2.71043300	-3.37754200	0.78459400
H	3.16376800	-4.09214200	-0.78012700
C	3.07612000	-0.25760300	2.56653300
H	3.28412200	0.21443600	3.53283900
H	4.02665600	-0.46795600	2.06945000
H	2.56226900	-1.20750000	2.74227400
C	3.00579300	2.39255100	1.50059500
H	2.42927700	3.17116200	0.99672000
H	3.93042900	2.24120300	0.93887000
H	3.24099500	2.71252200	2.52150200
C	0.65868500	1.24086900	2.66683200
H	0.01212400	0.37096500	2.80539400
H	0.05294500	2.04293900	2.23845700
H	1.04951300	1.56179900	3.63809200
F	-2.15630100	-1.13554000	2.36426000
F	-3.44117400	-0.27753600	-2.09593400
Fe	1.40379900	0.14132300	-0.49850800
H	2.57879200	0.93743300	-1.11210700
N	-0.30285900	-0.75604300	0.03726500
H	-0.47281500	-1.70488800	0.36187400
P	2.73885400	-1.63654000	-0.95112300
P	2.02357500	0.82751800	1.48014700

G= -2261.543783 au

P^{C-H}

C	-2.92877500	-0.60735700	-0.27435600
C	-3.37032800	-1.84959200	0.19518700
C	-4.62665900	-2.37099900	-0.08935000
H	-4.90598700	-3.33693000	0.31570900

C	-5.49360800	-1.62365700	-0.88747900
H	-6.47905000	-2.01321600	-1.12188600
C	-5.10373500	-0.38114500	-1.38946800
H	-5.75484000	0.21519100	-2.01835000
C	-3.83788400	0.09647900	-1.07253100
C	-1.57449100	-0.07538300	0.04484100
C	-1.34492300	1.10675600	0.85163400
C	-2.37894200	1.86264600	1.44104200
H	-3.41785500	1.57103200	1.30640200
C	-2.06552300	2.97858600	2.20268800
H	-2.85133500	3.57074000	2.66320800
C	-0.71609900	3.33077000	2.37027600
H	-0.46242700	4.20629400	2.96537600
C	0.29798100	2.57236600	1.78682100
H	1.32928800	2.87978300	1.94326300
C	0.04106200	1.42435700	1.00321100
C	1.96776100	-3.26186000	-0.66114500
H	2.44248400	-3.97089200	-1.34787000
H	0.88702900	-3.43370200	-0.67683200
H	2.31773900	-3.46912300	0.35131900
C	4.16427400	-1.55832800	-1.33040700
H	4.61893400	-1.63200900	-0.34006600
H	4.51698700	-0.63006400	-1.78545100
H	4.49076900	-2.40683800	-1.94135100
C	1.80579600	-1.69398400	-2.94107600
H	2.04621500	-0.80504200	-3.52634300
H	0.72207500	-1.83813800	-2.99002900
H	2.29293600	-2.55946100	-3.40274100
C	0.54726700	-2.08486700	2.69052900
H	0.81038000	-2.41068000	3.70277900
H	0.57005600	-2.94851100	2.02107900
H	-0.47475600	-1.69714900	2.69301400
C	3.34894600	-1.55529500	2.33557400
H	4.12209300	-0.80536900	2.14732600
H	3.51974700	-2.39545400	1.66003600
H	3.44517000	-1.91585500	3.36514900
C	1.71939500	0.34509600	3.54980000
H	0.74128600	0.79833800	3.71179600
H	2.44230200	1.14899800	3.39218500
H	2.00811300	-0.22959200	4.43590900
C	1.34620600	3.50684600	-1.06156600
H	1.51758400	4.14185900	-1.93691500
H	2.11946300	3.70443400	-0.31564900
H	0.38003100	3.74906400	-0.61850700

C	2.96083200	1.81456300	-2.56976700
H	3.15351400	0.88850800	-3.11395800
H	3.79987900	1.99008700	-1.89078800
H	2.90929000	2.63556500	-3.29266600
C	0.10351400	1.73282200	-2.88517100
H	-0.88345700	1.79046500	-2.41750600
H	0.14890500	0.80286200	-3.45805100
H	0.22423800	2.57848900	-3.57084400
F	-2.53357100	-2.57364100	0.97047300
F	-3.45562600	1.29050500	-1.57108100
Fe	1.26242300	0.16489300	0.06002700
H	2.56766900	0.91164700	0.46402200
N	-0.49156700	-0.66173100	-0.39056800
H	-0.68806700	-1.49072400	-0.94782000
P	2.31699600	-1.49300400	-1.15421600
P	1.68750700	-0.75594900	2.05710100
P	1.40362800	1.71866000	-1.54968000

G= -2261.549139 au

TS3

C	-1.08247200	0.24228400	0.21629200
C	-2.04215600	0.87822900	-0.57517100
C	-3.27279100	0.30800300	-0.88076400
H	-3.96859400	0.85236900	-1.50911300
C	-3.57266100	-0.95427800	-0.36630500
H	-4.53049900	-1.41294500	-0.59022600
C	-2.65118400	-1.63079800	0.43356000
H	-2.85933000	-2.60968400	0.85039800
C	-1.43141400	-1.01926400	0.70081500
C	0.21539500	0.93789200	0.61394200
C	1.49832900	0.31984200	0.12274900
C	1.51722900	-0.71067800	-0.82721600
H	0.58453700	-1.09315900	-1.22877400
C	2.72870100	-1.23921000	-1.27544100
H	2.72918800	-2.03335600	-2.01659900
C	3.93483400	-0.74952500	-0.77348600
H	4.87764900	-1.16383000	-1.11947100
C	3.92576500	0.27738000	0.17642200
H	4.86236000	0.66130900	0.57114500
C	2.71736300	0.80782800	0.61608800
F	-1.75616200	2.09562600	-1.07862700
F	-0.53765400	-1.67088500	1.47588800
H	2.68752800	1.60948900	1.34750800
N	0.17329300	1.96795100	1.30946800

H 0.13881800 2.78524800 1.86458900
G= -755.024684 au
Imaginary frequency: -1147.8937 cm⁻¹

R^{C-F}

C	1.09181000	0.24710200	-0.23343000
C	2.15973000	0.84587400	0.44742700
C	3.35235200	0.18060000	0.71247100
H	4.13661800	0.69980100	1.25125100
C	3.50109200	-1.13567900	0.27671900
H	4.42842700	-1.66510600	0.47111500
C	2.46833400	-1.77823800	-0.40682500
H	2.55852000	-2.79802200	-0.76274100
C	1.29291000	-1.07633100	-0.64144300
C	-0.17308300	0.98762500	-0.54571500
C	-1.46578800	0.38179100	-0.10076100
C	-1.54188700	-0.37127900	1.08059200
H	-0.64234600	-0.54591600	1.66282000
C	-2.76371900	-0.87853200	1.52100400
H	-2.80904100	-1.44812500	2.44469400
C	-3.92402200	-0.65777100	0.77694700
H	-4.87418700	-1.06050400	1.11554200
C	-3.85670200	0.07509100	-0.41052000
H	-4.75244000	0.23585300	-1.00337700
C	-2.63812900	0.59269800	-0.84374700
F	2.02372000	2.10460600	0.89403300
F	0.29857900	-1.69271200	-1.31177900
H	-2.58806400	1.14078100	-1.78064900
N	-0.05685200	2.10272600	-1.16447700
H	-0.97759800	2.53741600	-1.28391600

G= -755.064376 au

IM5

C	2.06978100	1.35685000	0.04748000
C	1.01653800	2.18174500	0.49582200
C	1.00740300	3.56612500	0.51364200
H	0.14972000	4.08992600	0.92130100
C	2.12789500	4.24728500	0.03804000
H	2.15585900	5.33118100	0.03955000
C	3.21570600	3.50611300	-0.44115800
H	4.10072700	3.98687400	-0.84375500
C	3.16596900	2.12389400	-0.44141800
C	1.96814100	-0.08273300	-0.03599000

C	3.16112500	-0.94732100	-0.00234600
C	4.24601000	-0.67711200	0.86082500
H	4.21011100	0.20751300	1.48975600
C	5.34213900	-1.53024400	0.93799100
H	6.15550600	-1.29366300	1.61942400
C	5.39856600	-2.69123600	0.16041800
H	6.25377900	-3.35762300	0.22456900
C	4.34041700	-2.97576400	-0.70537600
H	4.37583200	-3.86109900	-1.33556400
C	3.24563500	-2.11819700	-0.78873900
C	-1.70009000	-1.58479600	-3.08242200
H	-2.00415200	-2.48216600	-3.63302900
H	-0.68195900	-1.30997800	-3.37039600
H	-2.35990400	-0.75922800	-3.36041600
C	-3.44779100	-2.55080600	-1.03213800
H	-4.19492400	-1.75865000	-1.10992100
H	-3.53855900	-3.00628200	-0.04194500
H	-3.66071500	-3.31557000	-1.78646600
C	-0.76250100	-3.43364400	-1.15697000
H	-0.70346900	-3.78800400	-0.12478100
H	0.25541400	-3.27891000	-1.52359800
H	-1.22955700	-4.20902500	-1.77242200
C	-1.81976600	2.41593300	-2.26151200
H	-2.51804600	3.19595600	-2.58849100
H	-1.59402600	1.75711100	-3.10412600
H	-0.88118900	2.87814200	-1.94444300
C	-4.19712800	1.04424300	-1.50724700
H	-4.79945100	0.56628300	-0.72924300
H	-4.14837500	0.36866100	-2.36547900
H	-4.69840600	1.96534700	-1.82387500
C	-2.95224000	2.78599700	0.32059100
H	-2.05660100	3.15835400	0.82057300
H	-3.63198400	2.40323100	1.08728600
H	-3.44293900	3.61319600	-0.20371600
C	-1.33225800	0.25462100	3.43985400
H	-1.72665800	-0.13840400	4.38302700
H	-1.63606200	1.29932400	3.33535900
H	-0.24014100	0.22305000	3.46441300
C	-3.77058200	-0.71747300	2.35690900
H	-4.30434800	-1.33832100	1.63201300
H	-4.15109300	0.30437100	2.26756000
H	-3.98887100	-1.08539100	3.36619200
C	-1.53831200	-2.44535600	2.60337500
H	-0.45266700	-2.57522900	2.61603900

H	-1.96176900	-3.20150800	1.93551700
H	-1.93142100	-2.61570200	3.61251900
F	-0.08418700	1.55742400	1.07343100
F	4.22438700	1.47295500	-0.97067800
Fe	-1.04123000	-0.13338500	0.02772000
H	2.46328300	-2.33206800	-1.51293700
N	0.74066700	-0.65428300	-0.19287300
H	0.88699200	-1.65271200	-0.30551000
P	-1.73786400	-1.84730100	-1.24120900
P	-2.49150700	1.40750300	-0.84581600
P	-1.94078700	-0.73241100	1.98381500

G= -2261.521949 au

TS4

C	-1.82063200	1.46317000	-0.08853200
C	-0.52828500	1.96154100	-0.44875100
C	-0.23847100	3.34271800	-0.50034400
H	0.70251400	3.68191600	-0.91862200
C	-1.15875300	4.24378000	-0.00856300
H	-0.92016700	5.30228500	0.02815900
C	-2.42829200	3.79576100	0.43694600
H	-3.17051600	4.48208500	0.82817000
C	-2.72764800	2.45578200	0.37178700
C	-1.98499800	0.04913900	0.02152400
C	-3.29589600	-0.63269200	-0.02416500
C	-4.31544200	-0.19934800	-0.89499600
H	-4.13452300	0.66336500	-1.52787000
C	-5.53363000	-0.86930700	-0.96746100
H	-6.29965000	-0.51418800	-1.65173900
C	-5.77121500	-1.99754300	-0.17761000
H	-6.72121800	-2.52076400	-0.23742700
C	-4.77300600	-2.44241700	0.69172800
H	-4.94823700	-3.30857800	1.32465400
C	-3.55492800	-1.76993600	0.76803000
C	1.84336100	-0.14673400	3.36599500
H	1.96625400	-0.76151900	4.26470400
H	1.01732600	0.55329300	3.51425200
H	2.75628600	0.43457600	3.21449800
C	2.94600100	-2.35359700	1.94282700
H	3.85262600	-1.85384400	1.59610100
H	2.76097500	-3.20875800	1.28593400
H	3.11230800	-2.72693000	2.95895500
C	0.19284100	-2.30296300	2.58424800
H	-0.08310300	-3.08084300	1.86637000

H	-0.69721400	-1.71574200	2.81805900
H	0.55841300	-2.78631200	3.49585500
C	2.89814200	2.71463800	1.03946400
H	3.76660000	3.34721100	0.82195100
H	2.95257200	2.39152400	2.08216300
H	1.98251000	3.29618200	0.92329100
C	4.54992600	0.56501300	0.29847500
H	4.77573000	-0.29985500	-0.32989200
H	4.61619700	0.25347900	1.34467000
H	5.30706300	1.33673900	0.12421700
C	3.17172000	1.99743700	-1.72355500
H	2.26024500	2.46145000	-2.10372800
H	3.46883900	1.22074200	-2.43490300
H	3.96719800	2.74783100	-1.66975000
C	0.94537000	-1.17164400	-3.27706300
H	1.12054000	-1.96713200	-4.00918800
H	1.47991800	-0.27163800	-3.59318800
H	-0.12104400	-0.93348900	-3.25015200
C	3.22760800	-2.24858800	-1.95654700
H	3.68866700	-2.67241200	-1.06017700
H	3.83893500	-1.40364800	-2.28508300
H	3.23122600	-3.00832500	-2.74649500
C	0.66046400	-3.32546700	-1.44383000
H	-0.42290600	-3.18179100	-1.40683500
H	0.96941300	-3.83325000	-0.52511300
H	0.90083900	-3.97080600	-2.29619800
F	0.13614400	1.18621900	-1.45464900
F	-3.95058800	2.06254100	0.79959900
Fe	0.97465000	-0.12224600	-0.04593200
H	-2.80650400	-2.11081700	1.47824600
N	-0.85534500	-0.66614700	0.20666600
H	-1.07610500	-1.65263900	0.30027700
P	1.49234500	-1.18696500	1.86408200
P	2.84113100	1.21597200	-0.06619600
P	1.49979600	-1.66629200	-1.57380600

G= -2261.51406 au

Imaginary frequency: -177.4697 cm⁻¹

P^{C-F}

C	-1.61116400	1.37586400	-0.04439300
C	-0.20163600	1.61798600	-0.03355400
C	0.17617200	2.97213000	0.04205600
H	1.22807700	3.23938300	0.08972200
C	-0.74702100	4.02079000	0.07238000

H	-0.40027700	5.05085600	0.12471500
C	-2.11946300	3.76423500	0.04728500
H	-2.86341600	4.55230700	0.08125900
C	-2.52469500	2.44066300	0.00366600
C	-1.97065600	-0.03779400	0.03109900
C	-3.33811600	-0.60558100	-0.13065800
C	-4.10656900	-0.31196800	-1.26770500
H	-3.72332100	0.38751600	-2.00307400
C	-5.34203900	-0.92589200	-1.45867600
H	-5.92235000	-0.69947600	-2.34850200
C	-5.83692000	-1.82664400	-0.51140600
H	-6.80531100	-2.29595700	-0.65948800
C	-5.08441400	-2.11738300	0.62686900
H	-5.46634700	-2.80856600	1.37288100
C	-3.83895200	-1.51581500	0.81208200
C	0.47620800	1.40147800	3.10185600
H	0.69420100	1.32000000	4.17177500
H	-0.60355400	1.34290000	2.94422600
H	0.80474100	2.37544400	2.73420700
C	3.04018300	0.21729800	2.78888800
H	3.45565000	1.18302600	2.49104600
H	3.67634100	-0.56888700	2.37326500
H	3.06393700	0.15074500	3.88177100
C	0.73548700	-1.41196600	3.13334500
H	1.28471300	-2.31006000	2.83935300
H	-0.32673800	-1.58015800	2.93714100
H	0.87936500	-1.25159200	4.20694900
C	3.83729900	2.14535900	-0.24488800
H	4.45965600	2.69808200	-0.95665100
H	4.49462400	1.56451900	0.40888100
H	3.29378100	2.86469300	0.37259100
C	3.95256300	0.00510600	-2.04788000
H	3.47031600	-0.55346600	-2.85128900
H	4.46167900	-0.70000100	-1.38472200
H	4.70240800	0.66982100	-2.48977700
C	2.07296200	2.02885400	-2.54288000
H	1.54414500	2.91028700	-2.17961600
H	1.35632600	1.39594600	-3.06977300
H	2.89874400	2.33214300	-3.19446900
C	0.46993500	-3.67956400	0.06926100
H	0.90939000	-4.67198100	-0.07242000
H	-0.41356800	-3.60919800	-0.57251100
H	0.15494500	-3.58220500	1.11169800
C	1.91227900	-2.77924800	-2.19192700

H	2.95188800	-2.63621700	-2.49328800
H	1.27275400	-2.07627500	-2.73297200
H	1.63045200	-3.81631100	-2.39651900
C	3.21738900	-3.04196500	0.37833100
H	3.12262600	-3.04018900	1.46835500
H	4.08041500	-2.42350400	0.11645600
H	3.41030700	-4.06795300	0.04779800
F	0.37897900	-0.28980200	-1.99458100
F	-3.86078500	2.19978300	0.03802000
Fe	0.84357700	-0.08464400	-0.12327300
H	-3.25860200	-1.73453200	1.70462700
N	-0.95968300	-0.82750300	0.24564300
H	-1.22008900	-1.80937800	0.24792900
P	1.30486300	0.05285000	2.13725400
P	2.66934100	0.99480900	-1.13265000
P	1.67980500	-2.34192300	-0.40632700

G= -2261.593961 au