Supporting Information

A three-coordinate iron-silylene complex stabilized by ligand-ligand dispersion forces

Mikko M. Hänninen,[a,b] Kuntal Pal,[a] Benjamin M. Day,[a] Thomas Pugh,[a] and Richard A. Layfield*[a]

General synthetic details

All syntheses were carried out using standard Schlenk and glove-box techniques, using an inert atmosphere of argon. Toluene and pentane were dried by refluxing over molten potassium, distilled and degassed by freeze-pump-thaw cycles prior to use. Pentane was dried using an IT Inc. SPS. Deuterated NMR solvents (toluene-d_8 and benzene-d_6) were dried by refluxing over potassium before vacuum transferring to a J. Young's ampoule. NMR spectra were acquired on Bruker Avance-III 400 MHz or 500 MHz spectrometers. X-ray diffraction data were collected on a Bruker APEX-II diffractometer, using CuKα radiation. Elemental analyses were carried out by Mr. Stephen Boyer at London Metropolitan University, U.K. Literature procedures were used to synthesize 1,3-bis(2,6-diisopropylphenyl)-1,3-diaza-2-silacyclopent-4-en-2-ylidene (^{Si}IPr) and Fe[N(SiMe$_3$)$_2$]$_2$.[1,2]

Synthesis of [(^{Si}IPr)Fe(N″)$_2$]·toluene (1·toluene)

A pale yellow solution of ^{Si}IPr (162 mg, 0.40 mmol) in toluene (5 ml) was slowly added to a pale green solution of [Fe{N(SiMe$_3$)$_2$}$_2$] (150 mg, 0.40 mmol) in toluene (5 ml) at –78°C, producing a light yellow solution. The reaction mixture was slowly warmed to room temperature, stirred for one hour, filtered, concentrated to a volume of ca. 1 ml, and stored at –30 °C. A batch of crystalline material formed after four days. The crystals were collected, washed with pentane (2 × 5 ml) that had be pre-cooled to –78°C (*n.b.* the complex is very soluble in common non-polar hydrocarbon solvents), and then dried under vacuum. Yield 70.0 mg (20 %). Anal. calcd. for $C_{45}H_{80}FeN_4Si_5$: C 61.88; H 9.23; N, 6.41. Found: C 62.08; H 9.42; N 6.58. ^{1}H NMR (500.19 MHz, toluene-d_8, δ/ppm, 298 K): 8.77 (2H, ^{Si}IPr backbone); 7.37 (2H, aryl C*H*); 7.26 (4H , aryl C*H*); 1.89 (12H, *i*Pr-C*H*$_3$); 1.51 (4H, iPr-C*H*); 0.72 (12H, *i*Pr-C*H*$_3$).

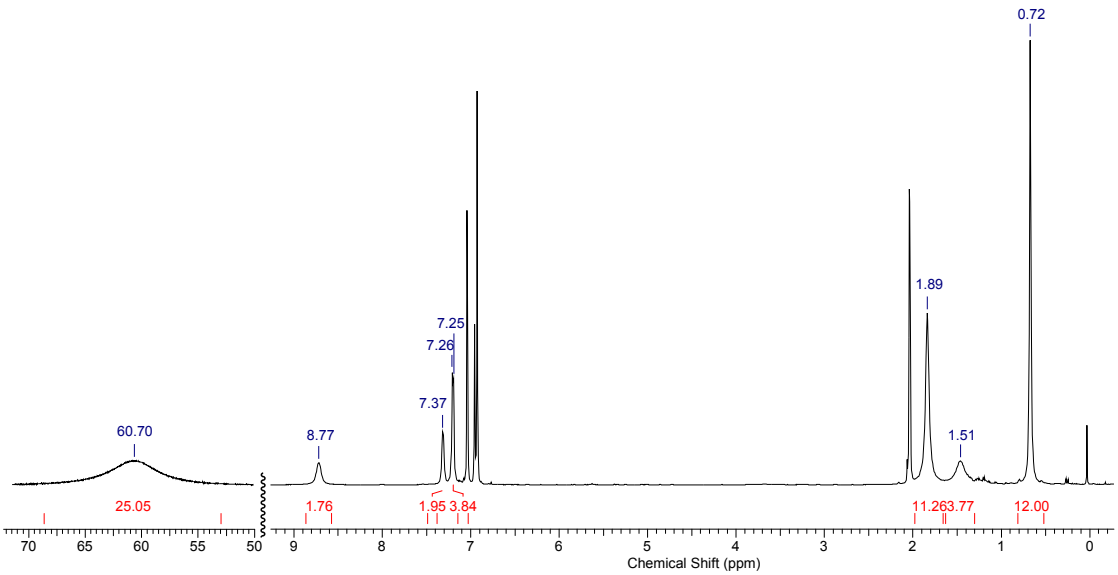

Figure S1. ^{1}H NMR spectrum of **1**·toluene at 298 K in toluene-D$_8$.

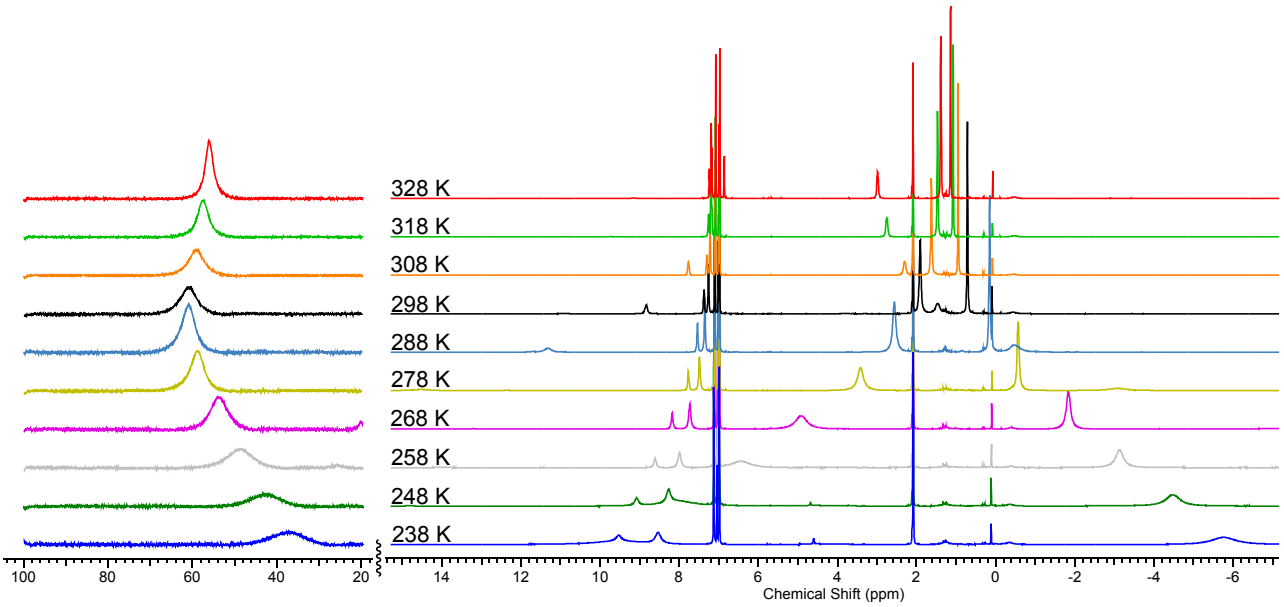

Figure S2. ^{1}H NMR spectrum of **1**·toluene at 10 K intervals in the range 238-328 K in toluene-D_8.

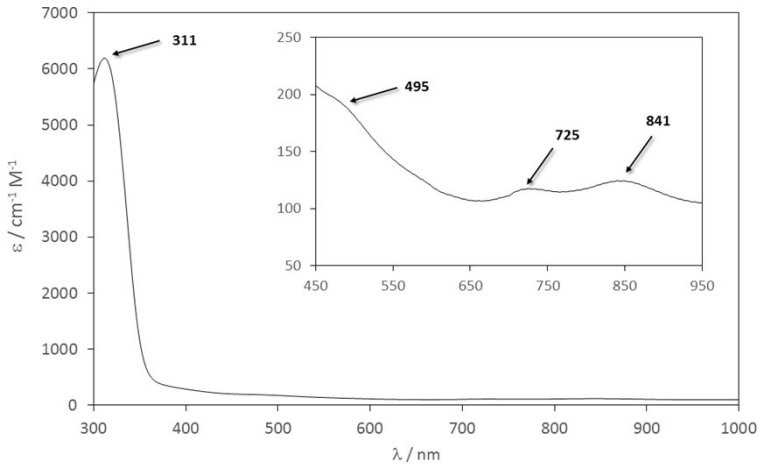

Figure S3. UV/vis spectrum of **1**·toluene in toluene.

Magnetic property measurements

The magnetic properties of a polycrystalline samples of **1**·toluene was measured using a Quantum Design MPMS-7 SQUID magnetometer at temperatures in the range 1.8-300 K. In a glove box, the polycrystalline sample was transferred to an NMR tube, restrained in eicosane and flame sealed under vacuum. The magnetic susceptibility and magnetization data were fitted simultaneously, using the following Hamiltonian and the PHI software.[3] The best fit was found with $S = 2$, $D = -22.6$ cm^{-1}, and $g_{x,y} = 2.14$ and $g_z = 2.32$.

$$\hat{H} = \mu_B\left(g_{xy}\left(\hat{S}_x B_x + \hat{S}_y B_y\right) + g_z \hat{S}_z B_z\right) + D\left(\hat{S}_z{}^2 - \frac{1}{3}S(S+1)\right) \quad (1)$$

Table S1. Crystal data and structure refinement for **1**·toluene.

CCDC ref. code	1463752
Empirical formula	$C_{41.5}H_{76}FeN_4Si_5$
Formula weight	827.36
Temperature/K	150.01(13)
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	11.3552(4)
b/Å	12.5187(4)
c/Å	18.5545(6)
α/°	78.705(3)
β/°	89.821(3)
γ/°	75.266(3)
Volume/Å^3	2498.40(15)
Z	2
ρ_{calc} / g cm^{-3}	1.100
μ/mm^{-1}	0.452
F(000)	898.0
Crystal size/mm^3	0.1 × 0.05 × 0.05
Radiation	Mo-K_α (λ = 0.71073 Å)
2θ range for data collection/°	6.61 to 52.744
Reflections collected	31256
Independent reflections	10197 [R_{int} = 0.0381, R_{sigma} = 0.0495]
Data/restraints/parameters	10197/57/505
Goodness-of-fit on F^2	1.031
Final R indexes [I>2σ(I)]	R_1 = 0.0433, wR_2 = 0.0958
Final R indexes [all data]	R_1 = 0.0624, wR_2 = 0.1057
Largest diff. peak/hole / e Å^{-3}	0.52/–0.45

Computational details

All calculations were performed using Turbomole (versions 6.6 and 7.0) or ADF2013 program packages.[4,5] Geometries were optimized with the PBE1PBE functional and the def2-SVP basis set for C, H, N, Si (amide ligand) atoms, and def2-TZVP for the Fe and Si (^{Si}IPr ligand) atoms. Dispersion correction by Grimme *et al.* (DFT-D3) with Becke-Johnson (BJ) damping was utilized in DFT calculations to include dispersion effects.[6,7] Full vibrational analysis was performed for all optimized structures to confirm that they represent a local minimum. Energy decomposition analysis (EDA) was performed as implemented in ADF2013 using PBE functional and DZP basis set for C, H, N, Si (amide ligand) atoms and TZVP for Fe and (^{Si}IPr ligand) atoms. DFT-D3 dispersion correction with BJ damping was also employed to include the dispersion effects in EDA analysis. EDA and ETS-NOCV analyses were performed as implemented in ADF2013 program package.

The geometry of complex **1** was also optimized using Hartree-Fock (HF) and second order Möller–Plesset perturbation theory (MP2) methods in order to gain further insight to the dispersion effects. For the MP2 calculation, all orbitals with energies below –3 a.u. were considered to be frozen. Frequency calculation was performed for the HF optimized structure whereas for MP2 optimized geometry the analysis of the vibrational frequencies could not be performed due to the computational resources. It should be noted that the bond lengths and angles obtained at MP2 level are in good agreement with DFT-D3 results hence the geometry can be also expected to be a minimum on the potential energy surface.

References

1. P. Zark, A. Schäfer, A. Mitra, D. Haase, W. Saak, R. West, T. Müller, *J. Organomet. Chem*., **2010**, *695*, 398.
2. R. A. Andersen, K. Faegri, J. C. Green, A. Haaland, M. F. Lappert, W. P. Leung, K. Rypdal, *Inorg. Chem*., **1988**, **27**, 1782.
3. N. F. Chilton, R. P. Anderson, L. D. Turner, A. Soncini, K. S. Murray, *J. Comput. Chem*., **2013**, *34*, 1164.
4. TURBOMOLE V6.6 2014, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.
5. ADF2014, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com
6. S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys*., **2010**, *132*, 154104.
7. S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem*., **2011**, *32*, 1456.

XYZ-Coordinates for [(^{Si}IPr)Fe(N″)$_2$]

PBE1PBE-D3 / Def2-mix (S = 2)
NIMAG = 0

Fe	11.58166	3.27162	4.60454
Si	9.21950	3.53552	3.86131
Si	12.21985	5.25406	6.95607
Si	13.16032	5.95394	4.12803
Si	12.03580	0.36294	5.72148
Si	13.02899	1.05731	2.91027
N	8.34796	4.66415	2.86345
N	7.73088	2.67079	4.11706
N	12.21007	4.98981	5.23058
N	12.09510	1.42649	4.33816
C	6.99693	4.36079	2.76348
H	6.33292	4.99901	2.18194
C	6.65508	3.24549	3.45404
H	5.66670	2.79194	3.51580
C	8.85835	5.84822	2.24661
C	8.72616	7.07291	2.92829
C	9.20953	8.22809	2.30450
H	9.12394	9.18963	2.81672
C	9.80869	8.16774	1.05307
H	10.18764	9.07894	0.58409
C	9.93764	6.94597	0.39921
H	10.42045	6.91314	-0.57863
C	9.46734	5.76249	0.97493
C	8.10636	7.16560	4.31032
H	7.75230	6.16153	4.58871
C	6.89071	8.09181	4.32681
H	7.16769	9.13053	4.08626
H	6.42432	8.09682	5.32440
H	6.13163	7.77067	3.59715
C	9.15224	7.57797	5.34626
H	10.00555	6.88347	5.34122
H	8.71457	7.58484	6.35711
H	9.54305	8.58820	5.14522
C	9.58663	4.43646	0.24330
H	9.75624	3.65943	1.00787
C	8.28240	4.08492	-0.47923
H	7.43179	4.02511	0.21359
H	8.37290	3.11017	-0.98419
H	8.04750	4.84340	-1.24318
C	10.76263	4.37651	-0.72672
H	10.59916	5.01763	-1.60764
H	10.89200	3.34726	-1.09258
H	11.70406	4.68327	-0.24825
C	7.55207	1.44932	4.83751
C	7.33452	1.49046	6.23260
C	7.14725	0.27502	6.89661
H	6.98494	0.27145	7.97549
C	7.17096	-0.93449	6.20859
H	7.02556	-1.87208	6.75045
C	7.39001	-0.95153	4.83729
H	7.41989	-1.90648	4.30677
C	7.58844	0.23585	4.12460

C	7.27965	2.80866	6.98566
H	8.00211	3.48774	6.50197
C	7.68421	2.69274	8.45209
H	6.92769	2.15268	9.04349
H	7.78551	3.69609	8.89136
H	8.64728	2.17548	8.57141
C	5.89686	3.45666	6.86475
H	5.61968	3.64181	5.81783
H	5.87720	4.42311	7.39289
H	5.12614	2.80865	7.31217
C	7.85777	0.18318	2.63212
H	7.93552	1.21848	2.26719
C	9.19679	-0.49698	2.34664
H	10.01619	0.00959	2.87814
H	9.41797	-0.47921	1.26767
H	9.19120	-1.55055	2.66856
C	6.70856	-0.47691	1.87079
H	6.58339	-1.53273	2.15907
H	6.90004	-0.45081	0.78664
H	5.75383	0.03699	2.06088
C	10.52546	4.80281	7.66041
H	9.77564	5.54260	7.34094
H	10.53848	4.77992	8.76183
H	10.18414	3.81697	7.31477
C	12.54709	7.04441	7.46077
H	13.52383	7.41199	7.10983
H	12.54481	7.10917	8.56130
H	11.76803	7.72370	7.08227
C	13.55255	4.19690	7.77761
H	13.45725	3.13660	7.49646
H	13.51840	4.26464	8.87704
H	14.54853	4.53087	7.44535
C	12.61523	7.75561	4.00711
H	11.59059	7.81805	3.61063
H	13.27815	8.28711	3.30431
H	12.64840	8.28635	4.96885
C	12.95723	5.25965	2.38573
H	13.38671	4.25440	2.26960
H	13.45653	5.91591	1.65515
H	11.88982	5.22650	2.11418
C	14.99441	5.91161	4.57934
H	15.17744	6.37030	5.56431
H	15.60237	6.45679	3.83916
H	15.35870	4.87278	4.62412
C	11.02520	1.19228	7.08152
H	11.50415	2.09617	7.48402
H	10.87882	0.49640	7.92299
H	10.02491	1.45593	6.70199
C	11.17025	-1.28127	5.39746
H	10.11411	-1.11141	5.13931
H	11.19572	-1.89016	6.31641
H	11.63487	-1.86687	4.59191
C	13.76548	0.00806	6.39356
H	14.37864	-0.53879	5.65937
H	13.72208	-0.60053	7.31141
H	14.28982	0.94783	6.62962
C	12.16540	1.79201	1.39858

H	11.23739	1.23838	1.18910
H	12.80547	1.74151	0.50328
H	11.89362	2.84614	1.54968
C	13.21896	-0.79049	2.56891
H	13.72615	-1.32306	3.38828
H	13.82898	-0.92287	1.66021
H	12.24607	-1.27490	2.39439
C	14.77093	1.77306	3.05849
H	14.74706	2.84682	3.30111
H	15.35419	1.64357	2.13245
H	15.31109	1.26918	3.87597

PBE1PBE / Def2-mix (S = 2)
NIMAG = 0

Fe	11.65211	3.26171	4.62176
Si	9.23286	3.53394	3.86664
Si	12.29549	5.29349	6.99586
Si	13.28051	5.90717	4.16607
Si	12.15955	0.37881	5.75297
Si	13.11461	0.99743	2.91371
N	8.35735	4.68150	2.88599
N	7.74383	2.65805	4.11341
N	12.31040	4.96748	5.27761
N	12.20904	1.42082	4.34885
C	7.00958	4.37124	2.78692
H	6.33978	5.01141	2.21424
C	6.67087	3.24676	3.46176
H	5.68052	2.79684	3.51824
C	8.84229	5.87681	2.26416
C	8.70429	7.10122	2.94975
C	9.15073	8.26560	2.31514
H	9.05486	9.22560	2.82856
C	9.71497	8.22090	1.04720
H	10.06212	9.14028	0.56950
C	9.83898	7.00415	0.38469
H	10.28332	6.98230	-0.61188
C	9.40530	5.81034	0.96901
C	8.07087	7.19780	4.32657
H	7.85709	6.17359	4.66798
C	6.73678	7.94583	4.26935
H	6.87496	8.98968	3.94481
H	6.26119	7.96610	5.26258
H	6.03546	7.46940	3.56752
C	9.02031	7.82438	5.34767
H	9.96421	7.26325	5.40611
H	8.55998	7.82849	6.34830
H	9.26371	8.86844	5.09425
C	9.49477	4.50280	0.19902
H	9.61904	3.69528	0.93975
C	8.19389	4.22854	-0.56414
H	7.32437	4.18075	0.10634
H	8.25643	3.26925	-1.10201
H	8.00619	5.02084	-1.30669
C	10.68735	4.43291	-0.75222
H	10.56266	5.10417	-1.61685
H	10.79010	3.41187	-1.14914

H	11.63043	4.69458	-0.25063
C	7.53902	1.42778	4.81704
C	7.26597	1.45415	6.20384
C	7.04397	0.23327	6.84799
H	6.83704	0.22291	7.91955
C	7.08078	-0.96978	6.15086
H	6.90521	-1.91118	6.67712
C	7.34076	-0.97301	4.78683
H	7.36542	-1.92203	4.24537
C	7.57435	0.21883	4.09207
C	7.15839	2.75884	6.97609
H	7.82689	3.48536	6.48490
C	7.60273	2.64570	8.43280
H	6.89097	2.05855	9.03473
H	7.65887	3.64677	8.88597
H	8.59407	2.17880	8.52581
C	5.73454	3.32162	6.90015
H	5.41684	3.50152	5.86348
H	5.66747	4.27791	7.44280
H	5.01660	2.62205	7.35788
C	7.82961	0.17231	2.59580
H	8.04277	1.19902	2.26160
C	9.05396	-0.67672	2.25396
H	9.94899	-0.30791	2.77573
H	9.25091	-0.64854	1.17061
H	8.91127	-1.73247	2.53438
C	6.58792	-0.30321	1.83782
H	6.32093	-1.33667	2.11109
H	6.76605	-0.28189	0.75112
H	5.71555	0.33321	2.05088
C	10.58237	4.92402	7.70857
H	9.84510	5.63313	7.29989
H	10.58359	5.03172	8.80565
H	10.23068	3.90764	7.47890
C	12.65786	7.09410	7.45106
H	13.65268	7.42769	7.11717
H	12.63295	7.18690	8.54961
H	11.90856	7.78846	7.04118
C	13.59499	4.26349	7.90645
H	13.48959	3.18496	7.71354
H	13.54196	4.41945	8.99653
H	14.60391	4.55510	7.57279
C	12.77404	7.72176	4.01985
H	11.72982	7.81020	3.68146
H	13.41063	8.21184	3.26416
H	12.88151	8.28191	4.95931
C	13.07712	5.20958	2.42171
H	13.43006	4.17279	2.32105
H	13.66203	5.81679	1.71154
H	12.02405	5.26162	2.10056
C	15.11825	5.84931	4.60978
H	15.31335	6.31138	5.59089
H	15.72456	6.38874	3.86367
H	15.47983	4.80961	4.65583
C	11.13938	1.21259	7.10756
H	11.56555	2.16611	7.45238
H	11.08372	0.55085	7.98743

H	10.10558	1.38543	6.76692
C	11.31221	-1.28608	5.46891
H	10.26995	-1.14412	5.14312
H	11.28980	-1.84357	6.42032
H	11.82381	-1.91486	4.72673
C	13.88772	0.04146	6.44371
H	14.51147	-0.51176	5.72324
H	13.83652	-0.55941	7.36655
H	14.40923	0.98314	6.67834
C	12.23637	1.66177	1.37532
H	11.27584	1.14064	1.23681
H	12.84663	1.49186	0.47316
H	12.02621	2.73976	1.43118
C	13.29797	-0.86439	2.63006
H	13.83163	-1.37105	3.44918
H	13.88591	-1.02045	1.71025
H	12.32673	-1.36404	2.49350
C	14.87676	1.68244	2.98083
H	14.90026	2.76998	3.14905
H	15.42728	1.47166	2.04923
H	15.42854	1.21423	3.81185

HF / Def2-mix (S = 2)
NIMAG = 0

Fe	11.92051	3.23428	4.71365
Si	9.06797	3.55219	3.81340
Si	12.53894	5.36796	7.06035
Si	13.49169	5.99577	4.23248
Si	12.35050	0.24912	5.82326
Si	13.31294	0.87619	2.99850
N	8.21876	4.69391	2.84355
N	7.61041	2.66744	4.05411
N	12.58201	5.03935	5.35759
N	12.45093	1.29611	4.44416
C	6.86490	4.37036	2.73434
H	6.20114	4.99759	2.16167
C	6.53265	3.26199	3.39489
H	5.55180	2.81807	3.44797
C	8.69061	5.89427	2.21348
C	8.59225	7.12083	2.91376
C	9.03910	8.28692	2.27332
H	8.98123	9.23481	2.79001
C	9.55136	8.24943	0.98058
H	9.89284	9.15969	0.50558
C	9.61293	7.03963	0.29440
H	9.99452	7.02986	-0.71624
C	9.18242	5.84183	0.88478
C	7.98076	7.23306	4.30942
H	7.74271	6.22951	4.65327
C	6.65989	8.01471	4.27819
H	6.81216	9.05221	3.97443
H	6.20031	8.02382	5.26885
H	5.94852	7.56627	3.58282
C	8.95734	7.83376	5.32678
H	9.88400	7.26248	5.36701
H	8.51254	7.82938	6.32415

H	9.21284	8.86744	5.08755
C	9.18756	4.55629	0.05800
H	9.11896	3.71689	0.74690
C	7.95776	4.49158	-0.86025
H	7.02804	4.55818	-0.29505
H	7.94428	3.55137	-1.41598
H	7.96646	5.30861	-1.58499
C	10.47242	4.36055	-0.75589
H	10.55060	5.07398	-1.57775
H	10.48381	3.36140	-1.19481
H	11.36307	4.46304	-0.13710
C	7.38790	1.43976	4.76389
C	7.03605	1.47774	6.13677
C	6.80318	0.25843	6.79073
H	6.53547	0.25648	7.83737
C	6.90027	-0.95595	6.11690
H	6.71959	-1.88376	6.64354
C	7.21850	-0.97292	4.76285
H	7.27496	-1.92115	4.24663
C	7.46065	0.21544	4.05660
C	6.82907	2.78645	6.89876
H	7.33200	3.57707	6.34575
C	7.43511	2.77330	8.30736
H	6.89044	2.11156	8.98260
H	7.39482	3.77573	8.73703
H	8.47744	2.45691	8.29645
C	5.33870	3.15344	6.96091
H	4.90181	3.23691	5.96569
H	5.20136	4.11129	7.46754
H	4.77201	2.39940	7.51149
C	7.74304	0.13860	2.55701
H	7.95254	1.14494	2.20287
C	8.97763	-0.71259	2.23947
H	9.85555	-0.34494	2.76932
H	9.19053	-0.68300	1.16877
H	8.83524	-1.75881	2.51540
C	6.51302	-0.35574	1.78285
H	6.25088	-1.38029	2.05384
H	6.70746	-0.33686	0.70835
H	5.64193	0.27215	1.97684
C	10.83095	4.93951	7.77444
H	10.07541	5.62719	7.38623
H	10.83324	5.03288	8.86429
H	10.50182	3.92536	7.54299
C	12.83222	7.18035	7.54262
H	13.81292	7.55255	7.23860
H	12.78051	7.26062	8.63271
H	12.07464	7.84859	7.12806
C	13.85240	4.37323	8.00480
H	13.78236	3.29875	7.82171
H	13.77289	4.53046	9.08456
H	14.85453	4.68508	7.69803
C	12.93147	7.80025	4.06590
H	11.87682	7.86253	3.78956
H	13.50791	8.28258	3.27039
H	13.07784	8.38501	4.97428
C	13.30522	5.27904	2.48387

H	13.71817	4.27437	2.37891
H	13.84035	5.91132	1.77003
H	12.25833	5.26244	2.16739
C	15.34822	6.02000	4.62834
H	15.55503	6.50197	5.58748
H	15.90584	6.56690	3.86228
H	15.75492	5.00628	4.67777
C	11.35835	1.09801	7.20210
H	11.83191	2.00380	7.58440
H	11.25679	0.41773	8.05216
H	10.34488	1.34474	6.87277
C	11.44398	-1.39094	5.52987
H	10.43081	-1.22138	5.15935
H	11.36014	-1.92899	6.47921
H	11.95513	-2.04895	4.82681
C	14.05473	-0.17412	6.54464
H	14.66433	-0.74855	5.84221
H	13.95782	-0.77181	7.45583
H	14.61302	0.73150	6.79693
C	12.43566	1.59254	1.47271
H	11.47426	1.09536	1.32116
H	13.03511	1.43343	0.57171
H	12.24375	2.66438	1.54166
C	13.45721	-0.98486	2.65345
H	13.99603	-1.52609	3.43414
H	14.01563	-1.12125	1.72232
H	12.48291	-1.46067	2.52439
C	15.09715	1.52614	3.02675
H	15.15287	2.60217	3.20563
H	15.61240	1.32070	2.08376
H	15.66313	1.03954	3.82581

MP2 / Def2-mix (S = 2)
NIMAG = Not available

Fe	11.55348	3.27537	4.59725
Si	9.18754	3.53891	3.85075
Si	12.07945	5.23798	7.11978
Si	13.17642	5.82768	4.29555
Si	12.16565	0.47289	5.60307
Si	13.00818	1.09129	2.69864
N	8.32235	4.64589	2.82546
N	7.69267	2.69521	4.13142
N	12.13752	4.95986	5.39843
N	12.13554	1.46054	4.16352
C	6.97161	4.36081	2.73136
H	6.31310	4.99783	2.14100
C	6.61783	3.25101	3.46023
H	5.62911	2.79781	3.53101
C	8.88370	5.82037	2.21475
C	8.87981	6.98322	2.91452
C	9.42707	8.08619	2.33626
H	9.43962	9.03265	2.88096
C	9.95373	8.01829	1.10410
H	10.39315	8.91075	0.65084
C	9.95304	6.84853	0.41626
H	10.40027	6.81459	-0.57745

C	9.42633	5.73268	0.95787
C	8.26758	7.09482	4.29958
H	7.98049	6.08473	4.62653
C	6.99451	7.94351	4.24772
H	7.22459	8.97687	3.94720
H	6.51571	7.97295	5.23858
H	6.27415	7.53209	3.52600
C	9.27396	7.63593	5.31407
H	10.16579	6.99561	5.35105
H	8.81938	7.66382	6.31636
H	9.58963	8.65991	5.06378
C	9.43022	4.42280	0.18620
H	9.54668	3.61319	0.92434
C	8.09369	4.21338	-0.53549
H	7.25034	4.19009	0.16552
H	8.10704	3.26065	-1.08721
H	7.92467	5.02903	-1.25482
C	10.58534	4.31416	-0.80666
H	10.44285	4.99005	-1.66332
H	10.63797	3.28910	-1.20020
H	11.54828	4.54889	-0.33318
C	7.55822	1.47307	4.87693
C	7.29764	1.52955	6.22264
C	7.18611	0.36729	6.89533
H	6.98747	0.37363	7.96730
C	7.33973	-0.82009	6.25648
H	7.25360	-1.75205	6.82132
C	7.60318	-0.85886	4.94150
H	7.73048	-1.82117	4.44111
C	7.71653	0.29269	4.22623
C	7.12861	2.85830	6.94180
H	7.80476	3.57829	6.45360
C	7.50905	2.79423	8.41929
H	6.77230	2.21746	8.99855
H	7.53532	3.81047	8.83755
H	8.49873	2.33961	8.56212
C	5.69508	3.38045	6.78901
H	5.42463	3.52918	5.73643
H	5.58609	4.34415	7.31024
H	4.98641	2.66405	7.23159
C	7.99016	0.21867	2.73449
H	8.14818	1.24307	2.36679
C	9.26146	-0.57564	2.43828
H	10.12294	-0.13027	2.95424
H	9.46136	-0.57531	1.35566
H	9.16683	-1.62415	2.75847
C	6.77398	-0.35343	2.00154
H	6.58096	-1.39101	2.31335
H	6.94743	-0.34862	0.91442
H	5.87125	0.23813	2.21180
C	10.32741	4.93250	7.76869
H	9.63440	5.68287	7.36111
H	10.29739	5.00112	8.86823
H	9.94449	3.94196	7.49017
C	12.52754	7.00926	7.60917
H	13.56381	7.26363	7.33954
H	12.43858	7.11174	8.70275

H	11.86027	7.75026	7.14571
C	13.28059	4.11972	8.06188
H	13.08612	3.05267	7.88359
H	13.22307	4.29739	9.14804
H	14.31366	4.32460	7.73947
C	12.93151	7.69930	4.21876
H	11.89995	7.94185	3.92593
H	13.60192	8.10584	3.44350
H	13.16166	8.21108	5.16274
C	12.75456	5.21571	2.55379
H	12.76181	4.11848	2.46523
H	13.48460	5.58391	1.81448
H	11.75931	5.58238	2.25568
C	15.00275	5.50022	4.65907
H	15.28694	5.93249	5.63200
H	15.66086	5.94171	3.89356
H	15.20390	4.41917	4.70480
C	10.96542	1.26700	6.83394
H	11.14257	2.34354	6.98042
H	11.05549	0.80688	7.83158
H	9.92739	1.12843	6.49174
C	11.54858	-1.30199	5.40850
H	10.50952	-1.31212	5.04941
H	11.56305	-1.78543	6.39937
H	12.16382	-1.90863	4.73066
C	13.89681	0.40127	6.35990
H	14.58788	-0.14025	5.69403
H	13.89982	-0.11452	7.33354
H	14.30151	1.41435	6.50516
C	12.03698	1.70141	1.19245
H	11.10226	1.13182	1.08608
H	12.62270	1.57274	0.26779
H	11.77070	2.76383	1.26827
C	13.28705	-0.76131	2.43819
H	13.91099	-1.20142	3.23080
H	13.81507	-0.91294	1.48291
H	12.34214	-1.32193	2.39379
C	14.72669	1.88308	2.67573
H	14.68487	2.97658	2.77922
H	15.26038	1.65186	1.73960
H	15.32831	1.49573	3.51309