Electronic Supplementary Information (ESI)

Core-Modified Hexaphyrin: Syntheses and Characterization of 31,34-Disilahexaphyrinoid

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CONTENTS

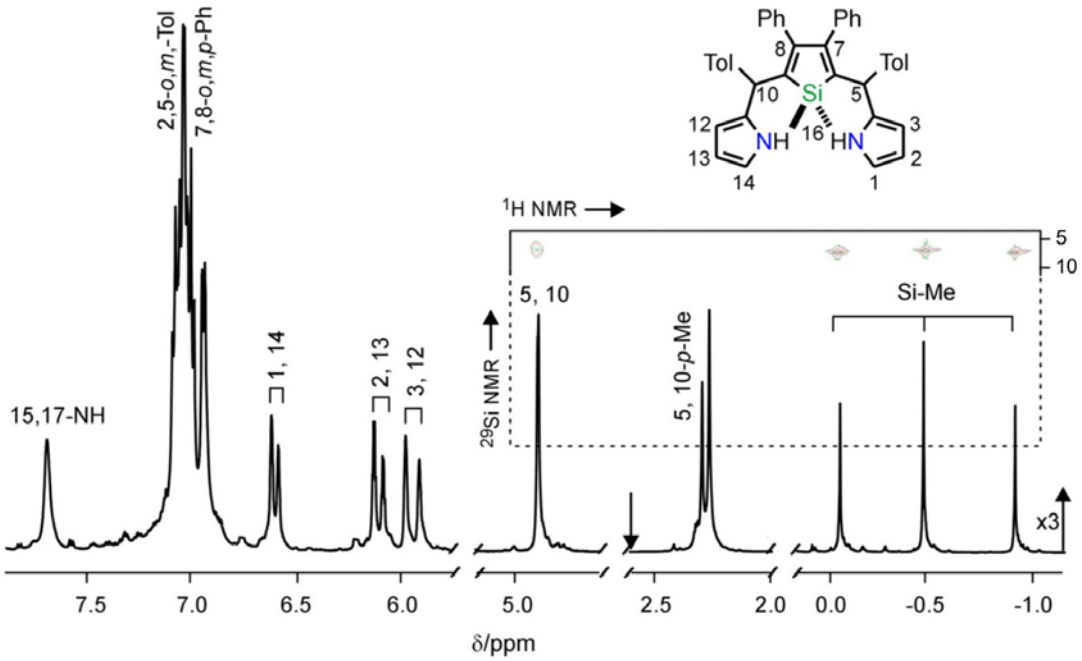

Figure S1. ^{1}H NMR spectrum of **3** (mixture of diastereomers) (dichloromethane-d_2, 298 K). Inset: ^{1}H - ^{29}Si NMR correlations.

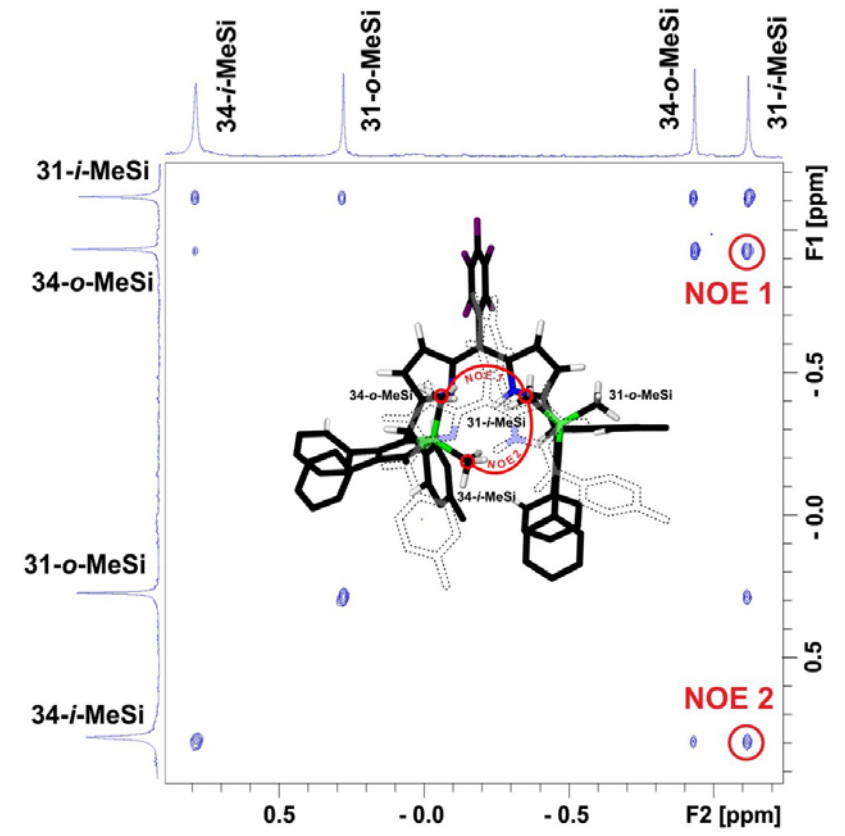

Figure S2. NOESY spectrum of **4**a (dichloromethane-d_2, 240 K). Only important correlations for Me-Si groups are shown

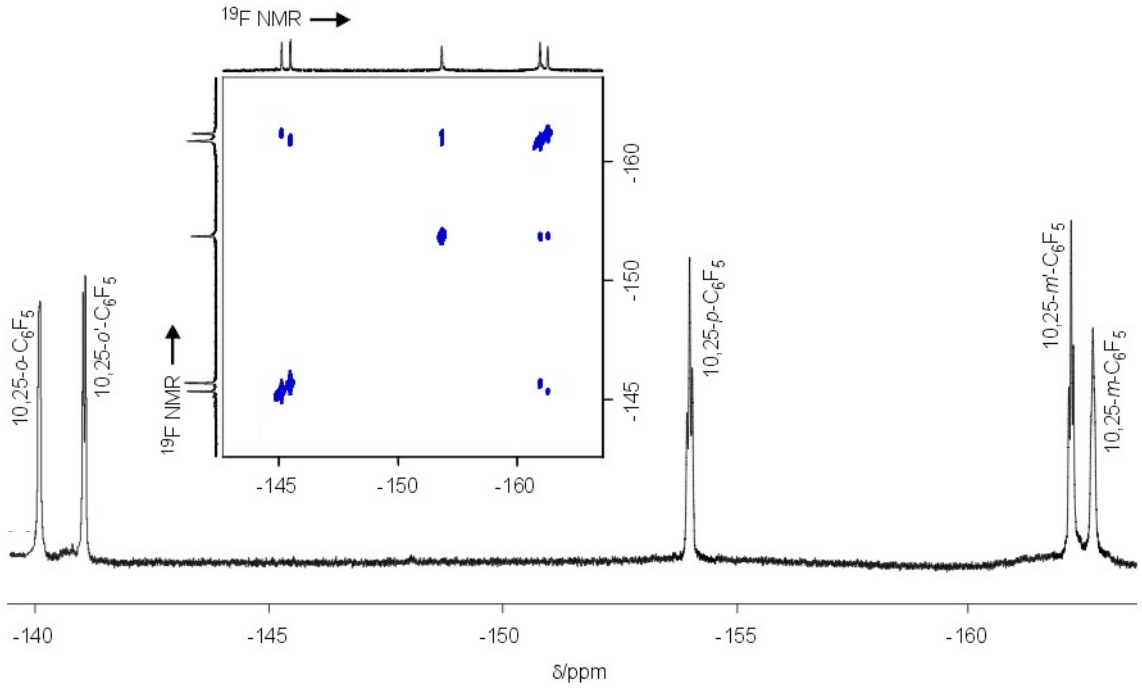

Figure S3. ^{19}F NMR spectrum of **4**a (dichloromethane-d_2, 240 K). Inset: ^{19}F - ^{19}F NMR correlations.

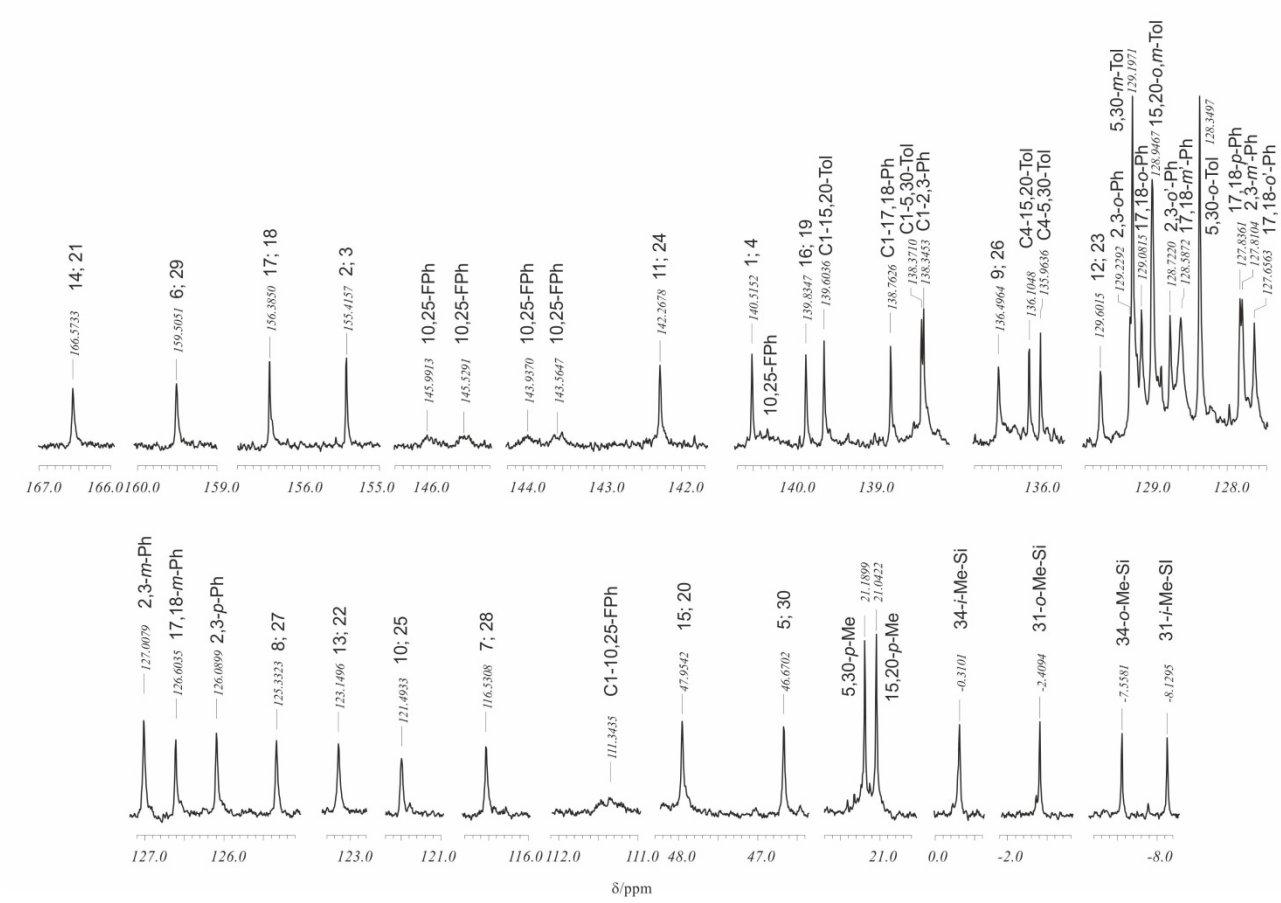

Figure S4. ^{13}C NMR spectrum of **4**a (dichloromethane-d_2, 240 K).

Table S1. ^{1}H NMR chemical shifts calculated for **4**a using the GIAO B3LYP/6-31G** method.

	δ [ppm]
H number	Calculated
NH	12,07
12, 23	6,45
13, 22	6,24
8, 27	5,99
7, 28	5,66
15, 20	4,46
5, 30	4,86
34-i-Si	1,64
31-o-Si	0,76
34-o-Si	-0,08
31-i-Si	-0,33

Table S2. Diagnostic spatial proximity for DFT models of 31,34-disilahexaphyrinoid. * - the shortest H ↔ H distances are given (in Å).

NOE connectivities	Rel. NOE intensities	Spatial proximity for diastereomer*			
		4a	**4**b	**4**c	**4**d
H(15,20) ↔ H(13,22)	1,00	2,48	4,01	2,48	4,01
NH ↔ H(5,30)	0,70	2,63	2,65	3,90	3,82
H(34-*i*-MeSi) ↔ H(5,30)	0,19	3,44	3,65	4,96	5,18
H(31-*i*-MeSi) ↔ H(5,30)	0,10	4,48	4,55	4,04	4,67

Table S3. Cartesian coordinates (.xyz format) for **4**a.

H 4.9188 2.0379 -2.0450	H -4.5642 -2.5895 2.9418
H 2.7966 -4.2523 -2.2759	C -5.4895 -2.2718 0.2384
C -1.3792 3.7502 1.1047	H -2.3431 -0.8217 -3.4081
N -0.0414 3.5175 1.0023	C 1.7604 -3.9051 -0.4930
C 0.5828 3.7465 2.2175	N 0.6250 -3.6780 0.1419
C -0.4221 4.1402 3.1174	C 0.8250 -4.1335 1.4555
C -1.6375 4.1476 2.4220	C 2.1688 -4.6634 1.5911
H -0.2682 4.3952 4.1556	C 2.7569 -4.5158 0.3713
H -2.6067 4.4335 2.8022	H 2.5950 -5.0973 2.4849
C -2.3427 3.5668 -0.0482	H 3.7595 -4.7942 0.0738
C -2.8589 2.1296 -0.1548	C -0.1493 -4.0687 2.4340
Si -2.9745 0.7688 1.1629	C 2.0364 -3.5355 -1.9357
C -3.6557 -0.4780 -0.0955	C 2.6759 -2.1516 -1.9950
C -3.9961 -1.9624 0.0676	C 3.5387 0.4329 -1.9010
C -3.3202 1.6076 -1.3223	C 3.8531 1.9314 -1.8253
C -3.7628 0.1638 -1.2895	C 3.6983 2.4617 -0.4128
C -4.1883 1.1772 2.5615	N 2.5606 2.7889 0.1745
C -1.3261 0.2850 1.9376	C 2.9046 3.1776 1.4815
C -3.4253 2.3745 -2.6041	C 4.3395 3.0710 1.6635
C -2.3607 2.4105 -3.5165	C 4.8363 2.6229 0.4781
C -4.6058 3.0608 -2.9244	H 4.8875 3.3228 2.5605
C -2.4763 3.1101 -4.7194	H 5.8687 2.4275 0.2190
C -3.6567 3.7869 -5.0276	C 1.9867 3.6008 2.4252
C -4.7206 3.7611 -4.1251	C 0.8412 -3.7395 -2.8755
C -4.2869 -0.4620 -2.5439	C 3.1430 2.7528 -2.9067
C -3.4161 -0.9039 -3.5505	C 0.1865 -4.5570 3.8064
C -3.9163 -1.4493 -4.7331	C 2.4829 3.9329 3.7962
C -5.2934 -1.5645 -4.9284	C 1.0499 -3.8403 4.6410
C -6.1686 -1.1366 -3.9296	C 1.3702 -4.2836 5.9223
C -5.6694 -0.5902 -2.7473	C 0.8184 -5.4709 6.3970
H -5.1729 1.4867 2.1995	C -0.0480 -6.2048 5.5904
H -4.3243 0.3023 3.2057	C -0.3541 -5.7428 4.3127
H -0.5820 0.0229 1.1834	C 2.9196 2.9340 4.6723
H -1.4572 -0.5775 2.5983	C 3.3812 3.2297 5.9530
H -0.9292 1.1111 2.5357	C 3.4104 4.5533 6.3850
H -1.4414 1.8802 -3.2872	C 2.9794 5.5701 5.5362
H -1.6427 3.1191 -5.4156	C 2.5223 5.2516 4.2599
H -3.7473 4.3292 -5.9643	F 1.5915 -2.6909 4.2199
H -5.6429 4.2871 -4.3542	F 2.1984 -3.5762 6.6986
H -3.2262 -1.7791 -5.5029	F 1.1199 -5.9058 7.6231
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H -6.3539 -0.2607 -1.9725	F 2.8970 1.6503 4.2936
C -3.2168 -2.6036 1.1963	F 3.7910 2.2531 6.7698
N -1.9407 -3.0537 1.0521	F 3.0122 6.8425 5.9484
C -1.4651 -3.5465 2.2564	F 2.1230 6.2536 3.4664
C -2.5050 -3.3990 3.1907	H -3.7856 1.9867 3.1788
C -3.5933 -2.8180 2.5281	H -1.7812 3.7764 -0.9687
H -2.4585 -3.6890 4.2301	H -3.6871 -2.4635 -0.8598

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C -3.1385 5.9476 -0.3867
C -4.0862 6.9623 -0.3036
C -5.3708 6.7146 0.2032
C -5.6644 5.4131 0.6193
C -4.7148 4.3913 0.5331
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C -5.9805 -3.5173 -0.1770
C -7.3205 -3.8535 -0.0106
C -8.2245 -2.9585 0.5801
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C -6.3867 -1.3779 0.8280
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H -2.1497 6.1699 -0.7804
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C 4.3509 -0.4592 -2.5347
Si 2.1062 -0.5554 -1.1476
C 5.6489 -0.0954 -3.1837
C 4.7160 -2.9289 -3.2642
C 2.2877 -0.6593 0.7296
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C 7.9818 0.5811 -3.0055
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H 6.3288 -2.7725 -1.8416
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H 6.9160 -5.6748 -4.9557
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C 3.3126 3.9962 -4.9959
C 3.8965 3.2306 -3.9888
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H 3.9289 4.3566 -5.8166
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C -0.3885 -3.1974 -4.9068
C -1.1929 -4.3330 -4.7772
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H 0.1765 -5.5428 -1.8979
H -2.3041 -5.7317 -5.9991
H -3.2640 -4.3763 -5.4036
H -2.1169 -4.1286 -6.7241

Table S4. Cartesian coordinates (.xyz format) for **4**b.

C 3.6918 3.8393 -1.9297
C 3.8327 -3.7197 -1.8763
C -3.1073 3.2370 0.1485
N -1.7877 3.3685 0.4542
C -1.6346 3.7868 1.7663
C -2.9291 3.9237 2.2971

C	-3.8409	3.5837	1.2903
H	-3.1641	4.2495	3.2998
H	-4.9187	3.6038	1.3512
C	-3.5977	2.7879	-1.2133
C	-3.5813	1.2642	-1.3780
Si	-3.7331	-0.1058	-0.0701
C	-3.4389	-1.4590	-1.3673
C	-3.4477	-2.9790	-1.1986
C	-3.3419	0.6636	-2.5771
C	-3.2659	-0.8480	-2.5714
C	-5.4344	-0.2134	0.7577
C	-2.4180	-0.0297	1.2785
C	-3.1428	1.4036	-3.8630
C	-1.8935	1.4166	-4.5042
C	-4.2067	2.0957	-4.4626
C	-1.7101	2.1128	-5.6979
C	-2.7762	2.7979	-6.2833
C	-4.0253	2.7838	-5.6632
C	-3.0622	-1.5819	-3.8594
C	-1.8675	-2.2682	-4.1263
C	-1.6940	-2.9665	-5.3222
C	-2.7131	-2.9896	-6.2741
C	-3.9051	-2.3080	-6.0228
C	-4.0772	-1.6104	-4.8284
H	-6.2560	-0.3219	0.0444
H	-5.4613	-1.0770	1.4301
H	-1.4144	0.0447	0.8559
H	-2.4552	-0.9262	1.9055
H	-2.5761	0.8389	1.9253
H	-1.0627	0.8783	-4.0618
H	-0.7333	2.1166	-6.1733
H	-2.6341	3.3363	-7.2159
H	-4.8631	3.3107	-6.1110
H	-0.7604	-3.4895	-5.5090
H	-2.5794	-3.5325	-7.2051
H	-4.7046	-2.3199	-6.7579
H	-5.0077	-1.0839	-4.6411
C	-2.9635	-3.4006	0.1724
N	-1.6426	-3.4672	0.4911
C	-1.4811	-3.8521	1.8119
C	-2.7727	-4.0366	2.3359
C	-3.6907	-3.7558	1.3158
H	-3.0013	-4.3520	3.3434
H	-4.7672	-3.8204	1.3692
C	-4.7929	-3.6531	-1.5215
H	-1.0626	-2.2414	-3.3980
C	2.4138	-3.2577	0.2356
N	1.1261	-3.4503	0.4615
C	1.0127	-3.7834	1.8196
C	2.3296	-3.7910	2.4265
C	3.2067	-3.4467	1.4402
H	2.5522	-4.0021	3.4633
H	4.2774	-3.3191	1.5176
C	-0.2066	-3.9854	2.4421
C	2.8886	-2.7821	-1.1203
C	3.2858	-1.3038	-1.0186
C	3.2342	1.4206	-1.0342
C	2.7810	2.8812	-1.1587
C	2.2843	3.3587	0.1886
N	0.9885	3.4887	0.4142
C	0.8608	3.8399	1.7664
C	2.1765	3.9267	2.3698
C	3.0685	3.6112	1.3875
H	2.3900	4.1673	3.4021
H	4.1445	3.5432	1.4643
C	-0.3656	3.9922	2.3885
H	1.9678	-2.7788	-1.7185
H	1.8629	2.8336	-1.7592
C	-0.2184	-4.3463	3.8915
C	-0.3916	4.3770	3.8317
C	-0.6903	-3.4545	4.8609
C	-0.7084	-3.7801	6.2147
C	-0.2461	-5.0274	6.6281
C	0.2293	-5.9371	5.6874
C	0.2384	-5.5905	4.3381
C	-0.8191	3.4803	4.8172
C	-0.8507	3.8275	6.1653
C	-0.4475	5.1021	6.5569
C	-0.0174	6.0173	5.5998
C	0.0056	5.6489	4.2564
F	-1.1316	-2.2422	4.5006
F	-1.1589	-2.9032	7.1185
F	-0.2587	-5.3493	7.9239
F	0.6691	-7.1373	6.0821
F	0.6942	-6.4948	3.4625
F	-1.2037	2.2428	4.4784
F	-1.2580	2.9454	7.0846
F	0.3653	7.2435	5.9732
F	0.4158	6.5594	3.3649
H	-5.6179	0.6824	1.3599
H	-2.8953	3.1954	-1.9529
H	-2.7327	-3.3934	-1.9213
C	-4.9487	3.4573	-1.5033
C	-4.9689	4.7846	-1.9550
C	-6.1702	5.4392	-2.2087
C	-7.4017	4.7959	-2.0151
C	-7.3786	3.4723	-1.5657
C	-6.1731	2.8117	-1.3136
C	-8.7029	5.5184	-2.2722
C	-4.8553	-5.0555	-1.5585

C	-6.0405	-5.7152	-1.8627
C	-7.2170	-5.0019	-2.1414
C	-7.1511	-3.6076	-2.1086
C	-5.9587	-2.9422	-1.8072
C	-8.5022	-5.7256	-2.4659
H	-5.1805	2.0921	-3.9852
H	-4.0299	5.3085	-2.1156
H	-6.1532	6.4656	-2.5675
H	-8.3165	2.9438	-1.4127
H	-6.1912	1.7801	-0.9816
H	-9.5451	4.8224	-2.3177
H	-8.6731	6.0742	-3.2153
H	-8.9184	6.2444	-1.4786
H	-3.9614	-5.6357	-1.3441
H	-6.0543	-6.8024	-1.8885
H	-8.0435	-3.0255	-2.3259
H	-5.9387	-1.8586	-1.8127
H	-8.8406	-6.3377	-1.6216
H	-8.3761	-6.4006	-3.3200
H	-9.3046	-5.0242	-2.7103
F	-0.4731	5.4446	7.8472
H	-0.9632	3.2324	-0.1322
C	4.4961	-0.6844	-1.0665
C	4.4675	0.8476	-1.0716
Si	1.9980	0.0364	-0.7281
C	5.7750	1.5777	-1.0754
C	5.8304	-1.3645	-1.0777
C	1.4062	0.0370	1.0663
C	6.3255	2.0081	0.1408
C	7.5556	2.6661	0.1785
C	8.2576	2.9027	-1.0031
C	7.7239	2.4717	-2.2186
C	6.4976	1.8093	-2.2535
C	6.4285	-1.7294	0.1374
C	7.6824	-2.3413	0.1641
C	8.3611	-2.5960	-1.0273
C	7.7795	-2.2303	-2.2423
C	6.5293	-1.6136	-2.2665
C	0.5528	0.0076	-1.9385
H	5.7870	1.8128	1.0638
H	7.9647	2.9911	1.1311
H	9.2144	3.4161	-0.9776
H	8.2644	2.6505	-3.1438
H	6.0872	1.4838	-3.2037
H	5.9084	-1.5197	1.0679
H	8.1285	-2.6160	1.1160
H	9.3367	-3.0732	-1.0100
H	8.3011	-2.4241	-3.1753
H	6.0813	-1.3389	-3.2159
H	0.7957	0.9183	1.2775
H	2.2667	0.0533	1.7418
H	0.8210	-0.8588	1.2878
H	0.9043	-0.0853	-2.9714
H	-0.0373	0.9263	-1.8598
H	-0.1212	-0.8284	-1.7274
C	4.5962	-4.7280	-1.2816
C	5.3984	-5.5698	-2.0543
C	5.4650	-5.4419	-3.4449
C	4.6842	-4.4430	-4.0423
C	3.8842	-3.6035	-3.2733
C	4.3847	4.9104	-1.3598
C	5.1534	5.7686	-2.1493
C	5.2550	5.5940	-3.5323
C	4.5442	4.5304	-4.1058
C	3.7783	3.6750	-3.3205
H	4.5623	-4.8772	-0.2086
H	5.9798	-6.3452	-1.5612
C	6.3584	-6.3348	-4.2728
H	4.6965	-4.3285	-5.1239
H	3.2831	-2.8415	-3.7644
H	4.3197	5.0974	-0.2940
H	5.6794	6.5939	-1.6755
C	6.1113	6.5060	-4.3783
H	4.5844	4.3776	-5.1820
H	3.2305	2.8629	-3.7932
H	6.5048	-7.3086	-3.7960
H	7.3514	-5.8876	-4.4085
H	5.9417	-6.5059	-5.2702
H	7.1147	6.0864	-4.5250
H	6.2356	7.4870	-3.9103
H	5.6767	6.6579	-5.3714
H	-0.8194	-3.3009	-0.0898

Table S5. Cartesian coordinates (.xyz format) for **4**c.H 3.2123 0.0252 4.1793

H	-3.4442	0.0704	4.0609
C	3.2670	0.2878	-3.0778
N	3.3247	0.7368	-1.7934
C	3.7097	2.0681	-1.7696
C	3.8965	2.4614	-3.1052
C	3.6215	1.3524	-3.9135
H	4.2058	3.4433	-3.4313
H	3.6781	1.3001	-4.9916
C	2.9366	-1.1304	-3.5019
C	1.4889	-1.5197	-3.1806
Si	0.0458	-0.3554	-3.5742
C	-1.2494	-1.6709	-3.1447
C	-2.7288	-1.4704	-3.5092
C	0.9534	-2.7208	-2.8344

C	-0.5777	-2.8014	-2.8003
C	0.0067	0.0412	-5.4292
C	-0.0283	1.2451	-2.5809
C	1.7052	-3.9883	-2.5710
C	1.7654	-4.5358	-1.2816
C	2.3107	-4.6892	-3.6231
C	2.4200	-5.7447	-1.0508
C	3.0218	-6.4320	-2.1064
C	2.9657	-5.8990	-3.3943
C	-1.1797	-4.1320	-2.4674
C	-1.7266	-4.3799	-1.2021
C	-2.2266	-5.6412	-0.8767
C	-2.1900	-6.6755	-1.8114
C	-1.6517	-6.4389	-3.0775
C	-1.1479	-5.1804	-3.3994
H	0.0544	-0.8683	-6.0363
H	-0.9103	0.5797	-5.6911
H	-0.0227	1.0476	-1.5067
H	-0.9349	1.8115	-2.8152
H	0.8315	1.8817	-2.8101
H	1.3000	-4.0088	-0.4551
H	2.4555	-6.1522	-0.0447
H	3.5262	-7.3773	-1.9274
H	3.4311	-6.4247	-4.2232
H	-2.6436	-5.8098	0.1114
H	-2.5762	-7.6584	-1.5566
H	-1.6199	-7.2364	-3.8146
H	-0.7195	-5.0071	-4.3820
C	-3.2282	-0.0820	-3.1690
N	-3.3109	0.4624	-1.9227
C	-3.8207	1.7496	-1.9955
C	-4.0665	2.0135	-3.3529
C	-3.7013	0.8730	-4.0761
H	-4.4754	2.9316	-3.7480
H	-3.7699	0.7279	-5.1451
H	-2.7049	-1.4444	-4.6084
H	-1.7617	-3.5819	-0.4674
C	-3.4005	1.0044	2.1902
N	-3.4402	0.9569	0.8699
C	-3.8534	2.2360	0.4584
C	-4.0587	3.0842	1.6173
C	-3.7764	2.3118	2.7022
H	-4.3732	4.1182	1.6027
H	-3.8247	2.5869	3.7476
C	-4.0331	2.5927	-0.8647
C	-2.9643	-0.1305	3.0941
C	-1.4586	-0.0624	3.3214
C	1.2590	-0.1194	3.3645
C	2.7728	-0.1460	3.1873
C	3.2125	1.0425	2.3557
N	3.3174	1.0661	1.0386
C	3.6869	2.3838	0.7150
C	3.8074	3.1741	1.9263
C	3.5069	2.3345	2.9543
H	4.0753	4.2199	1.9798
H	3.4826	2.5543	4.0137
C	3.8663	2.8369	-0.5782
C	-3.4862	-1.5111	2.6739
C	3.3432	-1.4926	2.7280
C	-4.4826	3.9854	-1.1722
C	4.2518	4.2687	-0.7786
C	-3.6084	4.9111	-1.7515
C	-4.0055	6.2118	-2.0508
C	-5.3103	6.6123	-1.7717
C	-6.2046	5.7126	-1.1975
C	-5.7857	4.4160	-0.9069
C	3.3336	5.2032	-1.2675
C	3.6770	6.5382	-1.4657
C	4.9702	6.9652	-1.1730
C	5.9074	6.0575	-0.6863
C	5.5418	4.7265	-0.4965
F	-2.3456	4.5587	-2.0252
F	-3.1451	7.0765	-2.5990
F	-5.7022	7.8571	-2.0538
F	-7.4591	6.0953	-0.9338
F	-6.6752	3.5761	-0.3629
F	2.0812	4.8246	-1.5528
F	2.7753	7.4109	-1.9290
F	7.1506	6.4662	-0.4085
F	6.4700	3.8799	-0.0337
H	0.8516	0.6808	-5.7063
C	4.1182	-2.0383	-3.1484
C	-3.7855	-2.5351	-3.1866
H	2.9499	-1.0629	-4.5993
H	2.2651	-4.2816	-4.6286
F	5.3103	8.2432	-1.3580
H	3.1606	0.2354	-0.9224
C	-0.8760	-0.1132	4.5512
C	0.6368	-0.1473	4.5768
Si	-0.0762	0.1212	2.0419
C	1.3511	-0.1929	5.8892
C	-1.6419	-0.1865	5.8337
C	-0.0436	1.8728	1.3335
C	1.2479	0.8771	6.7940
C	1.9299	0.8545	8.0090
C	2.7241	-0.2425	8.3494
C	2.8333	-1.3133	7.4627
C	2.1537	-1.2887	6.2435
C	-2.3511	0.9286	6.3073
C	-3.0827	0.8618	7.4939

C -3.1180 -0.3239 8.2279
C -2.4142 -1.4391 7.7699
C -1.6808 -1.3702 6.5862
C -0.0695 -1.1773 0.6754
H 0.6304 1.7328 6.5392
H 1.8401 1.6946 8.6918
H 3.2528 -0.2612 9.2980
H 3.4483 -2.1719 7.7169
H 2.2456 -2.1256 5.5583
H -2.3154 1.8560 5.7423
H -3.6233 1.7366 7.8441
H -3.6877 -0.3786 9.1509
H -2.4360 -2.3662 8.3355
H -1.1338 -2.2412 6.2387
H 0.8311 2.0145 0.6943
H 0.0011 2.6138 2.1370
H -0.9430 2.0640 0.7426
H -0.1447 -2.1896 1.0814
H 0.8542 -1.1144 0.0926
H -0.9107 -1.0259 -0.0064
H -3.0811 0.0573 -1.0169
C 2.5880 -2.6699 2.7520
C 3.1702 -3.9090 2.4754
C 4.5304 -4.0196 2.1708
C 5.2860 -2.8384 2.1477
C 4.7052 -1.6005 2.4124
C 5.1554 -5.3568 1.8522
H 1.5360 -2.6225 3.0123
H 2.5554 -4.8055 2.5126
H 6.3506 -2.8895 1.9310
H 5.3222 -0.7071 2.3894
H 4.6836 -6.1648 2.4204
H 5.0438 -5.5991 0.7880
H 6.2255 -5.3642 2.0808
C -2.7424 -2.6779 2.8708
C -3.2940 -3.9377 2.6211
C -4.6108 -4.0787 2.1742
C -5.3571 -2.9066 1.9822
C -4.8067 -1.6503 2.2196
C -5.2065 -5.4364 1.8881
H -1.7281 -2.6075 3.2492
H -2.6902 -4.8254 2.7964
H -6.3922 -2.9789 1.6556
H -5.4159 -0.7654 2.0638
H -6.2637 -5.4776 2.1693
H -5.1449 -5.6770 0.8194
H -4.6821 -6.2269 2.4335
C 4.9743 -2.4544 -4.1736
C 6.1192 -3.2037 -3.9041
C 6.4525 -3.5566 -2.5937
C 5.6004 -3.1277 -1.5663
C 4.4559 -2.3825 -1.8334
C 7.6772 -4.3858 -2.2883
H 4.7470 -2.1843 -5.2025
H 6.7627 -3.5123 -4.7245
H 5.8348 -3.3745 -0.5355
H 3.8245 -2.0810 -1.0029
H 8.3634 -4.4157 -3.1394
H 8.2253 -3.9888 -1.4273
H 7.4058 -5.4212 -2.0475
C -4.1657 -3.4300 -4.1948
C -5.1742 -4.3682 -3.9907
C -5.8517 -4.4414 -2.7683
C -5.4789 -3.5400 -1.7648
C -4.4651 -2.6046 -1.9654
C -6.9294 -5.4730 -2.5347
H -3.6654 -3.3900 -5.1595
H -5.4441 -5.0469 -4.7964
H -5.9906 -3.5616 -0.8069
H -4.2236 -1.9260 -1.1542
H -7.5084 -5.6623 -3.4441
H -6.4976 -6.4321 -2.2214
H -7.6242 -5.1567 -1.7511

Table S6. Cartesian coordinates (.xyz format) for **4**d.

C 3.1141 4.1201 -1.6050
C 3.7151 -3.4670 -1.8756
C -3.6228 3.0225 0.4881
N -2.3083 3.2172 0.7797
C -2.1529 3.5526 2.1141
C -3.4421 3.5739 2.6754
C -4.3525 3.2463 1.6615
H -3.6746 3.8121 3.7029
H -5.4280 3.1787 1.7468
C -4.1275 2.6281 -0.8854
C -4.1583 1.1081 -1.0906
Si -3.7739 -0.2919 0.1306
C -3.9427 -1.6090 -1.2257
C -3.6714 -3.1178 -1.1736
C -4.6903 0.5106 -2.1929
C -4.5741 -0.9974 -2.2658
C -5.2560 -0.4686 1.3065
C -2.2177 -0.2205 1.1774
H -6.2019 -0.5146 0.7588
H -5.1568 -1.3807 1.9033
H -1.3106 -0.1247 0.5828
H -2.1310 -1.1274 1.7838

H	-2.2631	0.6287	1.8662
C	-3.1268	-3.5654	0.1678
N	-1.8004	-3.5799	0.4699
C	-1.6042	-4.0160	1.7692
C	-2.8780	-4.2935	2.2963
C	-3.8210	-4.0148	1.2975
H	-3.0776	-4.6640	3.2910
H	-4.8942	-4.1250	1.3647
C	2.2744	-3.1377	0.2432
N	0.9965	-3.4074	0.4446
C	0.8886	-3.8054	1.7858
C	2.1990	-3.7686	2.4090
C	3.0649	-3.3351	1.4495
H	2.4222	-4.0109	3.4388
H	4.1255	-3.1500	1.5490
C	-0.3197	-4.1026	2.3906
C	2.7441	-2.5851	-1.0876
C	3.0885	-1.0981	-0.9273
C	2.8805	1.6211	-0.8239
C	2.3075	3.0439	-0.8758
C	1.7841	3.4178	0.4963
N	0.4842	3.4719	0.7275
C	0.3426	3.7355	2.0983
C	1.6552	3.8504	2.7077
C	2.5585	3.6364	1.7094
H	1.8589	4.0382	3.7528
H	3.6368	3.6074	1.7862
C	-0.8851	3.7826	2.7338
H	1.8264	-2.5880	-1.6904
H	1.3891	2.9453	-1.4693
C	-0.3121	-4.5167	3.8265
C	-0.9148	4.0536	4.2034
C	-0.8072	-3.6740	4.8272
C	-0.8069	-4.0450	6.1694
C	-0.3015	-5.2898	6.5380
C	0.1983	-6.1511	5.5648
C	0.1881	-5.7591	4.2278
C	-1.2549	3.0504	5.1173
C	-1.2883	3.2847	6.4895
C	-0.9756	4.5515	6.9776
C	-0.6336	5.5709	6.0931
C	-0.6072	5.3143	4.7239
F	-1.2900	-2.4655	4.5087
F	-1.2811	-3.2145	7.1044
F	-0.2960	-5.6555	7.8222
F	0.6803	-7.3483	5.9167
F	0.6701	-6.6161	3.3195
F	-1.5505	1.8182	4.6823
F	-1.6112	2.3039	7.3396
F	-0.3375	6.7887	6.5612
F	-0.2816	6.3205	3.9033
H	-5.2949	0.3820	1.9941
F	-1.0030	4.7869	8.2917
H	-1.5014	3.1917	0.1561
C	4.2553	-0.4055	-1.0268
C	4.1375	1.1243	-0.9762
Si	1.7539	0.1532	-0.5024
C	5.3940	1.9333	-1.0711
C	5.6220	-1.0062	-1.1421
C	1.2991	0.0440	1.3292
C	6.0543	2.3231	0.1032
C	7.2381	3.0597	0.0488
C	7.7818	3.4186	-1.1845
C	7.1357	3.0329	-2.3600
C	5.9563	2.2913	-2.3036
C	6.2987	-1.3990	0.0222
C	7.5816	-1.9434	-0.0430
C	8.2102	-2.1040	-1.2779
C	7.5491	-1.7119	-2.4429
C	6.2701	-1.1606	-2.3747
C	0.2727	0.0959	-1.6639
H	5.6373	2.0366	1.0648
H	7.7348	3.3515	0.9700
H	8.7024	3.9934	-1.2302
H	7.5505	3.3099	-3.3250
H	5.4551	2.0025	-3.2218
H	5.8140	-1.2662	0.9855
H	8.0890	-2.2406	0.8706
H	9.2082	-2.5293	-1.3325
H	8.0308	-1.8339	-3.4089
H	5.7612	-0.8628	-3.2858
H	0.6581	0.8747	1.6321
H	2.2151	0.0866	1.9265
H	0.7887	-0.8933	1.5600
H	0.5992	0.1593	-2.7075
H	-0.4036	0.9313	-1.4662
H	-0.2859	-0.8343	-1.5368
C	4.5927	-4.3947	-1.3040
C	5.4162	-5.1889	-2.1010
C	5.3936	-5.0950	-3.4975
C	4.5088	-4.1742	-4.0701
C	3.6844	-3.3807	-3.2740
C	3.8563	5.1252	-0.9751
C	4.5336	6.0899	-1.7200
C	4.4933	6.0952	-3.1194
C	3.7425	5.0960	-3.7493
C	3.0637	4.1327	-3.0054
H	4.6336	-4.5147	-0.2278
H	6.0881	-5.8987	-1.6241
C	6.2851	-5.9676	-4.3493

H 4.4605 -4.0800 -5.1526
H 3.0046 -2.6756 -3.7471
H 3.9042 5.1709 0.1066
H 5.1035 6.8560 -1.1994
C 5.2221 7.1532 -3.9138
H 3.6841 5.0744 -4.8352
H 2.4856 3.3700 -3.5224
H 6.0417 -7.0297 -4.2272
H 7.3397 -5.8478 -4.0764
H 6.1855 -5.7250 -5.4110
H 6.2771 7.2141 -3.6245
H 4.7876 8.1470 -3.7515
H 5.1808 6.9463 -4.9870
H -1.0020 -3.3703 -0.1298
H -5.1622 2.9933 -0.9290
H -4.6323 -3.6368 -1.2886
C -3.3441 3.4155 -1.9468
C -2.2539 2.8762 -2.6369
C -1.4959 3.6611 -3.5063
C -1.8035 5.0091 -3.7245
C -2.9071 5.5407 -3.0453
C -3.6606 4.7607 -2.1702
C -0.9802 5.8504 -4.6707
C -2.7521 -3.6542 -2.2830
C -2.8056 -5.0133 -2.6137
C -1.9179 -5.5642 -3.5365
C -0.9388 -4.7805 -4.1592
C -0.8977 -3.4185 -3.8371
C -1.7891 -2.8638 -2.9185
C 0.0423 -5.3741 -5.1419
C -5.4188 1.2477 -3.2733
C -6.7386 1.6661 -3.0443
C -7.4531 2.3527 -4.0267
C -6.8573 2.6338 -5.2562
C -5.5453 2.2230 -5.4961
C -4.8338 1.5339 -4.5149
C -5.2030 -1.7344 -3.4077
C -6.4546 -2.3405 -3.2175
C -7.0789 -3.0369 -4.2529
C -6.4596 -3.1404 -5.4985
C -5.2143 -2.5434 -5.6999
C -4.5929 -1.8453 -4.6650
H -7.2077 1.4410 -2.0903
H -8.4750 2.6651 -3.8310
H -7.4109 3.1690 -6.0222
H -5.0725 2.4411 -6.4494
H -3.8098 1.2309 -4.7058
H -6.9427 -2.2563 -2.2503
H -8.0491 -3.4962 -4.0855
H -6.9426 -3.6828 -6.3060
H -4.7223 -2.6231 -6.6650
H -3.6181 -1.3984 -4.8282
H -2.0049 1.8290 -2.5081
H -0.6483 3.2160 -4.0225
H -3.1764 6.5830 -3.1973
H -4.5003 5.2075 -1.6434
H -1.2260 5.6320 -5.7175
H 0.0901 5.6606 -4.5408
H -1.1541 6.9179 -4.5092
H -3.5435 -5.6521 -2.1347
H -1.9831 -6.6235 -3.7722
H -0.1560 -2.7789 -4.3104
H -1.7466 -1.8018 -2.7065
H -0.0763 -4.9370 -6.1405
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H 1.0760 -5.1894 -4.8283