Supporting Information for

Synthesis and Structure of a Ferrocenylsilane-bridged Bisphosphine

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Contents

1. NMR spectra of the newly obtained compounds.

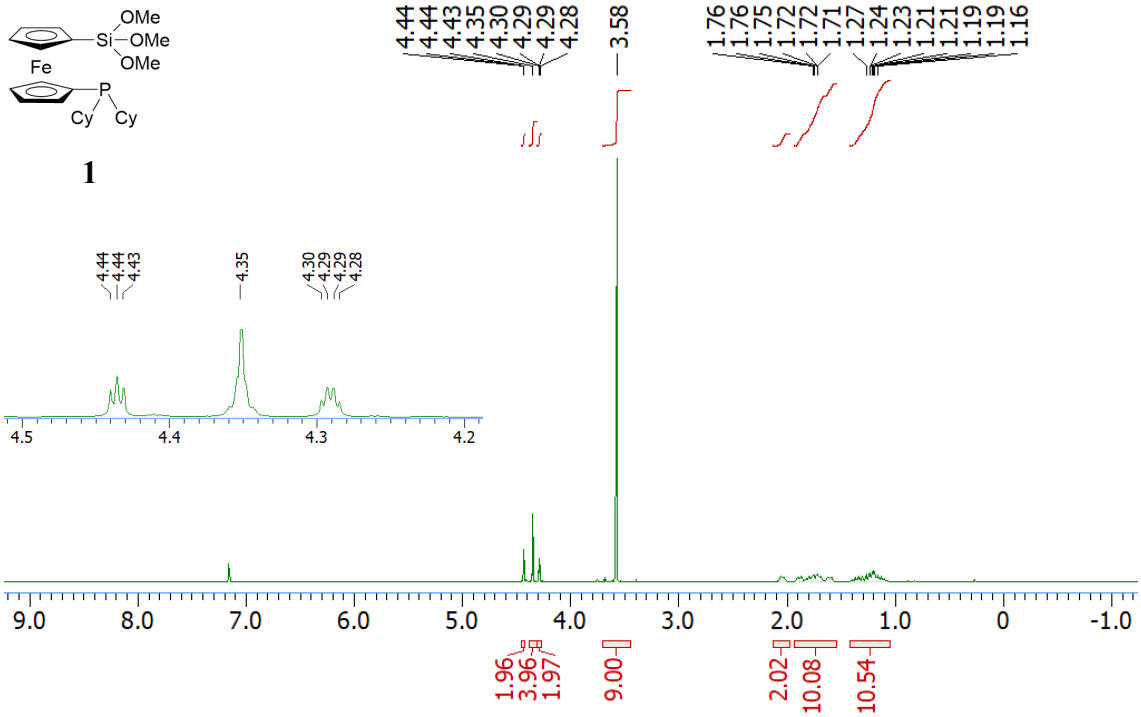


Figure S1. ^{1}H NMR spectrum (400 MHz) of **1** in C_6D_6 drawn in ppm.

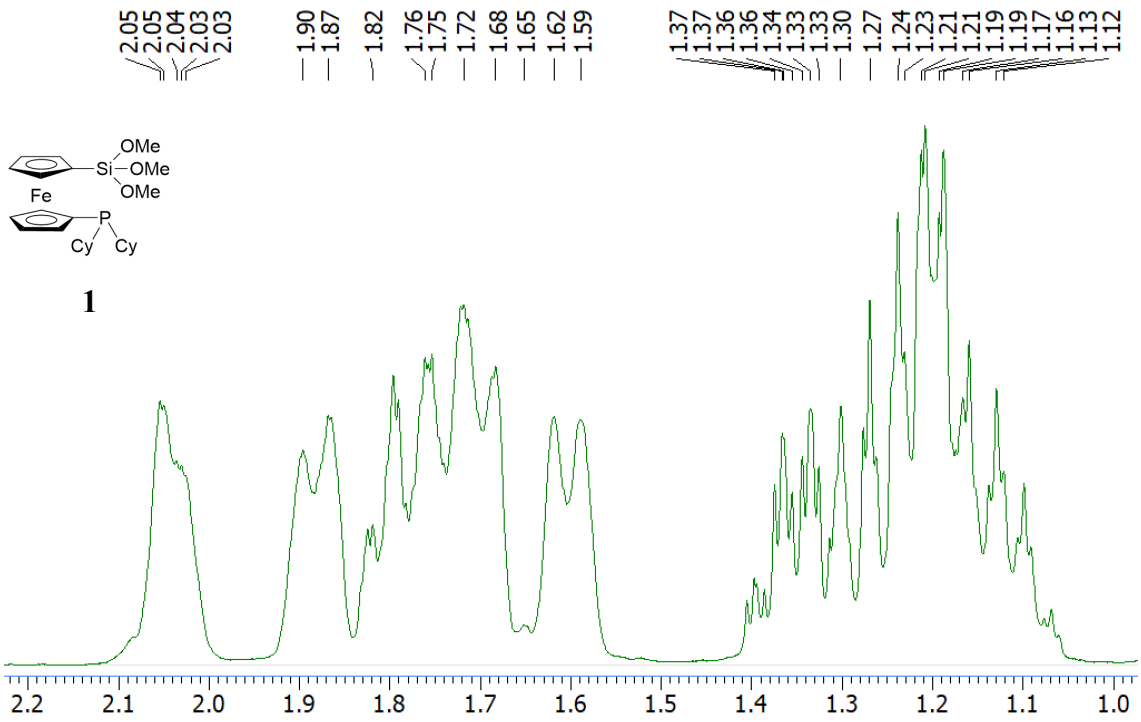


Figure S2. Selected region of ^{1}H NMR spectrum (400 MHz) of **1** in C_6D_6 drawn in ppm.

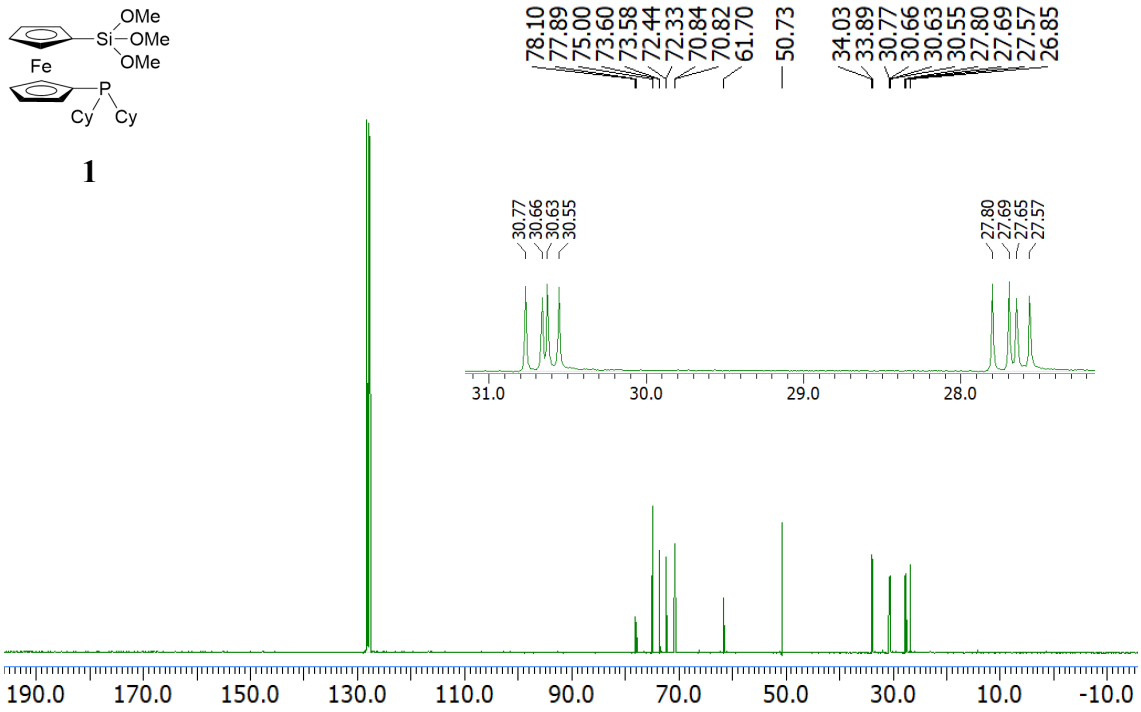


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **1** in C_6D_6 drawn in ppm.

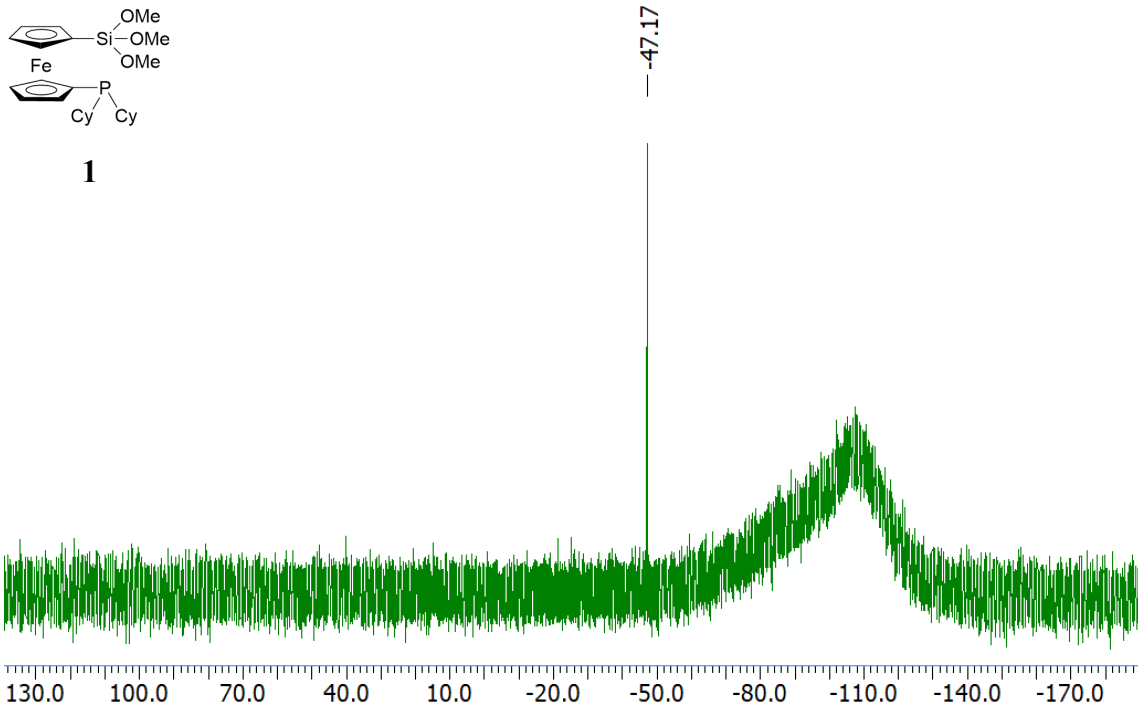
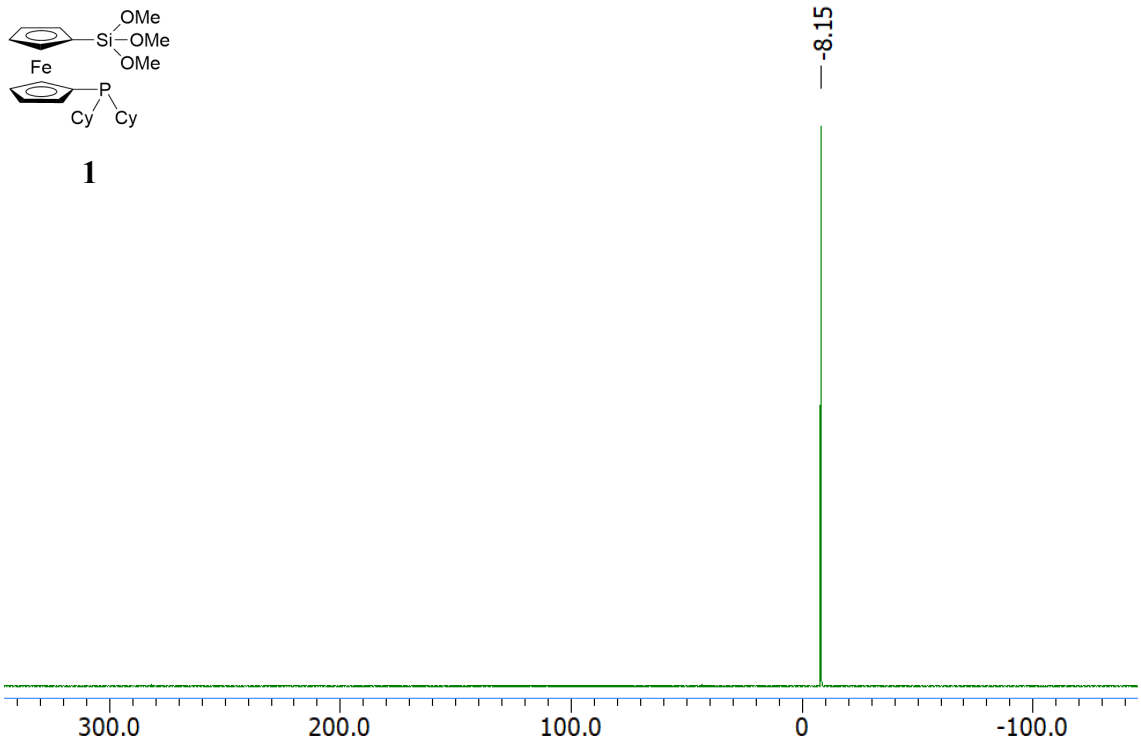


Figure S4. $^{29}Si\{^{1}H\}$ NMR spectrum (79.5 MHz) of **1** in C_6D_6 drawn in ppm.



1

Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of **1** in C_6D_6 drawn in ppm.

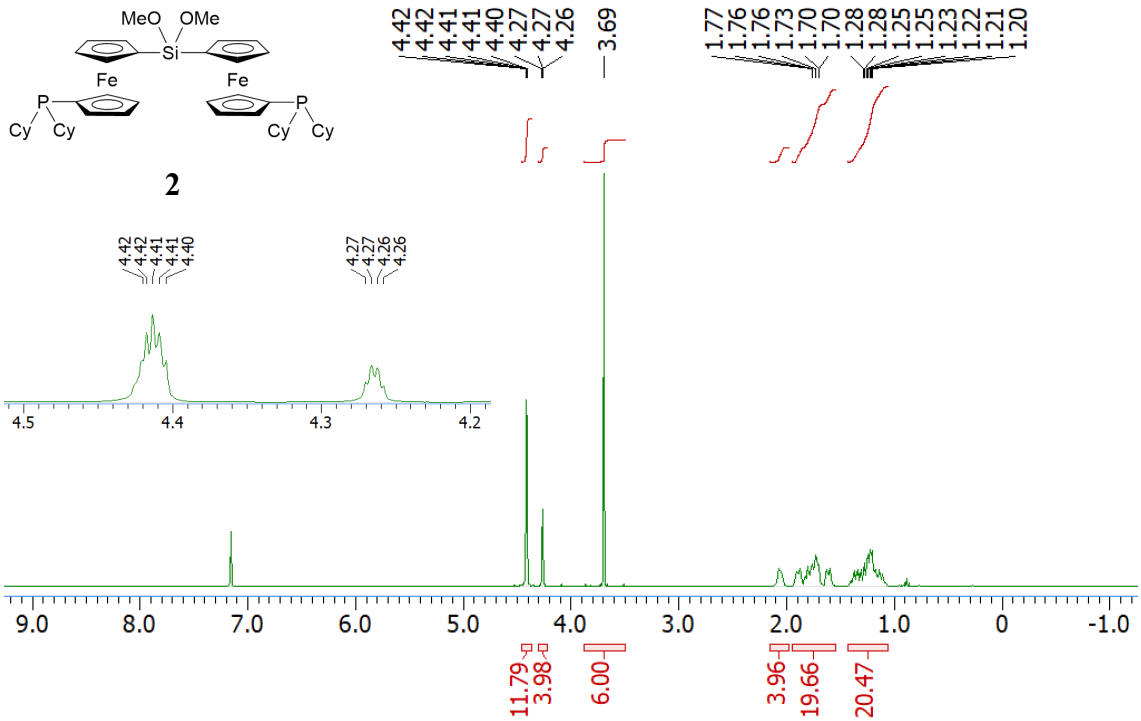


Figure S6. ^{1}H NMR spectrum (400 MHz) of **2** in C_6D_6 drawn in ppm.

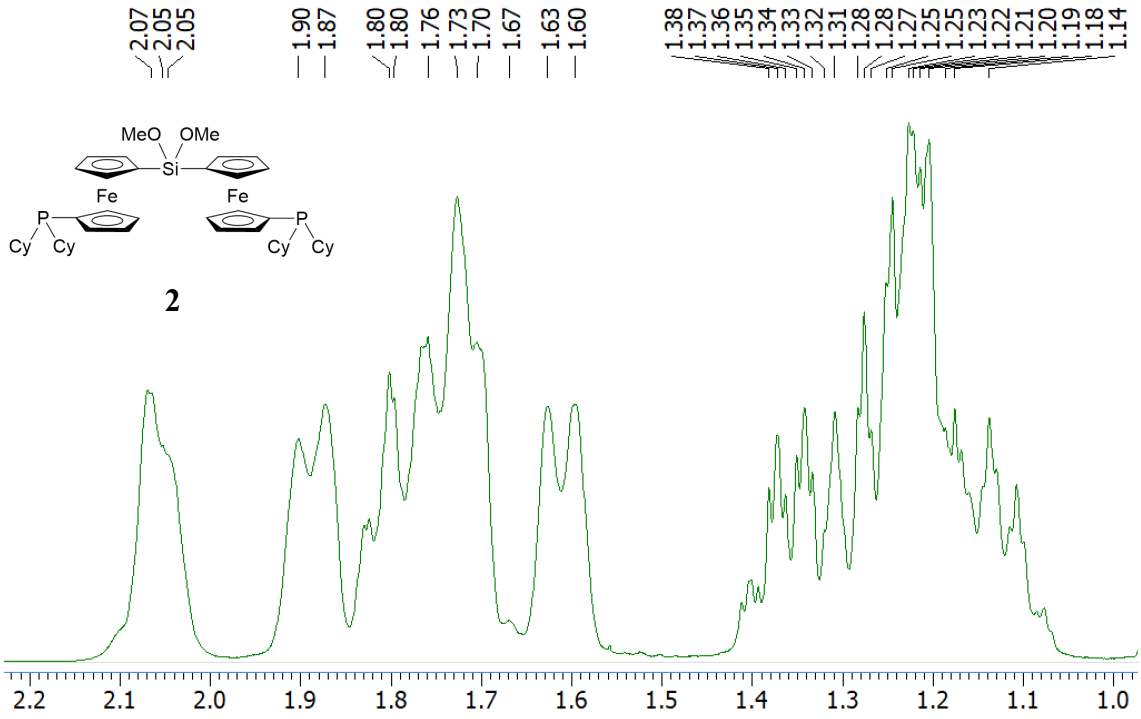


Figure S7. Selected region of ^{1}H NMR spectrum (400 MHz) of **2** in C_6D_6 drawn in ppm.

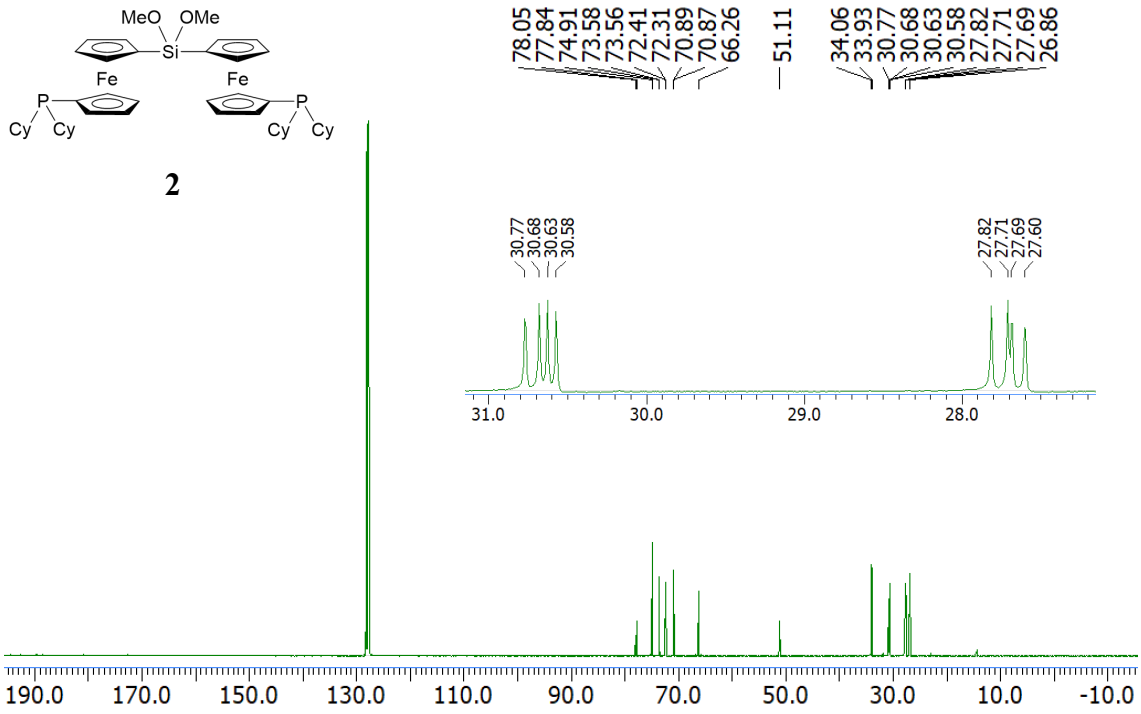


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz) of **2** in C_6D_6 drawn in ppm.

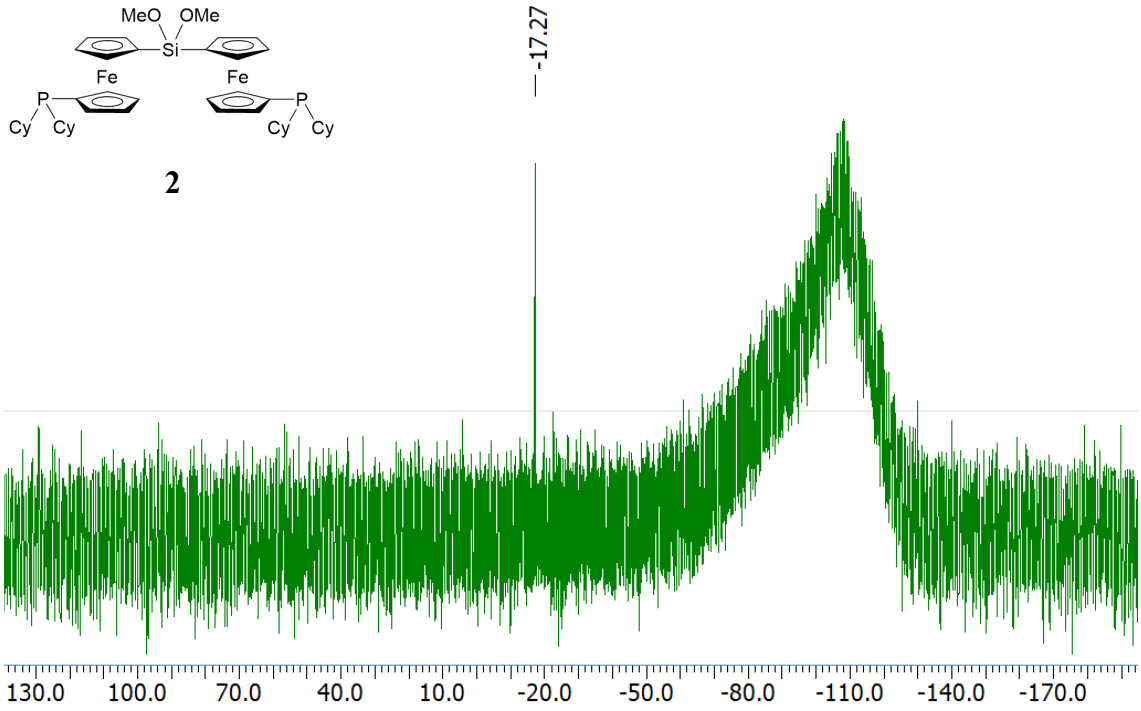
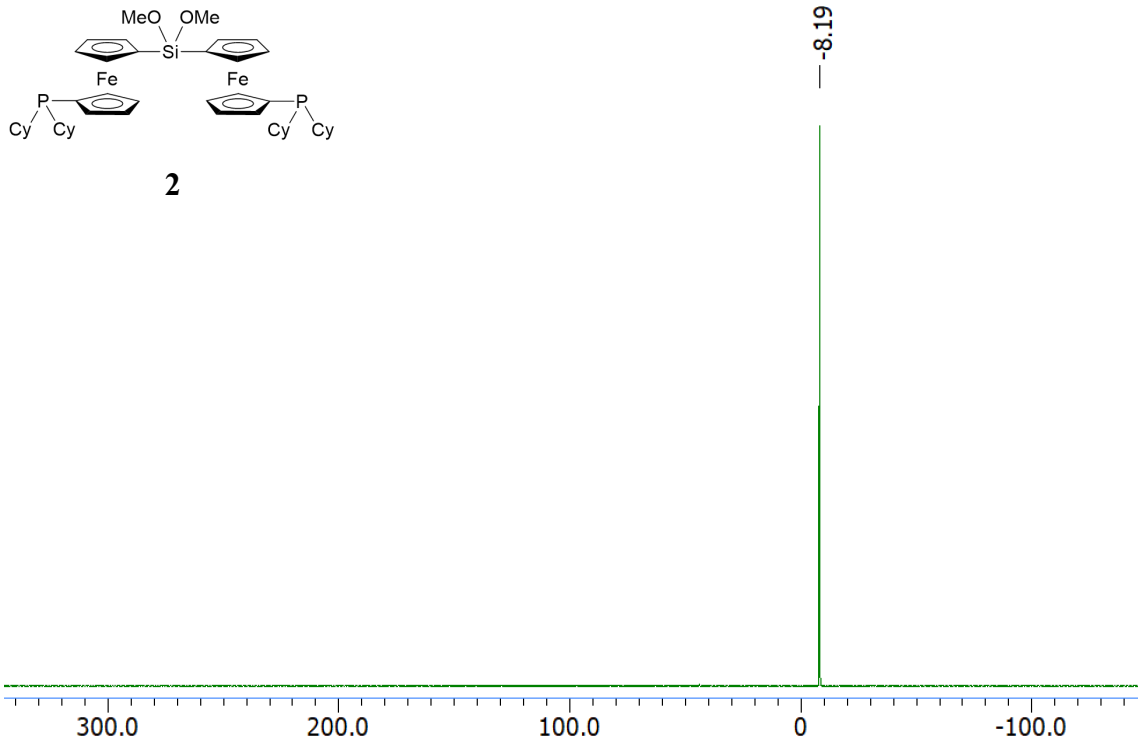


Figure S9. $^{29}Si\{^{1}H\}$ NMR spectrum (79.5 MHz) of **2** in C_6D_6 drawn in ppm.



2

Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz) of **2** in C_6D_6 drawn in ppm.

2. Crystallographic data

Table S1. Crystal data and structural refinement data for **1** and **2**.

Compound	**1**	**2**
Formula	$C_{25}H_{39}FeO_3PSi$	$C_{46}H_{66}Fe_2O_2P_2Si$
Molecular Weight	502.47	852.71
Temperature / ºC	−170	−170
λ / Å	0.71073	0.71073
Crystal size / mm^3	0.18 x 0.15 x 0.10	0.10 x 0.07 x 0.02
Crystal system	Triclinic	Monoclinic
Space group	*P*-1 (#2)	$P2_1/c$ (#14)
a / Å	10.4839(2)	10.1549(2)
b / Å	10.5500(2)	34.1666(7)
c / Å	24.0736(4)	12.6691(3)
α / º	93.5710(10)	90
β / º	96.4280(10)	104.079(2)
γ / º	111.368(2)	90
V / $Å^3$	2448.71(8)	4263.61(16)
Z	4	4
μ / mm^{-1}	0.755	0.820
$D_{calcd.}$ / $g \cdot cm^{-3}$	1.363	1.328
θ_{max} / º	25.242	25.242
Refl./restr./param.	12407/0/565	11086/0/478
Completeness / %	99.6	99.9
GOF	1.022	1.129
R_1 ($I>2\sigma(I)$)	0.0311	0.0634
wR_2 ($I>2\sigma(I)$)	0.0791	0.1187
R_1 (all data)	0.0381	0.0921
wR_2 (all data)	0.0827	0.1284
Largest diff. peak and hole / $e \cdot Å^{-3}$	0.641, −0.400	1.785, −0.654
CCDC number	2141476	2141477

3. Coordinates of theoretically optimized structures

Theoretical calculations: All calculations were carried out using the density functional theory (DFT) method with a B3PW91-D3(BJ) functional,[S1,S2] and geometry optimizations and vibrational frequencies were calculated in the gas phase using the 6-311G(3d) basis sets, as implemented in the Gaussian 16 program package.[S3] Computational time was generously provided by the Supercomputer Laboratory at the Institute for Chemical Research (Kyoto University). The coordinates of the optimized structures are shown below.

Optimized structures: .xyz file format.

· Compound **4**

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Compound_4, electronic energy = -3096.48322997 a.u

Fe	0.867712	-0.629374	0.330172
C	2.750097	-1.100952	-0.263853
C	2.283516	-2.040438	0.712936
H	2.725940	-2.201023	1.685787
C	1.109555	-2.664382	0.216326
H	0.510170	-3.393650	0.742648
C	0.835077	-2.125024	-1.071489
H	-0.019117	-2.353745	-1.691490
C	1.838368	-1.168632	-1.369019
H	1.878704	-0.543739	-2.249351
C	-0.923995	0.355929	0.241510
C	0.175809	1.239737	-0.008790
H	0.358872	1.768411	-0.932641
C	1.027572	1.241269	1.127653
H	1.962775	1.771777	1.221553
C	0.481405	0.344362	2.084204
H	0.928368	0.082557	3.032775
C	-0.717587	-0.195922	1.545123
H	-1.345778	-0.930919	2.026374
Si	4.112603	0.092638	-0.069437
O	5.586406	-0.493895	-0.509709
C	5.804288	-1.038510	-1.793943
H	5.117136	-1.866683	-1.996505
H	6.827295	-1.415531	-1.836865
H	5.676691	-0.282271	-2.575843
O	3.723178	1.359567	-1.039749
C	4.577668	2.466743	-1.222931
H	4.493743	3.166393	-0.384894
H	4.281124	2.984584	-2.136872
H	5.625380	2.162316	-1.320006
O	4.281894	0.505526	1.502050
C	5.496278	0.815647	2.152364

H	6.314322	0.187661	1.792858
H	5.361164	0.648733	3.222582
H	5.762683	1.865861	1.996050
P	-2.273024	0.093942	-0.945874
C	-3.274777	-1.208235	-0.076326
H	-3.351734	-0.948857	0.987047
C	-2.588012	-2.569444	-0.190878
H	-2.455793	-2.808662	-1.254147
H	-1.587739	-2.518330	0.241553
C	-3.401831	-3.671454	0.477283
H	-2.893344	-4.635052	0.363288
H	-3.457900	-3.475339	1.556506
C	-4.811856	-3.740576	-0.095614
H	-5.398528	-4.511324	0.415473
H	-4.756298	-4.039169	-1.150793
C	-5.506979	-2.388599	0.006010
H	-5.656541	-2.138758	1.064815
H	-6.504213	-2.435149	-0.444764
C	-4.689690	-1.280982	-0.652669
H	-5.205581	-0.324975	-0.527886
H	-4.627064	-1.462371	-1.734102
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H	-4.213493	1.460114	-1.178729
C	-3.650878	1.872183	0.853443
H	-2.725849	1.979690	1.431920
H	-4.179313	1.010439	1.271925
C	-4.505583	3.126689	1.014762
H	-5.473855	2.968317	0.520953
H	-4.723209	3.299034	2.074638
C	-3.827121	4.347435	0.404987
H	-4.469434	5.229601	0.499548
H	-2.909811	4.566945	0.967104
C	-3.468978	4.101485	-1.055928
H	-2.950719	4.971095	-1.474598
H	-4.390679	3.976695	-1.639774
C	-2.604504	2.853938	-1.207285
H	-1.652090	3.019789	-0.691335
H	-2.364688	2.673971	-2.260711

· Compound **5**

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Compound_5, electronic energy = -5442.81267319 a.u

Si	-0.146577	-1.789215	1.471889
O	-0.111868	-0.497820	2.481711
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H	-0.951855	0.835818	3.768558
H	-2.012300	0.334559	2.434741
H	-1.701217	-0.775661	3.787381
O	-0.990893	-2.959004	2.275934
C	-1.148116	-4.258038	1.756303
H	-1.504045	-4.910489	2.555690
H	-1.884639	-4.269398	0.945815
H	-0.201276	-4.659717	1.377960

Fe	2.944168	-1.084381	0.320338
C	1.566096	-2.341486	1.126184
C	2.012094	-2.827614	-0.148892
H	1.391186	-2.948179	-1.025066
C	3.412436	-3.041038	-0.090037
H	4.032181	-3.381630	-0.906638
C	3.857352	-2.687267	1.214081
H	4.881965	-2.679074	1.557247
C	2.727509	-2.265301	1.962191
H	2.744458	-1.888319	2.974736
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C	3.732354	0.125419	-1.125476
H	4.259132	-0.224961	-2.001073
C	2.326721	0.317904	-1.029008
H	1.597936	0.124228	-1.803334
C	2.035127	0.741466	0.295973
H	1.057212	0.917679	0.714257
C	3.254805	0.791196	1.018771
H	3.357970	1.019864	2.069589
P	6.063084	0.458619	0.668892
C	6.920408	-0.248111	-0.819316
H	6.486063	0.190305	-1.726629
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H	7.085684	-2.200817	0.064371
H	5.644234	-1.980642	-0.908292
C	7.432245	-2.393811	-2.053209
H	6.991706	-2.019031	-2.986905
H	7.278543	-3.478532	-2.051133
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H	9.376874	-2.530491	-1.147741
H	9.422750	-2.494525	-2.904220
C	9.143748	-0.559007	-1.976156
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C	6.408910	2.282353	0.458821
H	7.494461	2.363819	0.612204
C	6.060592	2.871876	-0.904475
H	4.986640	2.740674	-1.080877
H	6.574419	2.328511	-1.703022
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H	-1.186183	0.874300	0.081039
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H	-9.935043	0.155815	-2.061959
H	-9.770376	-1.586809	-2.220924
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H	-9.383613	-1.807415	0.213909
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H	-9.549863	0.156721	1.709261
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C	-7.793779	0.477875	0.488950
H	-7.462657	1.344337	1.069001
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C	-6.063373	3.540981	-0.517073
H	-5.897210	3.808061	-1.569323
H	-7.127492	3.308237	-0.420085
C	-5.719574	4.731078	0.374384
H	-6.323415	5.598771	0.087808
H	-5.994139	4.490614	1.410060
C	-4.235365	5.071606	0.316489
H	-4.007849	5.903086	0.991848
H	-3.982922	5.413927	-0.695748
C	-3.383698	3.855182	0.657228
H	-2.318416	4.095738	0.572135
H	-3.555778	3.573146	1.704746
C	-3.726106	2.673827	-0.242469
H	-3.126538	1.803657	0.025604
H	-3.470045	2.919753	-1.281233

· Cation **4**$^{+}$

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cation_4, electronic energy = -3096.26344823 a.u

Fe	0.893741	-0.849045	0.488386
C	2.750834	-1.165758	-0.309296
C	2.463116	-2.214490	0.623299
H	2.998758	-2.393127	1.545031
C	1.317208	-2.919180	0.180723
H	0.822621	-3.722925	0.708649
C	0.880005	-2.330751	-1.029352
H	-0.009988	-2.598408	-1.580628
C	1.753099	-1.257813	-1.336661
H	1.652602	-0.581303	-2.173189
C	-0.926337	0.275566	0.511790
C	0.232717	1.108021	0.429076
H	0.489575	1.746043	-0.403250
C	1.050140	0.884108	1.570172
H	2.010679	1.337042	1.766961
C	0.424869	-0.123825	2.354479
H	0.809426	-0.550501	3.270009
C	-0.781893	-0.496481	1.700355
H	-1.461246	-1.267188	2.032595
Si	4.062217	0.135172	-0.168566
O	5.489654	-0.300563	-0.808099
C	5.712568	-0.572078	-2.183013
H	5.325502	-1.559684	-2.446568
H	6.787320	-0.557386	-2.358988
H	5.239833	0.179002	-2.822022
O	3.390012	1.395155	-0.962375
C	4.068044	2.621398	-1.203558
H	5.125768	2.459821	-1.427489
H	3.985890	3.278248	-0.334229
H	3.599586	3.106490	-2.059537
O	4.303429	0.378851	1.419359
C	5.530794	0.748189	2.039877
H	6.380414	0.292811	1.529760
H	5.501618	0.401629	3.072448
H	5.644648	1.834402	2.033743
P	-2.163944	0.134038	-0.815133
C	-3.319131	-1.125817	-0.097667
H	-3.456913	-0.926304	0.972630
C	-2.736388	-2.531854	-0.273145
H	-2.560288	-2.703926	-1.342944
H	-1.761108	-2.611775	0.216907
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H	-3.243920	-4.594449	0.110800
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C	-5.046453	-3.511293	-0.407511
H	-5.726457	-4.258791	0.010816
H	-4.941671	-3.748188	-1.473904
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H	-6.594473	-2.044790	-0.778454
C	-4.688487	-1.038933	-0.778703
H	-5.133900	-0.053681	-0.620251
H	-4.559556	-1.154544	-1.862983
C	-3.063791	1.745104	-0.570192
H	-3.931302	1.634730	-1.234985
C	-3.559743	2.007298	0.849033
H	-2.694418	2.084223	1.519965
H	-4.163245	1.170603	1.212159
C	-4.368997	3.300221	0.914525
H	-5.285212	3.178624	0.322865
H	-4.688821	3.486137	1.944431
C	-3.573934	4.484277	0.378017
H	-4.185095	5.391210	0.396147
H	-2.717794	4.674190	1.038787
C	-3.067621	4.215370	-1.034096
H	-2.465259	5.055520	-1.392881
H	-3.920043	4.128610	-1.719258
C	-2.248240	2.928814	-1.091379
H	-1.355729	3.059239	-0.467700
H	-1.901295	2.733811	-2.111270

· Cation **5**$^{+}$

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cation_5, electronic energy = -5442.59683498 a.u

Si	-0.258210	-1.920870	1.672346
O	-0.168727	-0.630421	2.670872
C	-1.304599	-0.084604	3.329879
H	-0.970873	0.767651	3.921237
H	-2.049321	0.253190	2.605010
H	-1.759924	-0.822735	3.992863
O	-1.035912	-3.119177	2.461014
C	-1.445109	-4.341182	1.879044
H	-1.944698	-4.931122	2.646881
H	-2.143828	-4.165785	1.057685
H	-0.587126	-4.911097	1.507649
Fe	2.887002	-1.132129	0.538806
C	1.517733	-2.430984	1.390964
C	2.034285	-2.955941	0.160836
H	1.453721	-3.135254	-0.733171
C	3.439778	-3.131428	0.292351
H	4.115479	-3.483682	-0.472829
C	3.805857	-2.728748	1.602124
H	4.815502	-2.664594	1.984747
C	2.635476	-2.307225	2.272281
H	2.597537	-1.877753	3.263830
C	4.253367	0.456037	0.081660
C	3.487220	0.101566	-1.064179
H	3.888841	-0.268330	-1.995818
C	2.104940	0.252524	-0.769049
H	1.277408	0.020836	-1.424694
C	1.996487	0.706330	0.574900
H	1.084098	0.862077	1.130128

C	3.312575	0.804489	1.102177
H	3.564551	1.052702	2.122673
P	6.044364	0.323705	0.379884
C	6.658814	-0.188372	-1.291749
H	6.124850	0.376909	-2.066324
C	6.403847	-1.683755	-1.501464
H	6.884913	-2.239611	-0.686457
H	5.334496	-1.899976	-1.431978
C	6.949305	-2.167139	-2.840691
H	6.402940	-1.672147	-3.654225
H	6.766172	-3.240677	-2.952140
C	8.435653	-1.861220	-2.969719
H	8.990137	-2.442290	-2.221898
H	8.806946	-2.179733	-3.947993
C	8.705795	-0.377376	-2.757689
H	8.240120	0.196615	-3.569084
H	9.778878	-0.171189	-2.809880
C	8.154477	0.114552	-1.422619
H	8.693778	-0.371833	-0.599027
H	8.338000	1.187586	-1.325559
C	6.482721	2.130911	0.468200
H	7.580992	2.105141	0.472186
C	6.014585	2.977812	-0.711726
H	4.917299	2.977449	-0.736840
H	6.348901	2.545423	-1.659073
C	6.519861	4.413413	-0.588027
H	7.614314	4.414744	-0.668971
H	6.147529	5.011572	-1.425459
C	6.110902	5.037955	0.740410
H	5.018012	5.139739	0.771025
H	6.517790	6.049787	0.825151
C	6.567695	4.183196	1.916614
H	6.233962	4.620943	2.862354
H	7.664069	4.163678	1.952255
C	6.046348	2.753965	1.794453
H	4.951251	2.781314	1.841268
H	6.388697	2.141795	2.635040
Fe	-2.950637	-1.270074	-0.364775
C	-0.967276	-1.472138	0.048525
C	-1.349658	-2.314397	-1.051458
H	-1.293871	-3.393873	-1.075338
C	-1.874340	-1.498810	-2.089744
H	-2.290283	-1.850245	-3.022950
C	-1.827525	-0.146399	-1.657708
H	-2.219113	0.703003	-2.198368
C	-1.271360	-0.125491	-0.352252
H	-1.131063	0.754418	0.257974
C	-4.828775	-0.434859	-0.386565
C	-4.841902	-1.776357	-0.883670
H	-5.119912	-2.066519	-1.886305
C	-4.372497	-2.648238	0.134524
H	-4.255872	-3.718736	0.044373
C	-4.042508	-1.857073	1.267595
H	-3.618193	-2.217293	2.193719

C	-4.325126	-0.501646	0.948204
H	-4.172020	0.343186	1.602637
P	-5.378791	0.995938	-1.370544
C	-7.224623	0.803173	-1.196574
H	-7.619686	1.730333	-1.634799
C	-7.730175	-0.350918	-2.064049
H	-7.325993	-1.294080	-1.678425
H	-7.361057	-0.242699	-3.089448
C	-9.253706	-0.429428	-2.043880
H	-9.667892	0.476835	-2.504214
H	-9.593096	-1.271578	-2.655704
C	-9.778657	-0.559065	-0.619097
H	-9.443102	-1.515806	-0.197480
H	-10.872844	-0.585103	-0.615729
C	-9.272024	0.579456	0.257744
H	-9.620419	0.454369	1.288310
H	-9.695603	1.527194	-0.099661
C	-7.748469	0.672657	0.230482
H	-7.420237	1.517382	0.843213
H	-7.317424	-0.227998	0.684280
C	-5.032534	2.391760	-0.194716
H	-5.359841	2.102649	0.811882
C	-5.804497	3.647725	-0.603590
H	-5.547319	3.906159	-1.639392
H	-6.880882	3.458406	-0.588879
C	-5.482874	4.823650	0.314152
H	-6.026148	5.713785	-0.018190
H	-5.847793	4.597490	1.324550
C	-3.986529	5.104348	0.372087
H	-3.778820	5.925917	1.064868
H	-3.641892	5.435081	-0.616306
C	-3.214186	3.855007	0.776819
H	-2.136232	4.053232	0.775402
H	-3.479552	3.582288	1.807207
C	-3.533227	2.686905	-0.149136
H	-2.991193	1.793316	0.164047
H	-3.188371	2.921334	-1.164716

· Dication **5^{2+}(singlet)**

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Singletdiaction_5, electronic energy = -5442.26146074 a.u

Si	0.093231	-0.699458	1.830276
O	0.160728	0.894328	2.173677
C	-0.945572	1.603242	2.738887
H	-0.682733	2.659295	2.770187
H	-1.840824	1.473159	2.127014
H	-1.143972	1.251280	3.751910
O	-0.298406	-1.537746	3.159491
C	-0.836725	-2.847703	3.250291
H	-1.298770	-2.953510	4.230620
H	-1.591159	-3.012694	2.479843
H	-0.043614	-3.593572	3.154919
Fe	3.195323	-0.398742	0.030313

C	1.895201	-1.151877	1.471093
C	2.272735	-2.178617	0.540279
H	1.586941	-2.685028	-0.125038
C	3.665080	-2.355089	0.574842
H	4.238345	-3.058217	-0.006754
C	4.184252	-1.440175	1.553362
H	5.218465	-1.372660	1.863685
C	3.098049	-0.700214	2.085403
H	3.164196	0.086824	2.821870
C	3.928309	0.941842	-1.259337
C	3.152184	-0.032678	-2.003666
H	3.534914	-0.718064	-2.744565
C	1.832448	0.043165	-1.528647
H	1.001705	-0.585339	-1.819248
C	1.760563	1.057427	-0.528256
H	0.891990	1.304166	0.063143
C	3.029905	1.626511	-0.358990
H	3.297707	2.394081	0.348720
P	5.333876	0.261670	-0.487039
C	6.411366	-0.664597	-1.661181
H	6.182453	-0.182434	-2.621306
C	6.080984	-2.156514	-1.768109
H	6.291439	-2.634999	-0.804268
H	5.019592	-2.304853	-1.980376
C	6.934353	-2.807803	-2.852801
H	6.666184	-2.379369	-3.826320
H	6.693566	-3.872671	-2.905893
C	8.419499	-2.601085	-2.589463
H	8.707242	-3.135190	-1.675652
H	9.009155	-3.036223	-3.399378
C	8.746705	-1.122583	-2.440141
H	8.575237	-0.604493	-3.391340
H	9.802800	-0.980478	-2.197361
C	7.901028	-0.459262	-1.353088
H	8.137858	-0.908829	-0.381239
H	8.151213	0.601994	-1.292695
C	6.262964	1.414949	0.571447
H	7.220330	0.897727	0.709131
C	6.517280	2.705048	-0.236756
H	5.560561	3.209111	-0.410686
H	6.932783	2.476184	-1.222925
C	7.453505	3.622218	0.544341
H	8.436996	3.145329	0.632312
H	7.604296	4.541469	-0.027811
C	6.898866	3.928542	1.928727
H	5.969925	4.504282	1.831304
H	7.596541	4.562886	2.480108
C	6.628344	2.650166	2.711243
H	6.195875	2.878248	3.688675
H	7.573562	2.128797	2.904840
C	5.687978	1.710133	1.957913
H	4.700962	2.172632	1.871788
H	5.559019	0.785632	2.524779
Fe	-2.867541	-1.203034	0.178693

C	-0.846728	-1.042361	0.313308
C	-1.222734	-2.306943	-0.267420
H	-1.018737	-3.285000	0.146772
C	-1.967429	-2.058647	-1.451383
H	-2.427938	-2.808694	-2.077944
C	-2.070837	-0.652940	-1.627934
H	-2.643482	-0.154315	-2.396734
C	-1.391577	-0.024881	-0.552618
H	-1.332095	1.041247	-0.388134
C	-4.837963	-0.611408	0.067768
C	-4.717719	-2.031632	0.189758
H	-5.043542	-2.750508	-0.547196
C	-4.050398	-2.335584	1.405321
H	-3.813174	-3.327220	1.763254
C	-3.728128	-1.107239	2.041905
H	-3.198057	-0.992262	2.976919
C	-4.209880	-0.052169	1.221960
H	-4.114380	1.002224	1.433148
P	-5.631879	0.209275	-1.352406
C	-7.420877	-0.109977	-0.954667
H	-7.951874	0.513057	-1.687438
C	-7.799209	-1.562671	-1.248678
H	-7.266492	-2.222657	-0.554069
H	-7.483674	-1.840180	-2.259876
C	-9.298806	-1.781799	-1.070739
H	-9.840628	-1.186972	-1.816748
H	-9.548382	-2.828921	-1.267996
C	-9.751434	-1.378618	0.327395
H	-9.284229	-2.045141	1.064394
H	-10.832213	-1.512100	0.430996
C	-9.364251	0.062052	0.637530
H	-9.655340	0.327076	1.658880
H	-9.917319	0.737776	-0.027314
C	-7.866809	0.292855	0.448475
H	-7.625378	1.341186	0.647492
H	-7.308890	-0.302178	1.182202
C	-5.432090	1.996720	-0.891834
H	-5.657262	2.117927	0.175357
C	-6.406196	2.870259	-1.685950
H	-6.249854	2.700375	-2.759362
H	-7.438761	2.583694	-1.472787
C	-6.214203	4.349694	-1.365768
H	-6.902661	4.950460	-1.967205
H	-6.485339	4.526175	-0.316951
C	-4.776840	4.798016	-1.596817
H	-4.656998	5.850637	-1.323633
H	-4.541490	4.724653	-2.666360
C	-3.803264	3.928701	-0.810791
H	-2.769280	4.230440	-1.015155
H	-3.966579	4.081913	0.264499
C	-3.993730	2.452637	-1.142116
H	-3.303364	1.839228	-0.558873
H	-3.748671	2.280689	-2.198435

· Dication **5^{2+}(triplet)**

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Tripletdication_5, electronic energy = -5442.29812254 a.u

Si	-0.082664	-1.526187	1.276294
O	0.165400	-0.081600	1.996167
C	-0.801973	0.617029	2.767399
H	-0.314500	1.480795	3.216472
H	-1.625240	0.966981	2.137780
H	-1.203752	-0.013147	3.564002
O	-0.860509	-2.614429	2.208063
C	-0.282143	-3.284670	3.326544
H	-0.034639	-2.577206	4.121345
H	-1.014274	-3.996852	3.702654
H	0.618681	-3.828012	3.032014
Fe	3.047733	-1.022667	-0.116549
C	1.604418	-2.138311	0.819448
C	1.991277	-2.779738	-0.404313
H	1.352606	-2.946117	-1.260479
C	3.367914	-3.113157	-0.329086
H	3.958206	-3.557529	-1.118056
C	3.851289	-2.699279	0.933145
H	4.880453	-2.739571	1.262090
C	2.783962	-2.096997	1.638869
H	2.858595	-1.636794	2.614067
C	4.535047	0.513301	-0.278120
C	4.115844	0.055201	-1.561558
H	4.756943	-0.397368	-2.303261
C	2.713257	0.249385	-1.693597
H	2.117368	-0.012139	-2.556627
C	2.240311	0.819654	-0.479821
H	1.218725	1.062696	-0.232194
C	3.351332	0.952369	0.396381
H	3.304110	1.283219	1.423109
P	6.146303	0.327537	0.536549
C	7.197813	-0.317622	-0.843132
H	6.935339	0.201826	-1.773764
C	6.957938	-1.821103	-1.018654
H	7.182519	-2.322277	-0.068343
H	5.903451	-2.023612	-1.232587
C	7.839384	-2.403773	-2.118351
H	7.562362	-1.955022	-3.081209
H	7.655862	-3.478676	-2.211812
C	9.312109	-2.134650	-1.836949
H	9.612039	-2.678703	-0.932579
H	9.930882	-2.522136	-2.650663
C	9.567889	-0.646390	-1.640375
H	9.377791	-0.115360	-2.581716
H	10.617584	-0.467281	-1.392044
C	8.678942	-0.055454	-0.549695
H	8.938800	-0.499294	0.420318
H	8.870080	1.016981	-0.465034
C	6.644150	2.110310	0.714001
H	7.684604	2.023267	1.054909
C	6.613304	2.917884	-0.581027

H	5.576225	2.980983	-0.936208
H	7.184292	2.417502	-1.367969
C	7.160242	4.325072	-0.352468
H	8.224648	4.256690	-0.095846
H	7.103717	4.899067	-1.282101
C	6.413397	5.039882	0.766908
H	5.373726	5.210714	0.457180
H	6.848955	6.027337	0.941961
C	6.426939	4.221821	2.052742
H	5.852901	4.725849	2.835876
H	7.454948	4.139423	2.425773
C	5.866883	2.820103	1.822342
H	4.814334	2.913892	1.527708
H	5.894049	2.233832	2.746494
Fe	-3.209064	-1.246239	-0.196271
C	-1.141157	-1.345621	-0.233083
C	-1.722952	-2.405526	-1.006935
H	-1.639905	-3.461467	-0.789983
C	-2.469648	-1.834924	-2.074540
H	-3.059475	-2.375237	-2.801660
C	-2.358930	-0.427578	-1.980586
H	-2.887898	0.287967	-2.594996
C	-1.555067	-0.124538	-0.858744
H	-1.335627	0.871526	-0.500908
C	-5.201182	-0.512850	0.090013
C	-5.153142	-1.935039	-0.074369
H	-5.616863	-2.482595	-0.881750
C	-4.350457	-2.496361	0.954646
H	-4.120019	-3.543971	1.084429
C	-3.853495	-1.424794	1.745156
H	-3.175393	-1.520390	2.579376
C	-4.370139	-0.213688	1.208406
H	-4.154330	0.778218	1.575517
P	-5.930911	0.618491	-1.124652
C	-7.742635	0.311012	-0.846548
H	-8.204851	1.102360	-1.452035
C	-8.195904	-1.026063	-1.433175
H	-7.741899	-1.847406	-0.865473
H	-7.860879	-1.124199	-2.470699
C	-9.713936	-1.160963	-1.338487
H	-10.181385	-0.393861	-1.967731
H	-10.024633	-2.127483	-1.745444
C	-10.192727	-1.005756	0.099927
H	-9.808140	-1.839565	0.701809
H	-11.283103	-1.071095	0.144745
C	-9.718936	0.310952	0.702899
H	-10.027928	0.389683	1.749368
H	-10.195392	1.146977	0.175912
C	-8.202428	0.460076	0.601603
H	-7.892671	1.424550	1.014171
H	-7.716567	-0.313776	1.210320
C	-5.603877	2.265401	-0.345580
H	-5.770809	2.193540	0.736920
C	-6.560918	3.321836	-0.907554

H	-6.465664	3.350694	-2.000896
H	-7.597646	3.054640	-0.690356
C	-6.258226	4.700441	-0.327539
H	-6.937171	5.437733	-0.764401
H	-6.467277	4.687949	0.749628
C	-4.809123	5.108369	-0.558219
H	-4.609741	6.079235	-0.096672
H	-4.632588	5.233463	-1.633888
C	-3.851427	4.056228	-0.013135
H	-2.813887	4.335097	-0.224983
H	-3.945387	4.007600	1.079782
C	-4.152821	2.684028	-0.606246
H	-3.457423	1.937595	-0.208618
H	-3.988316	2.711186	-1.691057

4. References

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