Supporting Information

for

Synthesis, Structure, and Theoretical Investigation of Amidinato Supported 1,4-disilabenzene

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S1. Synthesis and experimental details of 2

2: Toluene (20 mL) was added to a mixture of **1** (0.1 g, 0.19 mmol) and diphenyl alkine (0.07 g, 0.39 mmol) at ambient temperature. The mixture was stirred overnight. The volatiles were removed *in vacuo* and cyclopentane (10 mL) was added to the residue. The reaction mixture once again was stirred overnight. The cyclopentane was removed in vacuum and THF (2 mL) and toluene (10 mL) was added to the reaction mixture. The solution was concentrated and stored at room temperature for two days to yield dark red crystals of **2** (0.05 g, 29.41%). Mp 154-158 °C. Anal. calcd for **2**, $C_{58}H_{66}N_4Si_2$ (874.34) C, 79.58; H, 7.60; N, 6.40; found: C, 80.51; H, 7.29; N, 6.55; Due to the high sensitivity of the crystals the reported values deviated from the calculated one. ^{1}H NMR (200 MHz, C_6D_6, 25 °C): δ 1.31 (s, 36 H, *t*Bu), 6.86-6.96 (m, 10 H, Ph); 7.92-8.19 ppm (m, 20 H, Ph) ^{13}C{^{1}H} NMR (125.75 MHz, C_6D_6, 25 °C): δ 30.8(C*Me*$_3$), 57.2 (*C*Me$_3$), 125.6, 126.4, 127.0, 127.8, 127.9, 128.5, 128.9, 129.4, 129.9, 130.2, 133.0, 136.4, 138.9, 139.0, 140.2, 141.5 (Ph), 171.37 ppm (NCN); ^{29}Si{^{1}H} NMR (99.36 MHz, C_6D_6, 25 °C): δ –18.05 ppm. EI-MS: *m*/*z*: 874 [M^+] (30%).

S2. Crystallographic data for the structural analysis of 2

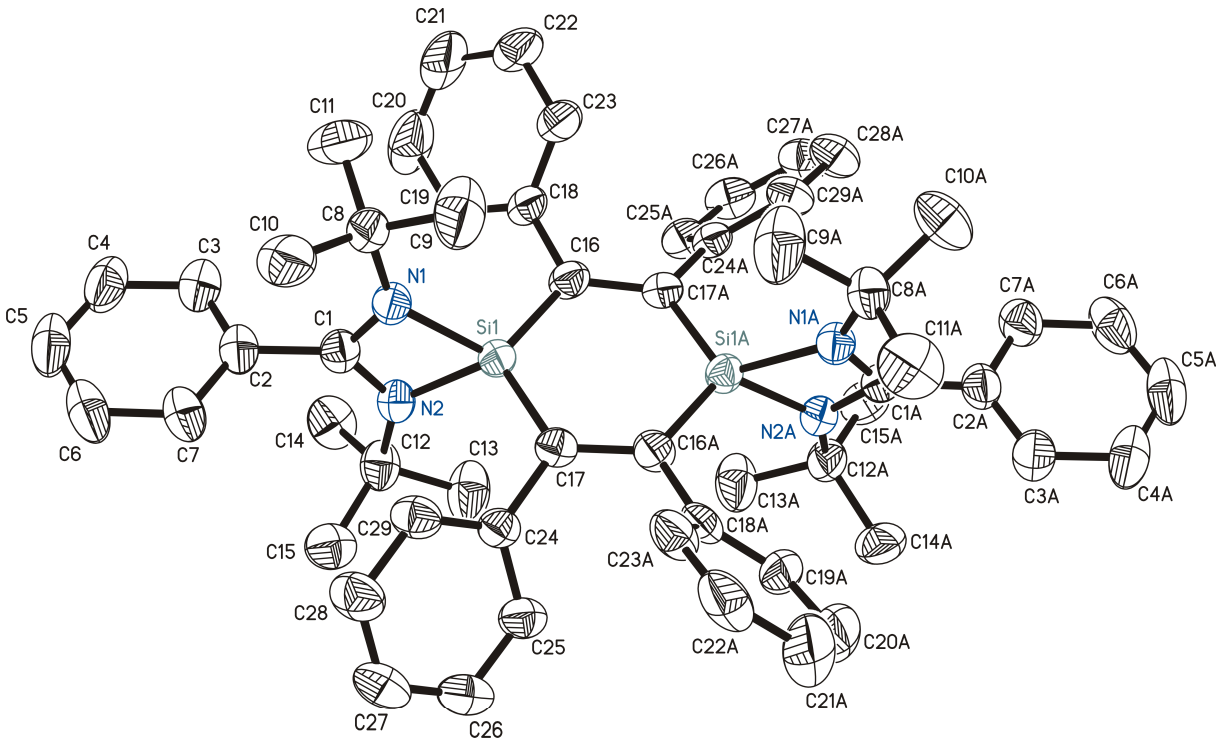


Figure 1: The solid state structure of **2**; anisotropic displacement parameters are depicted at the 50% probability level; the disordered phenyl group (C18 to C23), the solvent molecules (THF and cyclopentane) and H atoms are omitted for clarity reasons.

Empirical formula	C65.84 H81.67 N4 O0.36 Si2	
Formula weight	991.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P 3_1 2 1	
Unit cell dimensions	a = 14.0399(8) Å	α= 90°.
	b = 14.0399(8) Å	β= 90°.
	c = 28.1188(16) Å	γ = 120°.
Volume	4800.2(5) $Å^3$	
Z	3	
Density (calculated)	1.028 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	1607	
Crystal size	0.18 x 0.12 x 0.11 mm	
Theta range for data collection	1.67 to 26.37°.	
Index ranges	-17<=h<=17, -17<=k<=17, -35<=l<=35	
Reflections collected	93952	
Independent reflections	6572 [R(int) = 0.0278]	
Completeness to theta = 26.37°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9896 and 0.9831	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6572 / 306 / 441	
Goodness-of-fit on F^2	1.134	
Final R indices [I>2sigma(I)]	R1 = 0.0685, wR2 = 0.1932	
R indices (all data)	R1 = 0.0708, wR2 = 0.1961	
Absolute structure parameter	0.08(17)	
Largest diff. peak and hole	0.768 and -0.507 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for p3121. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4699(2)	7971(2)	150(1)	40(1)
C(2)	4103(2)	8598(2)	184(1)	45(1)
C(3)	3875(3)	8870(3)	626(1)	55(1)
C(4)	3310(3)	9455(3)	652(2)	66(1)
C(5)	2979(3)	9741(3)	246(2)	69(1)
C(6)	3214(3)	9476(3)	-193(2)	66(1)
C(7)	3784(3)	8906(3)	-228(1)	52(1)
C(8)	3116(2)	5985(2)	239(1)	45(1)
C(9)	3130(3)	4940(3)	126(2)	88(2)
C(10)	2326(3)	6107(4)	-80(1)	65(1)
C(11)	2795(3)	5977(4)	757(1)	74(1)
C(12)	6697(2)	9544(2)	25(1)	48(1)
C(13)	7738(3)	9467(3)	-5(2)	70(1)
C(14)	6768(3)	10240(3)	459(1)	60(1)
C(15)	6573(3)	10056(3)	-432(1)	55(1)
C(16)	6057(2)	6494(2)	565(1)	39(1)
C(17)	5980(2)	6696(2)	-504(1)	36(1)
C(18)	5718(12)	6632(11)	1048(4)	39(2)
C(19)	5716(15)	7560(14)	1206(3)	52(3)
C(20)	5260(20)	7620(20)	1636(4)	90(6)
C(21)	4790(20)	6700(20)	1932(4)	103(7)
C(22)	4788(14)	5760(18)	1784(3)	68(4)
C(23)	5221(11)	5712(14)	1343(4)	51(3)
C(18')	5429(13)	6309(14)	1026(5)	40(3)
C(19')	5353(12)	7165(15)	1231(5)	56(3)
C(20')	4785(12)	7021(18)	1654(4)	72(4)
C(21')	4302(11)	6004(18)	1874(4)	75(4)
C(22')	4388(13)	5158(19)	1676(5)	69(4)
C(23')	4973(12)	5299(14)	1259(5)	51(3)
C(24)	5824(2)	7255(2)	-922(1)	36(1)
C(25)	6691(3)	7864(2)	-1237(1)	45(1)
C(26)	6555(3)	8432(3)	-1613(1)	52(1)
C(27)	5584(3)	8420(3)	-1686(1)	56(1)
C(28)	4717(3)	7800(3)	-1392(1)	56(1)

C(29)	4830(2)	7224(2)	-1010(1)	45(1)
N(1)	4264(2)	6889(2)	165(1)	38(1)
N(2)	5782(2)	8396(2)	86(1)	39(1)
Si(1)	5629(1)	7002(1)	69(1)	35(1)
O(70)	199(13)	2179(13)	1383(7)	89(5)
C(71)	877(16)	3219(18)	1609(8)	74(5)
C(72)	283(16)	3821(16)	1723(6)	77(6)
C(73)	-905(16)	2930(20)	1669(10)	94(7)
C(74)	-901(15)	1960(18)	1436(11)	100(7)
C(81)	720(20)	1530(20)	823(8)	297(10)
C(82)	557(17)	362(16)	932(8)	279(9)
C(83)	1689(16)	785(14)	1174(5)	222(8)
C(84)	2502(16)	1877(15)	925(7)	257(8)
C(85)	1770(20)	1792(18)	497(6)	289(10)

Table 3. Selected bond lengths [Å] and angles [°] for p3121.

C(1)-N(1)	1.325(4)
C(1)-N(2)	1.339(4)
C(1)-C(2)	1.490(4)
C(8)-N(1)	1.486(4)
C(12)-N(2)	1.485(4)
C(16)-C(17)#1	1.415(4)
C(16)-C(18)	1.484(11)
C(16)-Si(1)	1.800(3)
C(17)-C(16)#1	1.415(4)
C(17)-C(24)	1.490(3)
C(17)-Si(1)	1.799(2)
N(1)-Si(1)	1.861(2)
N(2)-Si(1)	1.859(2)
N(1)-C(1)-N(2)	106.5(2)
N(1)-C(1)-C(2)	127.1(3)
N(2)-C(1)-C(2)	126.4(2)
N(1)-C(1)-Si(1)	53.29(13)
N(2)-C(1)-Si(1)	53.23(13)
C(2)-C(1)-Si(1)	178.2(2)
C(17)#1-C(16)-C(18')	118.6(6)
C(18)-C(16)-Si(1)	117.6(5)
C(16)#1-C(17)-C(24)	119.6(2)
C(16)#1-C(17)-Si(1)	123.18(17)
C(24)-C(17)-Si(1)	116.88(18)
C(1)-N(1)-C(8)	131.7(2)
C(1)-N(1)-Si(1)	91.89(17)
C(8)-N(1)-Si(1)	136.42(19)
C(1)-N(2)-C(12)	132.2(2)
C(1)-N(2)-Si(1)	91.51(16)
C(12)-N(2)-Si(1)	136.18(18)
C(17)-Si(1)-C(16)	114.36(12)
C(17)-Si(1)-N(2)	111.85(11)
C(16)-Si(1)-N(2)	120.84(12)
C(17)-Si(1)-N(1)	120.16(11)
C(16)-Si(1)-N(1)	112.83(11)
N(2)-Si(1)-N(1)	70.07(10)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z

Selected bond lengths [Å] and angles [°] for **2**.

C(1)-N(1)	1.325(4)	N(1)-C(1)-N(2)	106.5(2)
C(1)-N(2)	1.339(4)	N(1)-C(1)-C(2)	127.1(3)
C(1)-C(2)	1.490(4)	N(2)-C(1)-C(2)	126.4(2)
C(8)-N(1)	1.486(4)	N(1)-C(1)-Si(1)	53.29(13)
C(12)-N(2)	1.485(4)	N(2)-C(1)-Si(1)	53.23(13)
C(16)-C(17)#1	1.415(4)	C(2)-C(1)-Si(1)	178.2(2)
C(16)-C(18)	1.484(11)	C(17)#1-C(16)-	118.6(6)
C(16)-Si(1)	1.800(3)	C(18)-C(16)-Si(1)	117.6(5)
C(17)-C(16)#1	1.415(4)	C(16)#1-C(17)-C(24)	119.6(2)
C(17)-C(24)	1.490(3)	C(16)#1-C(17)-Si(1)	123.18(17)
C(17)-Si(1)	1.799(2)	C(24)-C(17)-Si(1)	116.88(18)
N(1)-Si(1)	1.861(2)	C(1)-N(1)-C(8)	131.7(2)
N(2)-Si(1)	1.859(2)	C(1)-N(1)-Si(1)	91.89(17)
		C(8)-N(1)-Si(1)	136.42(19)
		C(1)-N(2)-C(12)	132.2(2)
		C(1)-N(2)-Si(1)	91.51(16)
		C(12)-N(2)-Si(1)	136.18(18)
		C(17)-Si(1)-C(16)	114.36(12)
		C(17)-Si(1)-N(2)	111.85(11)
		C(16)-Si(1)-N(2)	120.84(12)
		C(17)-Si(1)-N(1)	120.16(11)
		C(16)-Si(1)-N(1)	112.83(11)
		N(2)-Si(1)-N(1)	70.07(10)

S3. Theoretical Calculations of 2 and 3

All theoretical calculations were performed with Gaussian 09 (Rev. A.02) on the UB3LYP/6-311G* level of theory.[19]

Coordinates of the singlet state of **2**

Si	-1.694411	0.000002	0.000040
N	-3.271482	0.111432	1.071280
N	-3.271532	-0.111428	-1.071120
C	-0.714705	1.523803	0.028913
C	-4.065913	0.000002	0.000098
C	-0.714707	-1.523799	-0.028886
C	-1.439315	2.805814	0.257711
C	-5.554397	-0.000002	0.000133
C	-1.439327	-2.805809	-0.257653
C	-6.261098	1.204415	-0.100145
H	-5.719409	2.140359	-0.179749
C	-3.214583	4.397786	-0.289400
H	-4.036508	4.686518	-0.939292
C	-4.197473	1.762065	2.700225
H	-3.563892	2.533706	2.262458
H	-4.302773	1.972574	3.768650
H	-5.190205	1.831052	2.253404
C	-6.261084	-1.204426	0.100443
H	-5.719383	-2.140364	0.180021
C	-1.765549	4.841034	1.572986
H	-1.458694	5.470832	2.403097
C	-7.653415	1.201170	-0.099542
H	-8.190988	2.140542	-0.177158
C	-8.353500	-0.000014	0.000197
H	-9.438505	-0.000018	0.000221
C	-3.584830	-0.363298	-2.503619
C	-2.523496	3.213315	-0.539698
H	-2.809576	2.600466	-1.386264
C	-3.584713	0.363303	2.503792
C	-2.843003	5.220769	0.771004
H	-3.375703	6.146378	0.964938
C	-4.531302	-0.704987	3.081295
H	-5.522922	-0.666400	2.630725
H	-4.651529	-0.542229	4.156032
H	-4.127888	-1.710341	2.940777
C	-1.078474	3.659530	1.320308
H	-0.245012	3.380950	1.955283
C	-7.653401	-1.201192	0.099904
H	-8.190963	-2.140568	0.177544
C	-1.078533	-3.659523	-1.320268
H	-0.245099	-3.380941	-1.955280
C	-4.197596	-1.762062	-2.700025
H	-3.563995	-2.533703	-2.262288
H	-4.302943	-1.972569	-3.768446
H	-5.190308	-1.831051	-2.253160
C	-4.531449	0.704989	-3.081076
H	-5.523049	0.666395	-2.630463
H	-4.651722	0.542235	-4.155808
H	-4.128034	1.710345	-2.940572
C	-2.523472	-3.213313	0.539802
H	-2.809515	-2.600465	1.386382
C	-3.214570	-4.397784	0.289532
H	-4.036467	-4.686518	0.939459

C	-2.247191	-0.293246	-3.260657
H	-1.776539	0.686177	-3.150862
H	-2.418414	-0.470726	-4.325543
H	-1.546432	-1.046652	-2.898413
C	-1.765618	-4.841027	-1.572919
H	-1.458800	-5.470823	-2.403045
C	-2.843037	-5.220764	-0.770891
H	-3.375745	-6.146373	-0.964803
C	-2.247039	0.293255	3.260769
H	-1.776389	-0.686166	3.150954
H	-2.418214	0.470735	4.325662
H	-1.546300	1.046664	2.898493
Si	1.694411	0.000001	-0.000046
N	3.271530	-0.111459	1.071119
N	3.271485	0.111460	-1.071275
C	0.714706	-1.523800	0.028839
C	4.065913	0.000000	-0.000094
C	0.714705	1.523803	-0.028881
C	1.439326	-2.805817	0.257572
C	5.554397	-0.000004	-0.000124
C	1.439315	2.805820	-0.257645
C	6.261085	-1.204424	-0.100471
H	5.719384	-2.140361	-0.180081
C	3.214569	-4.397777	-0.289654
H	4.036466	-4.686494	-0.939588
C	4.197583	-1.762139	2.699983
H	3.563980	-2.533766	2.262224
H	4.302927	-1.972675	3.768398
H	5.190296	-1.831120	2.253119
C	6.261098	1.204410	0.100195
H	5.719408	2.140351	0.179827
C	1.765614	-4.841070	1.572784
H	1.458795	-5.470887	2.402892
C	7.653402	-1.201190	-0.099927
H	8.190965	-2.140564	-0.177595
C	8.353500	-0.000015	-0.000178
H	9.438505	-0.000019	-0.000199
C	3.584722	0.363372	-2.503780
C	2.523472	-3.213300	-0.539893
H	2.809516	-2.600428	-1.386456
C	3.584822	-0.363369	2.503611
C	2.843033	-5.220786	0.770746
H	3.375741	-6.146401	0.964635
C	4.531442	0.704901	3.081100
H	5.523044	0.666316	2.630489
H	4.651712	0.542118	4.155828
H	4.128031	1.710261	2.940619
C	1.078530	-3.659559	1.320164
H	0.245096	-3.380993	1.955183
C	7.653415	1.201165	0.099597
H	8.190988	2.140535	0.177245
C	1.078475	3.659564	-1.320219
H	0.245013	3.381000	-1.955202
C	4.197477	1.762143	-2.700171
H	3.563891	2.533769	-2.262386
H	4.302780	1.972681	-3.768590
H	5.190207	1.831122	-2.253345
C	4.531318	-0.704897	-3.081307
H	5.522936	-0.666317	-2.630732
H	4.651549	-0.542110	-4.156039
H	4.127909	-1.710257	-2.940817
C	2.523496	3.213300	0.539774

H	2.809576	2.600428	1.386325
C	3.214583	4.397778	0.289509
H	4.036508	4.686493	0.939408
C	2.247052	0.293341	-3.260764
H	1.776406	-0.686086	-3.150980
H	2.418231	0.470852	-4.325652
H	1.546308	1.046736	-2.898469
C	1.765549	4.841075	-1.572867
H	1.458694	5.470895	-2.402961
C	2.843002	5.220789	-0.770874
H	3.375703	6.146404	-0.964783
C	2.247181	-0.293333	3.260646
H	1.776533	0.686095	3.150878
H	2.418400	-0.470843	4.325528
H	1.546421	-1.046726	2.898379

Coordinates of the triplet state of **2**

Si	-1.666043	0.000015	0.000043
N	-3.211776	0.014538	1.076981
N	-3.211826	-0.014499	-1.076822
C	-0.711702	1.548694	0.122242
C	-4.008565	0.000017	0.000098
C	-0.711727	-1.548674	-0.122207
C	-1.376629	2.793133	0.565800
C	-5.499351	0.000007	0.000133
C	-1.376695	-2.793100	-0.565742
C	-6.204350	1.207606	0.037428
H	-5.662880	2.146190	0.070178
C	-3.229888	4.396396	0.498690
H	-4.174828	4.706226	0.059227
C	-4.207834	1.384607	2.916901
H	-3.638069	2.247095	2.570267
H	-4.299517	1.449317	4.004940
H	-5.214244	1.442201	2.499680
C	-6.204333	-1.207602	-0.037128
H	-5.662850	-2.146178	-0.069902
C	-1.400592	4.774443	2.005264
H	-0.915337	5.371245	2.772622
C	-7.596994	1.204854	0.035549
H	-8.134628	2.146795	0.063822
C	-8.295985	-0.000014	0.000195
H	-9.380976	-0.000022	0.000219
C	-3.505475	-0.069608	-2.535288
C	-2.615073	3.229398	0.051038
H	-3.082547	2.658179	-0.742222
C	-3.505358	0.069631	2.535461
C	-2.632314	5.179045	1.484109
H	-3.106956	6.091469	1.830668
C	-4.354808	-1.132633	2.984933
H	-5.344735	-1.130261	2.527688
H	-4.493050	-1.097508	4.068989
H	-3.862977	-2.077708	2.743945
C	-0.786102	3.614134	1.553845
H	0.171379	3.320059	1.969065
C	-7.596977	-1.204872	-0.035188
H	-8.134599	-2.146821	-0.063437
C	-0.786216	-3.614116	-1.553802

H	0.171262	-3.320066	-1.969046
C	-4.207962	-1.384592	-2.916677
H	-3.638180	-2.247073	-2.570052
H	-4.299690	-1.449321	-4.004712
H	-5.214354	-1.442183	-2.499413
C	-4.354947	1.132648	-2.984740
H	-5.344857	1.130276	-2.527457
H	-4.493230	1.097511	-4.068790
H	-3.863111	2.077728	-2.743780
C	-2.615141	-3.229327	-0.050953
H	-3.082583	-2.658093	0.742316
C	-3.230000	-4.396307	-0.498590
H	-4.174939	-4.706109	-0.059106
C	-2.143419	-0.009070	-3.245992
H	-1.599281	0.901431	-2.984020
H	-2.290161	-0.016813	-4.328653
H	-1.524140	-0.868043	-2.982039
C	-1.400750	-4.774409	-2.005205
H	-0.915529	-5.371224	-2.772575
C	-2.632471	-5.178976	-1.484021
H	-3.107146	-6.091386	-1.830568
C	-2.143272	0.009086	3.246105
H	-1.599143	-0.901410	2.984094
H	-2.289967	0.016812	4.328772
H	-1.524006	0.868064	2.982138
Si	1.666044	-0.000006	-0.000037
N	3.211825	-0.014583	1.076830
N	3.211779	0.014556	-1.076971
C	0.711709	-1.548687	0.122159
C	4.008567	-0.000012	-0.000087
C	0.711722	1.548686	-0.122193
C	1.376657	-2.793133	0.565671
C	5.499353	-0.000012	-0.000117
C	1.376664	2.793121	-0.565746
C	6.204343	-1.207620	0.037057
H	5.662866	-2.146202	0.069755
C	3.229942	-4.396363	0.498501
H	4.174882	-4.706167	0.059020
C	4.207911	-1.384759	2.916652
H	3.638104	-2.247210	2.569993
H	4.299622	-1.449524	4.004686
H	5.214306	-1.442370	2.499400
C	6.204343	1.207594	-0.037315
H	5.662866	2.146177	-0.069992
C	1.400667	-4.774480	2.005083
H	0.915429	-5.371309	2.772430
C	7.596987	-1.204879	0.035121
H	8.134615	-2.146827	0.063299
C	8.295986	-0.000014	-0.000166
H	9.380978	-0.000014	-0.000185
C	3.505365	0.069703	-2.535448
C	2.615103	-3.229364	0.050886
H	3.082562	-2.658116	-0.742363
C	3.505472	-0.069740	2.535295
C	2.632390	-5.179049	1.483904
H	3.107049	-6.091475	1.830433
C	4.354991	1.132473	2.984773
H	5.344891	1.130088	2.527468
H	4.493296	1.097292	4.068819
H	3.863179	2.077577	2.743860
C	0.786155	-3.614167	1.553702
H	-0.171326	-3.320116	1.968941

C	7.596987	1.204852	-0.035429
H	8.134615	2.146800	-0.063625
C	0.786117	3.614161	-1.553745
H	-0.171393	3.320126	-1.968925
C	4.207793	1.384718	-2.916843
H	3.638008	2.247172	-2.570158
H	4.299451	1.449480	-4.004881
H	5.214209	1.442324	-2.499640
C	4.354859	-1.132516	-2.984957
H	5.344778	-1.130134	-2.527693
H	4.493121	-1.097339	-4.069009
H	3.863052	-2.077616	-2.744020
C	2.615149	3.229331	-0.051037
H	3.082645	2.658076	0.742184
C	3.229982	4.396317	-0.498693
H	4.174954	4.706105	-0.059271
C	2.143282	0.009133	-3.246097
H	1.599180	-0.901385	-2.984109
H	2.289981	0.016888	-4.328764
H	1.523990	0.868087	-2.982114
C	1.400623	4.774461	-2.005166
H	0.915349	5.371297	-2.772487
C	2.632384	5.179011	-1.484063
H	3.107039	6.091426	-1.830624
C	2.143419	-0.009168	3.246002
H	1.599311	0.901355	2.984043
H	2.290163	-0.016932	4.328662
H	1.524112	-0.868117	2.982037

Coordinates of the singlet state of **3**

Si	1.701518	0.000001	0.000033
N	3.292469	1.075130	-0.000184
N	3.292468	-1.075129	0.000301
C	0.706554	0.000017	1.486159
C	4.089022	0.000000	0.000045
C	0.706585	-0.000013	-1.486113
H	1.194329	0.000202	2.462956
C	5.575931	-0.000001	-0.000004
H	1.194370	-0.000198	-2.462878
C	6.288384	-0.000462	1.207632
H	5.750103	-0.000762	2.149067
C	4.370826	2.933905	1.264220
H	3.832896	2.619977	2.162300
H	4.482086	4.021569	1.300888
H	5.370314	2.498261	1.288894
C	6.288304	0.000456	-1.207686
H	5.749960	0.000758	-2.149085
C	7.679884	-0.000428	1.204769
H	8.216626	-0.000748	2.147955
C	8.382121	-0.000006	-0.000097
H	9.466964	-0.000008	-0.000133
C	3.592236	-2.525739	-0.000017
C	3.592238	2.525741	0.000118
C	4.370126	2.934439	-1.264242
H	5.369497	2.498576	-1.289730
H	4.481626	4.022097	-1.300386
H	3.831573	2.621096	-2.162153

C	7.679804	0.000417	-1.204916
H	8.216483	0.000736	-2.148139
C	4.370886	-2.933865	-1.264094
H	3.832991	-2.619924	-2.162190
H	4.482164	-4.021527	-1.300780
H	5.370368	-2.498204	-1.288712
C	4.370064	-2.934475	1.264369
H	5.369439	-2.498626	1.289912
H	4.481550	-4.022135	1.300492
H	3.831475	-2.621146	2.162262
C	2.236872	-3.255279	-0.000618
H	1.646164	-2.994917	0.879457
H	2.402795	-4.336378	-0.000659
H	1.646822	-2.994766	-0.881096
C	2.236873	3.255280	0.000633
H	1.646207	2.994892	-0.879463
H	2.402795	4.336380	0.000649
H	1.646781	2.994794	0.881091
Si	-1.701518	0.000002	-0.000005
N	-3.292469	1.075131	0.000177
N	-3.292468	-1.075128	-0.000262
C	-0.706554	-0.000018	-1.486130
C	-4.089022	0.000001	0.000001
C	-0.706585	0.000022	1.486142
H	-1.194315	0.000144	-2.462900
C	-5.575932	-0.000001	0.000037
H	-1.194368	-0.000140	2.462901
C	-6.288374	-0.000604	-1.207606
H	-5.750084	-0.001020	-2.149036
C	-4.370775	2.933885	-1.264313
H	-3.832819	2.619924	-2.162366
H	-4.482016	4.021551	-1.301014
H	-5.370269	2.498258	-1.289009
C	-6.288316	0.000597	1.207713
H	-5.749981	0.001014	2.149117
C	-7.679874	-0.000574	-1.204755
H	-8.216607	-0.001009	-2.147947
C	-8.382122	-0.000007	0.000104
H	-9.466966	-0.000009	0.000130
C	-3.592237	-2.525738	0.000033
C	-3.592237	2.525742	-0.000172
C	-4.370173	2.934465	1.264150
H	-5.369541	2.498592	1.289613
H	-4.481685	4.022122	1.300262
H	-3.831650	2.621148	2.162087
C	-7.679816	0.000561	1.204930
H	-8.216504	0.000994	2.148148
C	-4.370776	-2.933919	1.264160
H	-3.832819	-2.619991	2.162223
H	-4.482023	-4.021585	1.300823
H	-5.370269	-2.498287	1.288869
C	-4.370176	-2.934418	-1.264303
H	-5.369540	-2.498536	-1.289754
H	-4.481698	-4.022074	-1.300448
H	-3.831649	-2.621080	-2.162230
C	-2.236873	-3.255278	0.000487
H	-1.646243	-2.994882	-0.879632
H	-2.402795	-4.336377	0.000500
H	-1.646744	-2.994799	0.880922
C	-2.236871	3.255279	-0.000650
H	-1.646242	2.994910	0.879476
H	-2.402791	4.336378	-0.000698

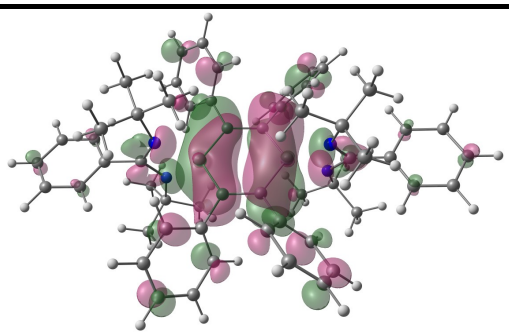
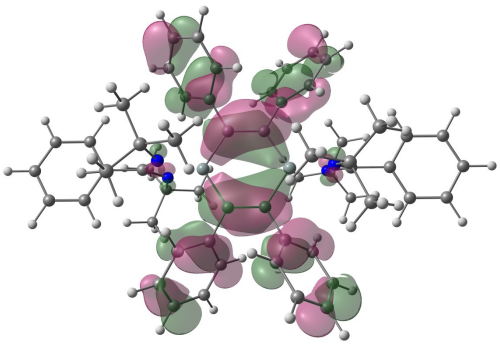
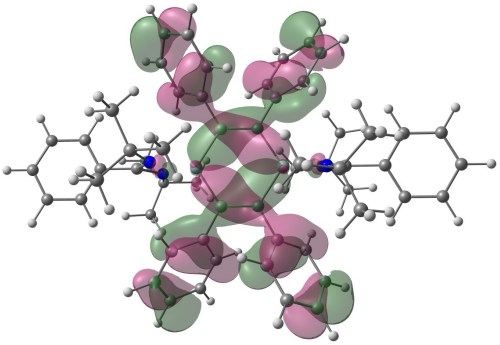
H	-1.646743	2.994770	-0.881077

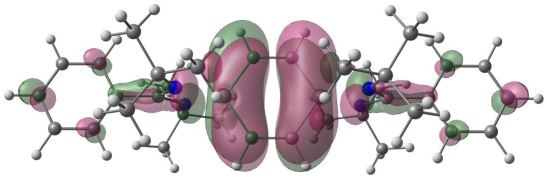
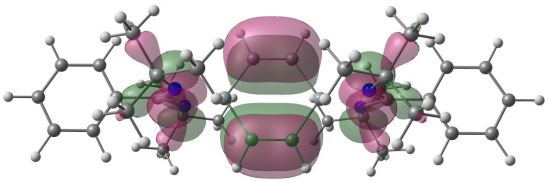
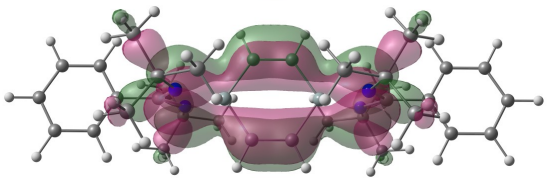
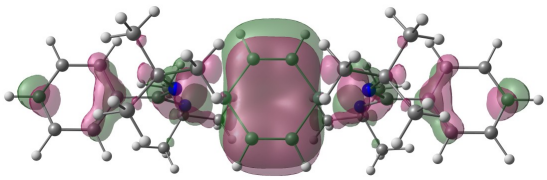
Coordinates of the triplet state of **3**

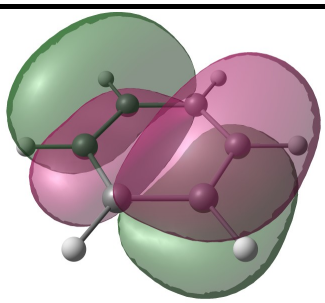
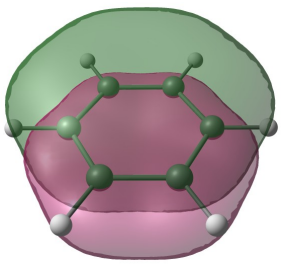
Si	-1.809412	0.000016	-0.000013
N	-3.222891	-1.096323	0.162978
N	-3.222909	1.096331	-0.162997
C	-0.721783	0.045189	1.491677
C	-4.116258	-0.000002	-0.000004
C	-0.721781	-0.045143	-1.491700
C	-5.545502	-0.000010	0.000010
H	-1.221508	-0.048889	-2.462345
C	-6.297558	-0.748580	0.952121
H	-5.768633	-1.287637	1.728481
C	-4.399755	-3.305874	0.429714
H	-4.158525	-3.259228	1.494964
H	-4.350288	-4.353291	0.116041
H	-5.425505	-2.969667	0.292604
C	-6.297584	0.748553	-0.952086
H	-5.768680	1.287615	-1.728456
C	-7.682818	-0.742029	0.947495
H	-8.217294	-1.307543	1.706426
C	-8.398548	-0.000024	0.000038
H	-9.483437	-0.000029	0.000049
C	-3.397914	2.468725	0.388082
C	-3.397877	-2.468715	-0.388114
C	-3.849557	-2.427080	-1.860964
H	-4.807905	-1.914688	-1.962214
H	-3.964448	-3.440043	-2.259862
H	-3.116271	-1.903051	-2.479970
C	-7.682844	0.741989	-0.947432
H	-8.217340	1.307498	-1.706353
C	-4.399804	3.305860	-0.429755
H	-4.158570	3.259209	-1.495004
H	-4.350356	4.353281	-0.116092
H	-5.425549	2.969637	-0.292646
C	-3.849595	2.427096	1.860932
H	-4.807936	1.914692	1.962185
H	-3.964501	3.440062	2.259820
H	-3.116302	1.903084	2.479943
C	-2.031507	3.170723	0.285696
H	-1.271921	2.678448	0.896923
H	-2.113900	4.205652	0.628104
H	-1.681423	3.182992	-0.750167
C	-2.031460	-3.170693	-0.285732
H	-1.271879	-2.678399	-0.896951
H	-2.113835	-4.205619	-0.628152
H	-1.681380	-3.182967	0.750133
Si	1.656425	0.000009	-0.000009
N	3.202666	-1.074431	0.052419
N	3.202678	1.074428	-0.052436
C	0.659938	-0.046231	-1.506572
C	4.002958	-0.000005	-0.000009
C	0.659936	0.046263	1.506552
H	1.162469	-0.062677	-2.475990
C	5.489693	-0.000009	-0.000002
H	1.162465	0.062716	2.475971
C	6.196748	-0.070196	-1.206733
H	5.658398	-0.137033	-2.145678
C	4.524748	-3.059802	-0.703552

H	4.216228	-2.860817	-1.732919
H	4.610256	-4.142965	-0.583215
H	5.515074	-2.631818	-0.550527
C	6.196739	0.070182	1.206734
H	5.658381	0.137026	2.145675
C	7.588639	-0.068252	-1.203633
H	8.126292	-0.123547	-2.144275
C	8.288521	-0.000014	0.000009
H	9.373224	-0.000016	0.000014
C	3.487151	2.513265	-0.291218
C	3.487110	-2.513269	0.291235
C	3.962488	-2.729467	1.739543
H	4.927838	-2.253920	1.922199
H	4.075926	-3.797488	1.944608
H	3.235293	-2.326363	2.448451
C	7.588629	0.068231	1.203646
H	8.126275	0.123525	2.144292
C	4.524747	3.059756	0.703637
H	4.216148	2.860784	1.732983
H	4.610313	4.142914	0.583305
H	5.515065	2.631725	0.550678
C	3.962614	2.729482	-1.739495
H	4.927969	2.253930	-1.922107
H	4.076072	3.797506	-1.944535
H	3.235454	2.326398	-2.448450
C	2.159836	3.259795	-0.079166
H	1.388475	2.912928	-0.769525
H	2.307456	4.329268	-0.247180
H	1.787085	3.123166	0.937987
C	2.159794	-3.259781	0.079125
H	1.388402	-2.912893	0.769439
H	2.307389	-4.329253	0.247162
H	1.787099	-3.123159	-0.938050
H	-1.221511	0.048954	2.462321

Highest occupied orbitals (number and energy in a.u.) of **2**, **3** and benzene. Positive (green) and negative (red) isosurface representation at 0.02 a.u..

235 -0.1043	
234 -0.1956	
233 -0.2042	

155 -0.0864	
154 -0.2055	
152 -0.2310	
151 -0.2406	

20 -0.2556		**21** -0.2555
17 -0.3691		

S4. Complete list of reference no 19

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.