Si-H Bond Activation by Electrophilic Phosphinidene Complexes

Supporting Information

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Table S1. Coordinates (Å) for optimized reactants $CpFe(CO)_2PNMe_2 + SiH_4$.

E(elec) = -1311.249376, E(Gibbs) = -1311.083925 (G_{rel} = 0 kcal/mol)

Fe	-1.05918600	-0.12053500	0.09381500
P	0.52697900	0.78039300	-1.12414200
N	1.48666700	1.92731200	-0.42585200
C	2.54575000	2.53742500	-1.26477000
H	2.51684800	2.11699800	-2.27052300
H	3.52370700	2.34006400	-0.81337600
H	2.38786300	3.61973400	-1.31581800
C	1.49451200	2.46569100	0.94298000
H	0.71833500	2.01084000	1.55135500
H	2.47043000	2.27185500	1.40151300
H	1.33581300	3.54897100	0.90701100
C	0.00904000	-0.47621900	1.47730400
O	0.68276800	-0.73940000	2.36650400
C	-1.66032600	1.43977600	0.71619600
O	-2.08149800	2.43111600	1.10736800
C	-2.69583500	-1.49462900	0.42111400
C	-1.55136500	-2.21522000	-0.03877400
C	-1.20438300	-1.73349500	-1.33486900
C	-2.13177500	-0.70582900	-1.68249400
C	-3.05267700	-0.56658700	-0.59963300
H	-3.19811700	-1.62766400	1.36977500
H	-1.03470200	-2.99703200	0.50328500
H	-0.39051700	-2.09667100	-1.94874900
H	-2.15755900	-0.15302200	-2.61233900
H	-3.87983000	0.13093000	-0.56088900

Si	3.76080400	-2.24055800	0.08882500
H	2.62824600	-1.43272700	-0.46370000
H	4.51732500	-1.38233800	1.03403200
H	3.18760100	-3.40951800	0.80032600
H	4.62296900	-2.67497300	-1.03484400

Table S2. Coordinates (Å) for optimized transition state 1 for $CpFe(CO)_2PNMe_2 + SiH_4$.

E(elec) = -1311.215957, E(Gibbs) = -1311.043740 (G_{rel} = +25 kcal/mol)

Fe	1.02461900	-0.15239700	0.05237900
P	-1.19359800	0.33330800	-0.44523500
N	-2.28783000	-0.93426500	-0.32184300
C	-3.52122000	-0.88174900	-1.12386700
H	-3.37769200	-0.24075100	-1.99620000
H	-4.37128400	-0.50502800	-0.53754000
H	-3.76283700	-1.89137900	-1.47238800
C	-2.37087600	-1.84789600	0.82169300
H	-1.39510500	-1.96838400	1.29304600
H	-3.07918000	-1.47741000	1.57717500
H	-2.71214800	-2.83057300	0.47983300
C	0.74764800	-0.41404000	1.80206500
O	0.60331500	-0.56016200	2.92903700
C	0.77928800	-1.86159300	-0.43608000
O	0.67151700	-2.95188700	-0.76692000
C	3.02039000	0.54677200	0.40612200
C	2.13619100	1.67056600	0.26093500
C	1.59922500	1.62661000	-1.05535200
C	2.09480900	0.46807400	-1.71095800
C	2.99333400	-0.19003800	-0.80320000

H	3.59727100	0.29874300	1.28761700
H	1.95875500	2.43969500	1.00079100
H	0.90047100	2.33630300	-1.47771400
H	1.87312400	0.16218000	-2.72449200
H	3.54582500	-1.09939100	-1.00184200
Si	-2.29310300	2.43838400	0.22942000
H	-1.43032200	1.08523900	0.93715500
H	-2.67032800	2.79962900	1.61933700
H	-1.25495900	3.34905600	-0.29500100
H	-3.51087400	2.30341100	-0.59717300

Table S3. Coordinates (Å) for optimized transition state 2 for $CpFe(CO)_2PNMe_2 + SiH_4$.

E(elec) = -1311.204948, E(Gibbs) = -1311.033446 (G_{rel} = +32 kcal/mol)

Fe	0.94606200	-0.18370100	0.09890600
P	-1.14119400	0.04182000	-0.92987700
N	-2.46399300	-0.75660100	-0.26745500
C	-3.52751600	-1.21389500	-1.17794600
H	-3.12600100	-1.35516800	-2.18388800
H	-4.35830700	-0.49635500	-1.22429800
H	-3.91702500	-2.17310500	-0.81978100
C	-2.87455000	-0.68767900	1.13749700
H	-2.02012500	-0.46578600	1.77923200
H	-3.64575000	0.07891100	1.30108500
H	-3.28649000	-1.65680400	1.43872500
C	0.57053400	0.48786400	1.71912800
O	0.38643300	0.91657100	2.76486200
C	0.48604100	-1.86757300	0.54536800
O	0.24343700	-2.94837500	0.82786400

C	3.03542900	0.23138400	0.28899000
C	2.38839300	1.33963400	-0.35953700
C	1.82807700	0.86116700	-1.57211300
C	2.10111700	-0.53512500	-1.68134800
C	2.87123900	-0.91168200	-0.53735900
H	3.56692900	0.26398700	1.23111300
H	2.35494000	2.35816900	0.00341100
H	1.26688700	1.45038400	-2.28592700
H	1.80682500	-1.18177800	-2.49662500
H	3.23974600	-1.90578100	-0.31797400
Si	-1.56840000	2.47479400	-0.06652400
H	-1.61415000	1.33149600	-1.52087400
H	-1.76237200	2.24681400	1.38165800
H	-0.32358100	3.21346400	-0.37158200
H	-2.76723500	3.11942500	-0.65202900

Table S4. Coordinates (Å) for optimized product for $CpFe(CO)_2PNMe_2 + SiH_4$.

E(elec) = -1311.271632, E(Gibbs) = -1311.095640 (G_{rel} = –7 kcal/mol)

Fe	0.97030700	0.07244500	0.11742800
P	-1.21411300	0.08097800	-0.58072500
N	-2.17983600	-1.15569200	0.09014100
C	-1.69780300	-2.53447700	-0.08037200
H	-0.62195400	-2.58616400	0.09906900
H	-1.90889000	-2.93062500	-1.08607300
H	-2.19540300	-3.17519700	0.65398100
C	-3.64384300	-1.06253100	-0.03154100
H	-4.00369000	-0.09719400	0.33303300
H	-3.99850300	-1.21199000	-1.06247000

H	-4.08890300	-1.83479500	0.60255300
C	0.91522800	1.76963700	0.68490500
O	0.93187100	2.85448500	1.05141800
C	0.51627200	-0.59725800	1.72290400
O	0.26727900	-1.03305800	2.75028500
C	3.02123800	-0.54226400	0.11936200
C	2.86210100	0.52309800	-0.80991100
C	1.91602500	0.12325200	-1.79888600
C	1.53409900	-1.22595600	-1.50833300
C	2.21016700	-1.63627500	-0.33324700
H	3.66559200	-0.53995900	0.98842300
H	3.34697800	1.48945100	-0.75144000
H	1.59423300	0.71194900	-2.64742700
H	0.84903100	-1.83014700	-2.08799900
H	2.12801100	-2.60360500	0.14531900
Si	-2.36082900	2.06077200	-0.37902800
H	-1.23430900	-0.05656700	-2.00307300
H	-2.54322800	2.32397400	1.06553400
H	-1.44498000	3.03685500	-1.01130800
H	-3.64391700	1.97006100	-1.10787400

Table S5. Mulliken partial charges (au)

	reactant	TS1	TS2	product
Fe	-0.708	-0.639	-0.603	-0.621
P	0.585	0.438	0.409	0.477
N	-0.417	-0.473	-0.477	-0.484
C	-0.330	-0.324	-0.321	-0.336
H	0.214	0.190	0.192	0.178
H	0.205	0.176	0.178	0.173
H	0.206	0.196	0.192	0.199

C	-0.336	-0.329	-0.327	-0.339
H	0.193	0.179	0.176	0.198
H	0.213	0.182	0.181	0.175
H	0.214	0.198	0.196	0.195
C	0.408	0.418	0.408	0.421
O	-0.219	-0.219	-0.214	-0.216
C	0.408	0.420	0.429	0.427
O	-0.219	-0.215	-0.206	-0.207
C	-0.083	-0.100	-0.110	-0.122
C	-0.106	-0.111	-0.092	-0.088
C	-0.113	-0.099	-0.112	-0.115
C	-0.112	-0.102	-0.095	-0.108
C	-0.105	-0.103	-0.090	-0.092
H	0.217	0.215	0.218	0.217
H	0.217	0.206	0.212	0.217
H	0.216	0.202	0.205	0.209
H	0.215	0.212	0.216	0.202
H	0.218	0.216	0.219	0.211
Si	0.265	0.381	0.282	0.275
H	-0.118	-0.071	-0.014	0.008
H	-0.047	-0.013	-0.018	-0.010
H	-0.048	-0.024	-0.028	-0.030
H	-0.034	-0.007	-0.005	-0.016