Supporting Information

"Synthesis of six-coordinate mono-, bis-, and tris(tetrazolato) complexes via [3+2] cycloadditions of nitriles to silicon-bound azido ligands"

Peter Portius, Martin Davis

Contents

1. General experimental conditions

All experiments were carried out under an atmosphere of argon using Schlenk or glove box techniques. Appropriate safety precautions were adopted during all experiments involving silicon azides. The glassware was baked out in vacuo prior to use. The solvents CH_2Cl_2, MeCN, THF and hexane were obtained from Grubbs columns, stirred over CaH_2, trap-to-trap condensed and stored in ampoules. Tolunitril, benzonitrile and pyridylnitrile (Aldrich) and the deuterated solvents MeCN-d_3 and $CDCl_3$ were stirred over CaH_2 and trap-to-trap condensed prior to use. Nujol was kept dry by standing over sodium. The compounds **1a** and **1b** were obtained using published procedures.[1] C, H, N microanalyses were performed by the Elemental Analysis service of the Department of Chemistry, University of Sheffield, using a Perkin Elmer 2400 CHNS/O Series II Elemental Analyser. Melting points were determined in sealed capillary tubes under argon using a Gallenkamp 7936B melting point apparatus and are uncorrected. Positive ion current mass spectra were obtained from VG AutoSpec (GC MS EI+, calibrated against PFK, 50 < *m*/*z* < 700 Da at temperatures of *ca*. 200ºC) and Waters LCT (TOF, ES+, 0.1 < m/z < 3.0 kDa) spectrometers. IR spectra were obtained from solutions in a specac$^{(R)}$ transmission cell equipped with CaF_2 windows (4000 – 1200 cm^{-1}) or from capillary layers of paraffin mulls between NaCl windows (4000 – 500 cm^{-1}) using Mattson Galaxy 2020 and Bruker Tensor 27 FTIR spectrometers with a resolution of 2 cm^{-1}. The following abbreviations were used for the relative intensities and shape of the absorption bands: vs: very strong; s: strong; m: medium; w: weak; vw: very weak; br: broad. The asymmetric and symmetric vibrational modes were denoted by the subscript symbols “as” and “sym”, respectively. For the IR spectra recorded in nujol mulls, only those bands with an absorption maximum exceeding 0.01 absorbance units were evaluated

and their intensities are given in parentheses relative to the main band (100%). ^{1}H and ^{13}C{^{1}H} NMR spectra were recorded on a Bruker 250 spectrometer (SF(^{1}H) = 249.9 MHz and SF(^{13}C) = 62.84 MHz) in dry and deoxygenated solvents at temperatures between 20°C and 25°C. The ^{1}H and ^{13}C{^{1}H} NMR spectra were calibrated against the residual proton and natural abundance ^{13}C resonances of the solvent relative to $SiMe_4$ (solvent acetonitrile-d_3, chloroform-*d* and dichloromethane-d_2 (δ(^{1}H) [ppm] = 1.94, 7.26, 5.32) and the natural abundance of ^{13}C in the solvent (δ (^{13}C) [ppm] = 1.3 and 118.3, 77.2, 53.8). Solid state NMR spectra are referenced against adamantane (38.5 ppm) and were recorded under the following conditions: ^{29}Si (99.34 MHz) CP, magic angle spinning at 8kHz, recycle delay of 10 s contact time of 2 ms; ^{15}N (50.67 MHz) CP, magic angle spinning at 8 kHz, recycle delay of 9 s, contact time of 2 ms; ^{13}C (125.76 MHz) CP, total sideband suppression (TOSS), magic angle spinning at 8 kHz, recycle delay of 5 s, contact time of 2 ms. The following abbreviations were used for the signal multiplicities: ddd: doublet of double doublets; dd: double doublet; s: singlet. Numbering of the ring protons according to IUPAC recommendations.[1] Suitable single crystals for the X-ray diffraction studies were obtained upon slow cooling saturated solutions from room temperature to approximately −30°C. Details of the crystallographic measurements can be found in section 4. Supplementary crystallographic data for this paper (CCDC 1493371-1493377) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

2. Additional analytical data on the title compounds

Complex 4a. IR (Nujol, cm^{-1}, A > 0.05 in parentheses): 3126(6), 3091(12), 3071(8), 2149(73), 2122(60), 1624(13), 1615(26), 1575(13), 1568(12), 1505(13 sh), 1495(38), 1478(31 sh), 1454(100), 1356(27), 1325(58), 1240(22), 1183(20), 1165(19), 1137(27), 1077(30), 1043(19), 1026(12), 783(27), 735(30), 726(25), 706(74), 676(18), 657(13), 593(12), 578(49), 554(48), 515(45).

Complex 4b. IR (Nujol, cm^{-1}, A > 0.05 in parentheses): 3132(6), 3101(8), 3078(7), 2157(100), 2122(38), 1627(8), 1618(17), 1576(7), 1570(8), 1505(13 sh), 1498(25), 1479(20 sh), 1451(57), 1366(26 sh), 1351(21), 1316(26), 1233(8), 1179(15), 1162(12), 1151(6), 1135(7), 1110(6), 1093(8), 1071(18), 1056(6), 1044(17), 1027(12), 779(17), 733(27), 727(17), 703(21), 696(25), 683(21), 671(12), 562(47), 536(32), 518(52).

Complex *OC-6-13*-[Si(N$_3$)$_2$(κ*N*(2)-ptz)$_2$(bpy)] (**5**). FTIR (CH_2Cl_2, cm^{-1}) ν_{as}(NN) = 2164vs, 2134w; (CH_3CN, cm^{-1}) ν_{as}(NN) = 2162vs, 2132w; (THF, cm^{-1}) ν_{as}(NN) = 2163vs, 2129m; (Nujol, cm^{-1}, A > 0.01 in parentheses): 3066(5), 2166(63), 2126(32), 1625(7), 1615(18), 1568(8 br), 1506(12), 1456(100), 1317(13), 1245(7), 1190(5), 1176(7), 1164(8), 1132(5), 1116(7), 1069(13), 1043(14), 791(9), 783(17), 733(30), 695(30), 586(16), 575(31), 547(29).

[1] Nomenclature of Organic Chemistry, J. Rigaudy, S. P. Klesney (Editors), Pergamon Press, **1979**.

Complex *OC-6-13*-[Si(N$_3$)$_2$(*κN*(2)-ttz)$_2$(bpy)]·CH$_3$CN (**6**). FTIR (CH_2Cl_2, cm^{-1}) ν_{as}(NN) = 2164vs, 2134w; (CH_3CN, cm^{-1}) ν_{as}(NN) = 2162vs, 2133w; (THF, cm^{-1}) ν_{as}(NN) = 2162vs, 2132w; (nujol, cm^{-1}, A > 0.05 in parentheses): ν_{as}(NN) = 3129(7), 3092 (8), 3072(13), 3066(14), 3039(14), 2248(5), 2156 (100), 2127(67), 1626(9), 1617(26), 1575(9), 1569(8), 1508(11), 1456(91), 1435(29 sh), 1335(20), 1324(25), 1242(11), 1187(15), 1164 (12), 1132(10), 1117(6), 1075(16), 1045(21), 1027(9), 1006(8), 829(19), 784(25), 773(6), 760 (18), 738(32), 723(10), 694(39), 622(10), 579(58), 549(38), 509(38).

Complex *OC-6-13*-[Si(N$_3$)$_2$(*κN*(2)-ptz)$_2$(phen)]·CH$_3$CN (**7·CH$_3$CN**). IR (Nujol, cm^{-1}, A > 0.05 in parentheses): 3095(9), 3068(13), 3032(11), 2250(5), 2164(95 sh), 2158(100), 2129(88), 1635(5), 1624(9), 1583(23), 1526(24), 1489(8), 1446(64), 1433(46), 1362(20 sh), 1328(20), 1247(12), 1232(11), 1209(6), 1189(16), 1149(17), 1131(9), 1114(23), 1072(6), 1040(9), 1024(11), 1006(6), 883(21), 859(31), 791(13), 757(34), 742(15 sh), 733(50), 726(67), 720(36 sh), 695(68), 660(7), 582(64), 562(48), 548(56), 540(49 sh).

Complex [Si(N$_3$)(mtz)$_3$(bpy)] (**8**). FTIR (CH_3CN, cm^{-1}) ν_{as}(NN) = 2159vs; (THF, cm^{-1}) ν_{as}(NN) = 2158vs; (py, cm^{-1}) ν_{as}(NN) = 2161vs; IR (Nujol, cm^{-1}, A > 0.05 in parentheses): 3133(8), 3116(6), 3092(8), 3076(13 sh), 3068(17), 3051(12), 3039(11), 2158(100), 1628(15), 1617(32), 1578(15), 1568(10), 1510(39), 1505(35 sh), 1482(25), 1461(55 sh nujol), 1454(66), 1430(28), 1378(44 nujol), 1360(32), 1320(32), 1293(7), 1253(8), 1238(26), 1182(37), 1162(18), 1140(15), 1128(16), 1116(10), 1105(21), 1084(11), 1073(25), 1056(12), 1045(35), 1031(23), 1017(12), 789(28), 772(12), 733(37), 727(23), 724(23), 706(44), 700(47), 676(24), 572(72), 524(55), 508(47).

Complex *OC-6-22*-[Si(N$_3$)$_2$(*κ*^{2}*N*(1),*N*'-pytz)$_2$] (**9**). FTIR (CH_3CN, cm^{-1}) ν_{as}(NN) = 2143s(br); (CH_2Cl_2, cm^{-1}) ν_{as}(NN) = 2141s(br), (Nujol, cm^{-1}, A > 0.10 in parentheses): 3103(15), 2164(90), 2122(65), 1631(38), 1569(10), 1543(10), 1451(100), 1408(17), 1328(27, br), 1294(20), 1162(28), 1113(20), 1094(20), 1059(51), 1050(35), 1030(16), 909(10), 802(26), 771(22), 733(40), 722(64), 682(30), 668(28), 586(52), 557(59), 531(28), 509(12).

Characteristic ^{1}H NMR data (250 MHz, r.t., CD_3CN, ppm) for the protons H6, H6' (bpy) and H2, H9 (phen) of the complexes studied *in situ* and of the starting complexes **1** and **2** for reference (H6,H6' and H2,H9 are isochronous, respectively): *OC-6-22*-[Si(N$_3$)$_4$(bpy)], δ = 9.40 (2H, ddd, 5.8, 1.5, 0.8 Hz); *OC-6-23*-[Si(N$_3$)$_3$(*κN*(1)-mtz)(bpy)], δ = 9.32 (2H, pd); *OC-6-23*-[Si(N$_3$)$_3$(*κN*(2)-mtz)(bpy)], δ = 9.64 (2H, pd); *OC-6-32*-[Si(N$_3$)$_2$(*κN*(2)-mtz)$_2$(bpy), δ = 9.72 (1H); *OC-6-23*-[Si(N$_3$)$_3$(ttz)(bpy)], δ = 9.69 (2H, ddd) ($CDCl_3$, 9.84 (2H, ddd)); *OC-6-22*-[Si(N$_3$)$_4$(phen)], δ = 9.60 (2H, dd, 5.4, 1.3 Hz);*OC-6-24*-[Si(N$_3$)$_2$(*κN*(1)-mtz)(*κN*(2)-mtz)(phen)], δ = 9.85 (2H, d, 5.4 Hz); *OC-6-13*-[Si(N$_3$)$_2$(*κN*(2)-mtz)$_2$(phen)], δ = 10.07 (2H, d, 5.5 Hz); *OC-6-23*-[Si(N$_3$)$_3$(*κN*(1)-mtz)(phen)], δ = 9.57 (2H, pd, *ca*. 5.5

Hz); *OC-6-23*-[Si(N_3)$_3$(κN(2)-mtz)(phen)], δ = 9.85 (2H); *OC-6-23*-[Si(N_3)$_2$(κN(2)-mtz)(phen), δ = 9.93 (1H); *OC-6-23*-[Si(N_3)$_3$(ptz)(phen)], δ = 9.90 (2H, dd, 5.5 Hz, 1.2 Hz).

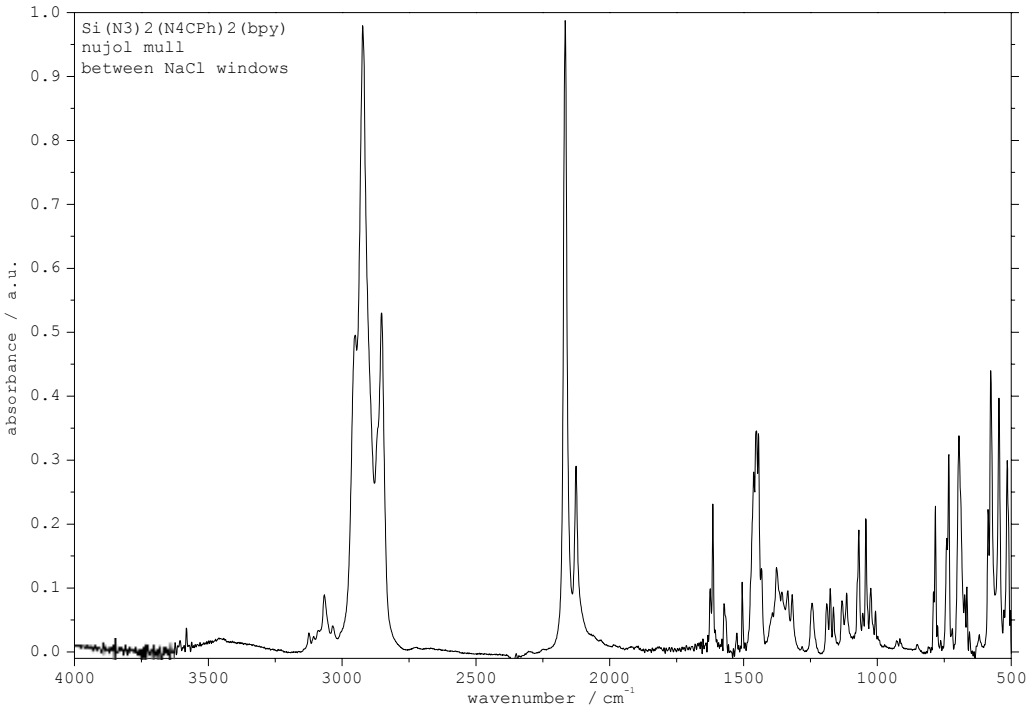


Fig. S1. IR spectrum of a nujol mull of analytically pure compound **5** between NaCl windows

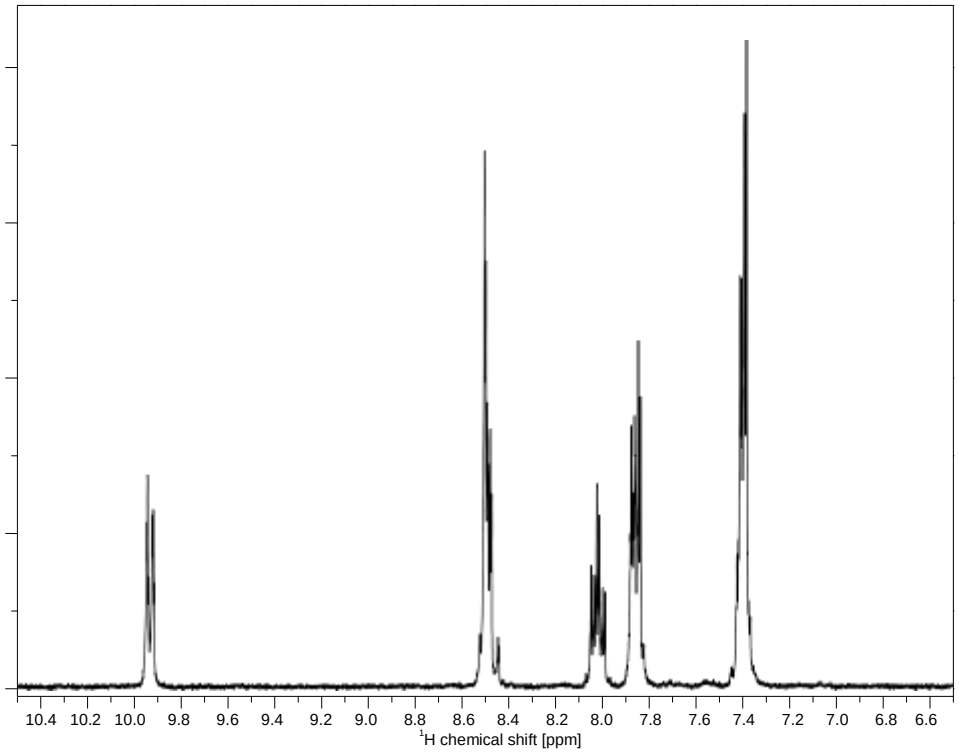


Fig. S2. 6.5 – 10.5 ppm section of the ^{1}H NMR spectrum of compound **5** in acetonitrile-d_3 solution.

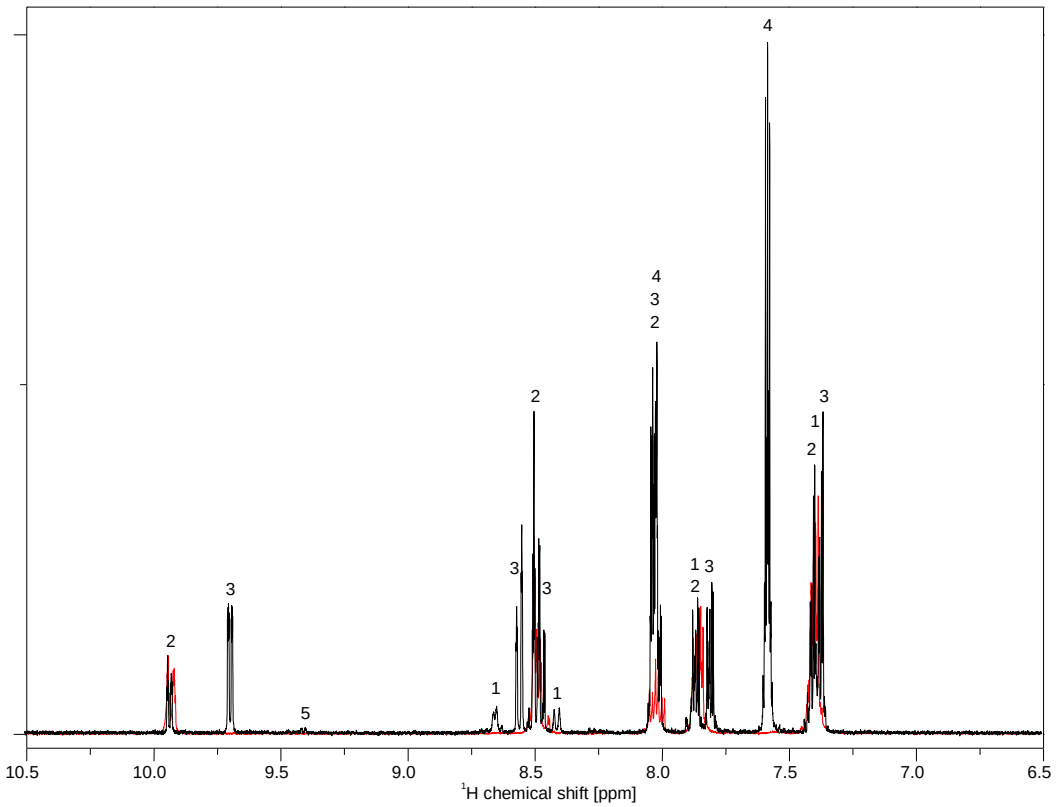


Fig. S3. 6.5 – 10.5 ppm section of the ^{1}H NMR spectrum in acetonitrile-d_3 solution of a sample of the reaction mixture during the synthesis of complex **5** after evaporation of the majority of the reaction solvent. Assignement: complex **5** (“2”), $Si(N_3)_3(N_4CPh)(bpy)$ (“3”) and PhCN (“4”), free bpy (“1”), complex **1** (“5”).

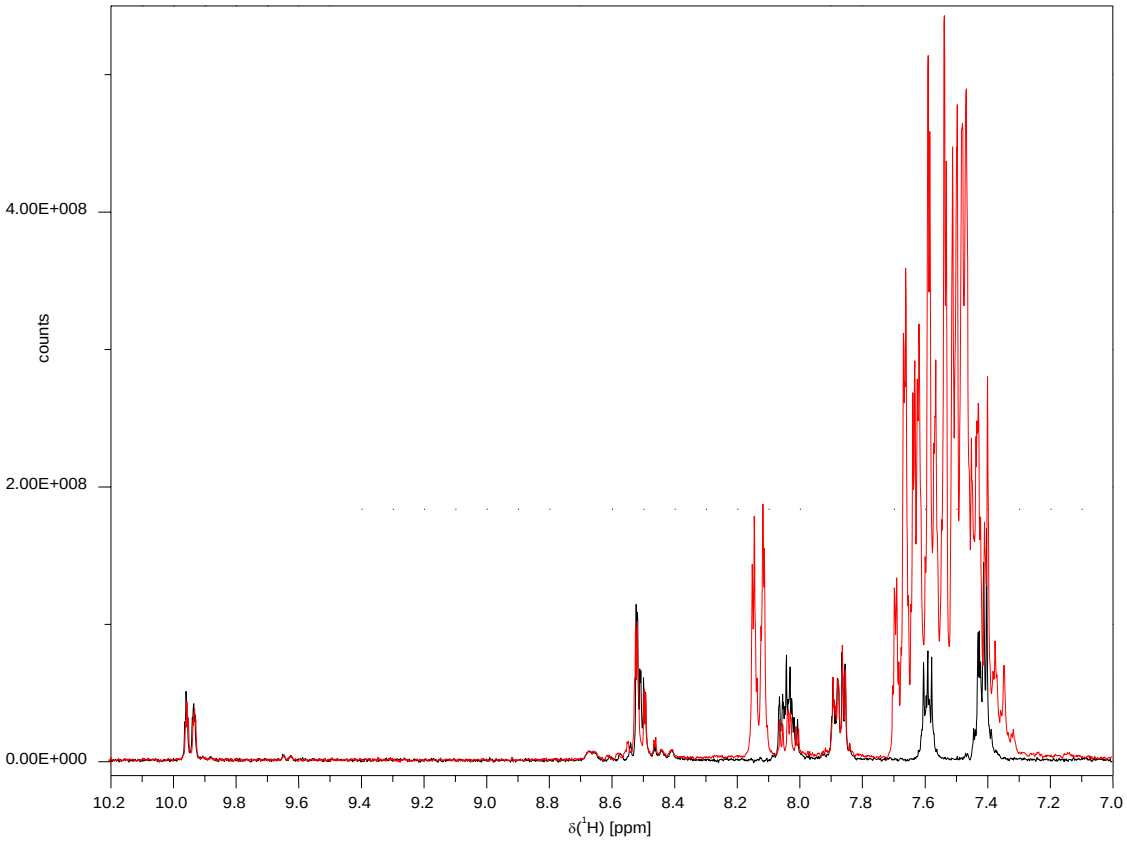


Fig. S4. 7.0 – 10.2 ppm section of the ^{1}H NMR spectrum of a mixture of compound **5** and Ph-CN.

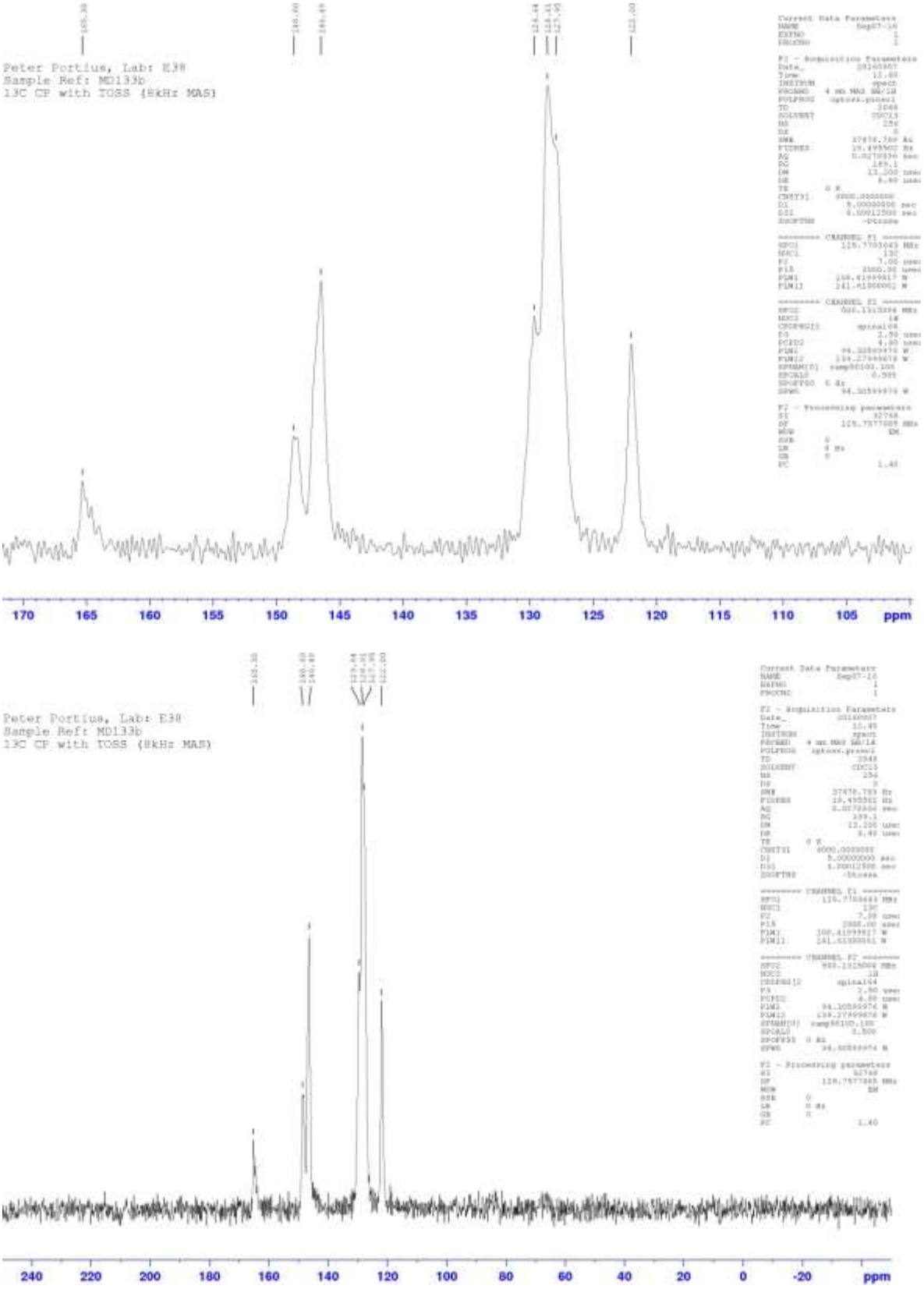


Fig. S5. ^{13}C ssNMR spectrum of $Si(N_3)_2(N_4C\text{-}Ph)_2(bpy)$ (**5**) in solid state (100 - 170 ppm expansion, top; overview, bottom).

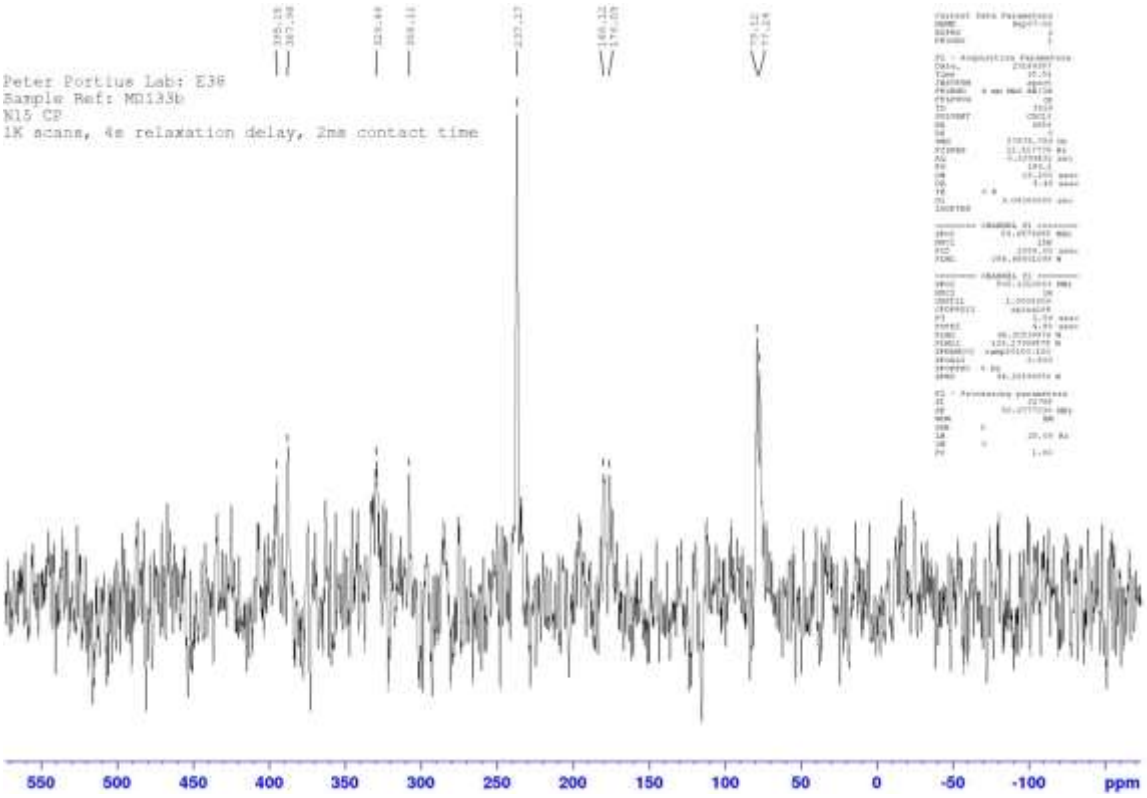


Fig. S6. ^{15}N ssNMR spectrum of $Si(N_3)_2(N_4C\text{-}Ph)_2(bpy)$ (**5**) in solid state (chemical shifts in unified scale).
(Note: $\delta(NH_3) = 0$ ppm), $\delta(CH_3NO_3) = 380$ ppm.)

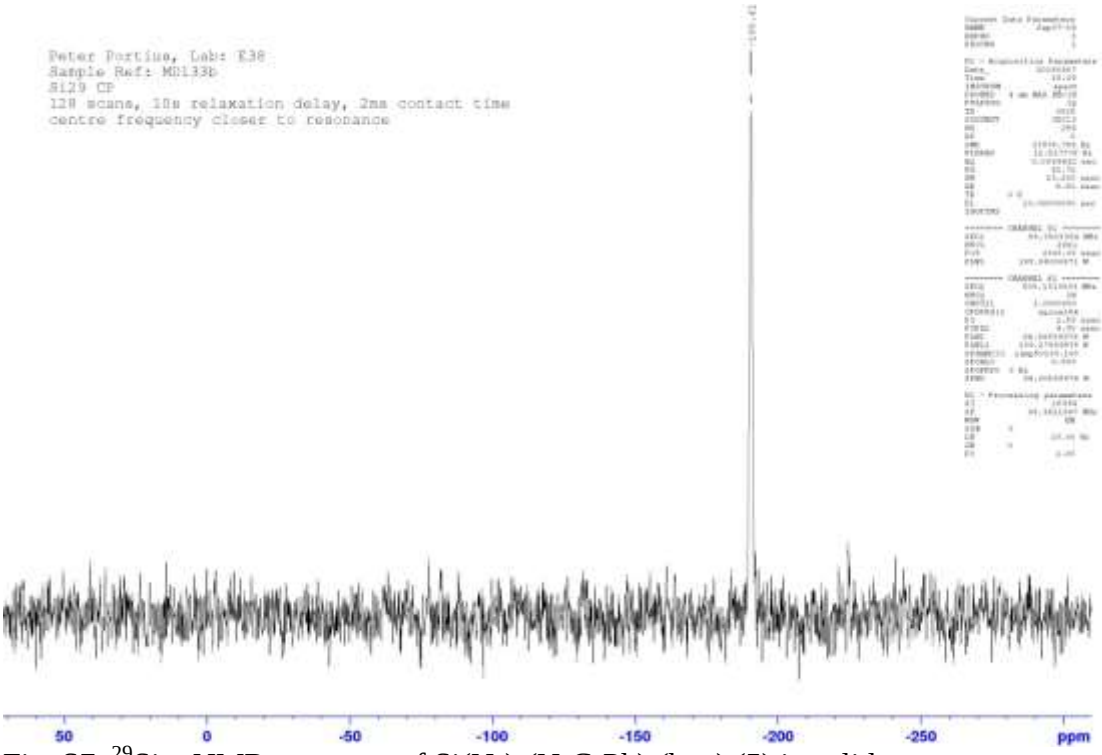


Fig. S7. ^{29}Si ssNMR spectrum of $Si(N_3)_2(N_4C\text{-}Ph)_2(bpy)$ (**5**) in solid state.

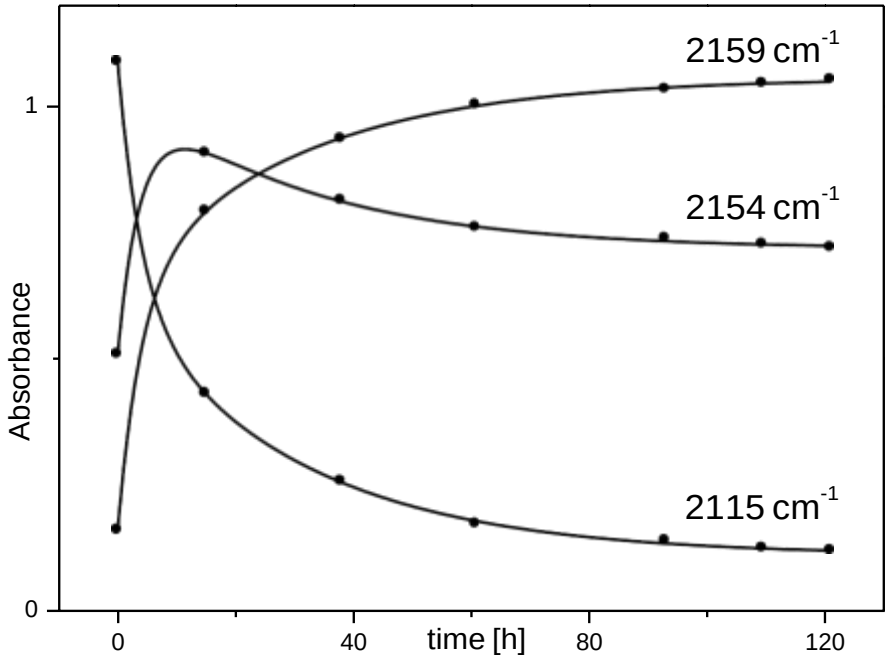


Fig. S8. Kinetic traces of $Si(N_3)_4(phen)$ (2115 cm^{-1}) and $Si(N_3)_2(N_4CPh)_2(phen)$ (2159 cm^{-1}) showing the conversion *via* the intermediary $Si(N_3)_3(N_4CPh)(phen)$ (2154 cm^{-1}) in Ph-CN at 120 °C obtained from FTIR spectral monitoring. Absorbance changes were recorded at the given wavenumbers which are close to but do not coincide exactly with the interpolated peak maxima of observed species due to data point spacing.

3. Details of the single crystal X-ray diffraction studies of compounds 4a,b, 5, 6 and 9

Diffraction data were collected on a Bruker Smart APEX II or Bruker Kappa APEX II with CCD area detectors[3] and an Oxford Cryosystems low temperature unit and Mo-K α radiation (λ = 0.71073 Å). Crystallographic and experimental details are summarized in Table S3. All measured reflections were corrected for Lorentz and polarisation effects and for absorption by semi empirical methods based on symmetry-equivalent and repeated reflections. The structures were solved by direct methods and refined by full matrix least squares methods on F^2. H atoms were placed geometrically and refined with a riding model and with U_{iso} constrained to be 1.2 times (1.5 for CH_3 groups) U_{eq} of the carrier atom. Complex scattering factors were taken from the program package SHELXTL as implemented on a Viglen Pentium computer.[4]

Table S1. Crystallographic data of crystals of compounds **4a**,**b**, **6**, **7** and **9**

Compound	**7·CH$_3$CN**	**6·CH$_3$CN**	**4a**	**4b**	**9**
rational formula	Si(N$_3$)$_2$-(N$_4$CPh-κ*N*2)$_2$(phen)	Si(N$_3$)$_2$-(N$_4$CTol-κ*N*2)$_2$(bpy)	Si(N$_3$)$_2$-(N$_4$CMe-κ*N*2)$_2$(bpy)	Si(N$_3$)$_2$(N$_4$CMe-κ*N*1)-(N$_4$CMe-κ*N*2)(bpy)	Si(N$_3$)$_2$-(N$_4$Cpy-κ*N*1)$_2$
dimensions / mm	0.42 × 0.26 × 0.22	0.26 × 0.24 × 0.04	0.40 × 0.30 × 0.20	0.26 × 0.20 × 0.08	0.33 × 0.05 × 0.05
Crystal symmetry	Triclinic	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Space group	*P*1	*P*2(1)/c	*C*2/c	*P*2(1)/c	*P*bcn
a / Å	11.1045(3)	10.8501(3)	11.7941(6)	10.8760(3)	12.030(4)
b / Å	11.9991(4)	24.9305(6)	13.5508(6)	14.5601(4)	9.833(3)
c / Å	12.7949(4)	11.6142(3)	12.6135(6)	14.9281(4)	13.979(4)
α / °	96.0600(10)	90	90	90	90
β / °	108.5450(10)	110.1040(10)	104.555(2)	110.732(2)	90
γ / °	111.1680(10)	90	90	90	90
U / Å^3	1459.66(8)	2950.20(13)	1951.19(16)	2210.87(10)	1653.6(9)
sum formula	C$_{28}$H$_{21}$N$_{17}$Si	C$_{28}$H$_{25}$N$_{17}$Si	C$_{14}$H$_{14}$N$_{16}$Si	C$_{16}$H$_{17}$N$_{17}$Si	C$_{12}$H$_8$N$_{16}$Si
Z	2	4	4	4	4
D_C / (Mg·m^{-3})	1.419	1.413	1.479	1.429	1.624
μ(Mo-K$_\alpha$) / (mm^{-1})	0.134	0.133	0.163	0.152	0.185
F(000)	644	1304	896	984	824
Reflections	18046	37864	11099	16411	7694
θ range / °	2.22 - 25.99	2.00 - 27.50	2.33 - 27.53	2.00 - 25.00	3.96 - 25.00
min. / max. transm. coeff.	0.9458 / 0.9711	0.9662 / 0.9947	0.9378 / 0.9589	0.9617 / 0.9880	0.9413 / 0.9908
indep. refls. $\|F\|/\sigma(\|F\|) > 4.0$	8948	6717	2237	3878	1453
R_1 (all data)	0.0359 (0.0377)	0.0392 (0.0560)	0.0316 (0.0368)	0.0473 (0.0806)	0.0442 (0.0854)
wR_2 (all data)	0.0977 (0.0998)	0.0885 (0.0959)	0.0837 (0.0876)	0.1070 (0.1266)	0.0999 (0.1212)
data, restraints, parameters	8948, 3, 831	6717, 0, 418	2237, 0, 142	3878, 0, 311	1453, 0, 132
min./max. res. e. density [e·Å^{-3}]	–0.233 / 0.334	–0.238 / 0.366	–0.329 / 0.285	–0.266 / 0.263	–0.354 / 0.258
Fw	623.71	627.74	434.50	475.56	404.43
T / K	100(2)	100(2)	130(2)	96(2)	110(2)

4. Differential Scanning Calorimetry (DSC) measurements

A Perkin Elmer "Pyris 1" Differential Scanning Calorimeter was operated under nitrogen flow and calibrated against indium. The samples were sealed in closed stainless steel cells, which could withstand an internal pressure of about 15 MPa. The heating rate was 10 K min^{-1}.

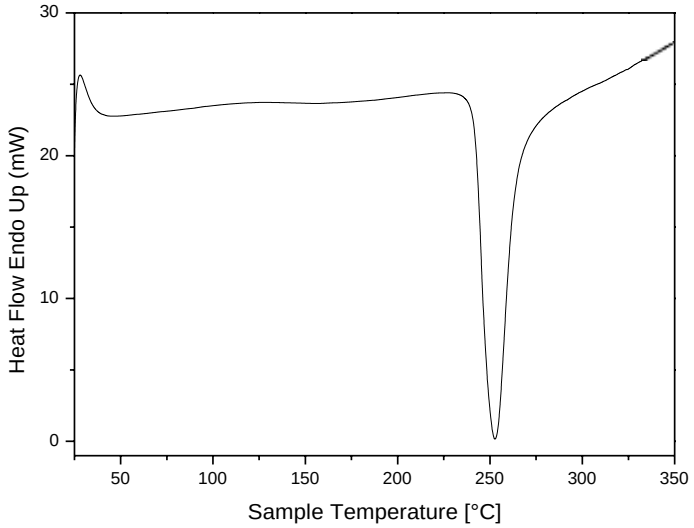


Fig. S9. DSC of compound **4a**, $[Si(N_3)_2(\kappa N(2)\text{-}mtz)_2(bpy)]$, heating rate 10 K min^{-1}.

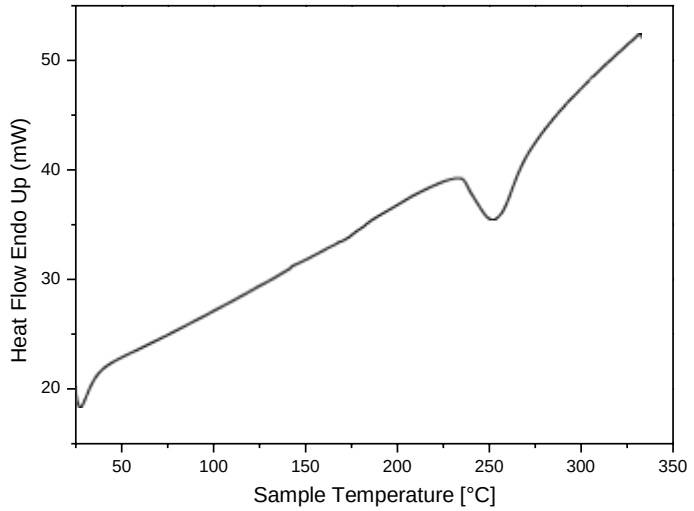


Fig. S10. DSC of compound 8, $[Si(N3)(\kappa N(2)\text{-}mtz)_3(bpy)]$, heating rate 10 K min^{-1}.

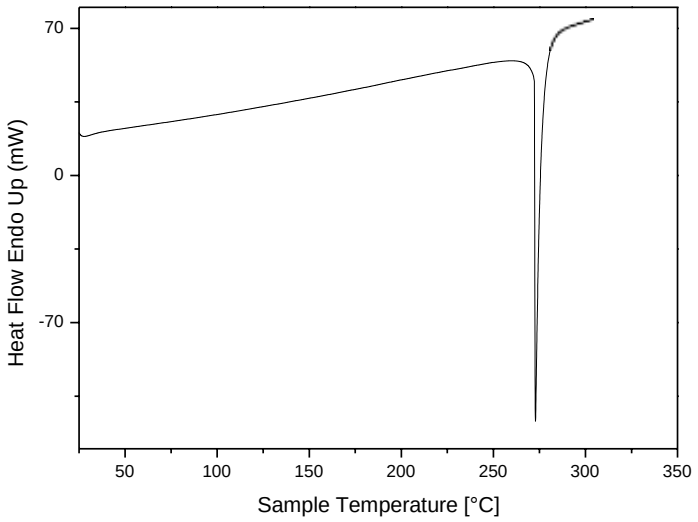
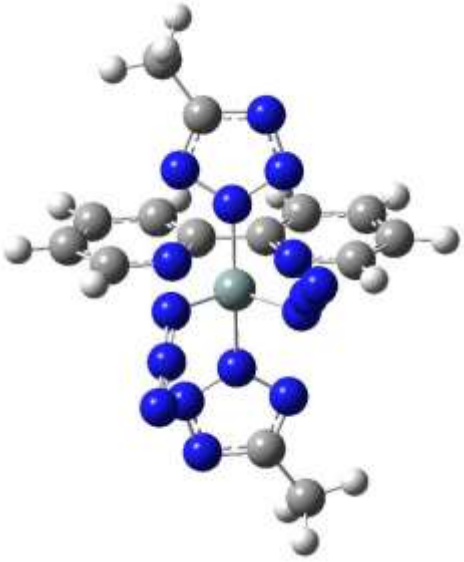


Fig. S11. DSC of compound **9**, [Si(N_3)$_2$(κN(1),N'-pytz)$_2$], heating rate 10 K min^{-1}.

5. Density functional theory (DFT) calculations.

DFT and HF calculations were carried out with the Gaussian03 package of programmes[2] on the B3LYP and HF levels of theory with the 6-311G(d,p) basis set. The Cartesian coordinates of the molecular start geometries of **4a,b** and **9** were obtained from the molecular structures as determined by X-ray diffraction. The nature of the minimum geometries was established by vibrational frequency calculations. The following symmetries were determined at the minimum: **4a** (C_2), **4b** (C_1), *OC-6-32-* (C_1) and *OC-6-33*-[Si(N_3)$_2$(κN(2)-mtz)$_2$(bpy)] (C_2), *OC-6-32-* (C_1) and *OC-6-13*-[Si(N_3)$_2$(κ^{2}N,N(1)-pytz)$_2$] (C_2), *OC-6-23*-[Si(N_3)$_3$(κN(1)-mtz)(bpy) (C_1) and *OC-6-33*-[Si(N_3)$_3$(κN(2)-mtz)(bpy)] (C_1), and *OC-6-33*-[Si(N_3)(κN(2)-mtz)$_3$(bpy)] (C_1) obtained from the DFT calculations with reference to **9** (C_2), *OC-6-23*-[Si(N_3)$_3$(κN(2)-mtz)(bpy)] (C_1) and *OC-6-31*-[Si(N_3)(κ(N_2)-mtz)$_3$(bpy)] (C_1). The temperature corrections to Δ*G* were obtained from Gaussian using the above minimum structures.

5.1. *OC-6-24*-Si(N$_3$)$_2$(*ax*-*κN*(2)-mtz)$_2$(bpy)] (Table 4 entry a)



Gaussian log file name: Si(N3)2(N4CMe)2(bpy)(2,5-2,5)_X-ray_b3lyp-6-311g(d,p)_C2_symmetry_opt_freq
Route: opt freq b3lyp/6-311g(d,p) geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]#N)(N=[N]#N)N2N:N:C(C):N2.C:3:C:C:C(:N:C:3)C:4:C:C:C:C:N:4
Formula: $C_{14}H_{14}N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1707.7370926 a.u.
Thermal correction to Gibbs Energy (298 K): 0.258938 a.u.

Cartesian Coordinates (*x y z* format)

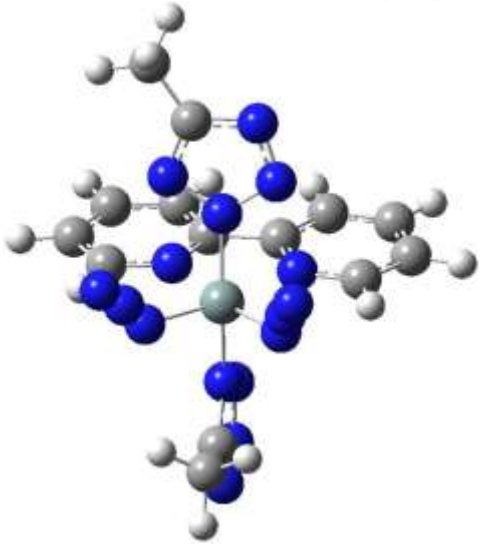
1	Si1	0.0000	0.0000	0.7333 Si
2	C2	0.0000	3.9254	0.3065 C
3	C3	-0.6245	5.2708	0.1554 C
4	H4	-0.1755	5.8139	-0.6793 H
5	H5	-0.4723	5.8696	1.0572 H
6	H6	-1.6959	5.1691	-0.0168 H
7	C7	2.5815	-0.4235	-0.6940 C
8	H8	2.9275	-0.4946	0.3267 H
9	C9	3.4190	-0.5513	-1.7935 C
10	H10	4.4758	-0.7237	-1.6396 H
11	C11	2.8768	-0.4532	-3.0687 C
12	H12	3.5061	-0.5468	-3.9456 H
13	C13	1.5116	-0.2339	-3.2101 C
14	H14	1.0673	-0.1562	-4.1923 H
15	C15	0.7268	-0.1148	-2.0674 C
16	N16	0.2805	1.8720	0.5296 N
17	N17	1.4926	2.4250	0.5349 N
18	N18	1.3368	3.7165	0.3960 N
19	N19	-0.6821	2.7892	0.3801 N
20	N20	1.3604	-0.2550	1.8795 N
21	N21	1.6087	0.4643	2.8316 N
22	N22	1.9027	1.0760	3.7400 N
23	N23	1.2686	-0.2053	-0.8364 N
24	C24	0.0000	-3.9254	0.3065 C
25	C25	0.6245	-5.2708	0.1554 C
26	H26	0.1755	-5.8139	-0.6793 H
27	H27	0.4723	-5.8696	1.0572 H
28	H28	1.6959	-5.1691	-0.0168 H

29	C29	-2.5815	0.4235	-0.6940 C
30	H30	-2.9275	0.4946	0.3267 H
31	C31	-3.4190	0.5513	-1.7935 C
32	H32	-4.4758	0.7237	-1.6396 H
33	C33	-2.8768	0.4532	-3.0687 C
34	H34	-3.5061	0.5468	-3.9456 H
35	C35	-1.5116	0.2339	-3.2101 C
36	H36	-1.0673	0.1562	-4.1923 H
37	C37	-0.7268	0.1148	-2.0674 C
38	N38	-0.2805	-1.8720	0.5296 N
39	N39	-1.4926	-2.4250	0.5349 N
40	N40	-1.3368	-3.7165	0.3960 N
41	N41	0.6821	-2.7892	0.3801 N
42	N42	-1.3604	0.2550	1.8795 N
43	N43	-1.6087	-0.4643	2.8316 N
44	N44	-1.9027	-1.0760	3.7400 N
45	N45	-1.2686	0.2053	-0.8364 N

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	32.6083	0.839
2	36.6579	0.3793
3	40.8417	1.4856
4	44.0093	0.0003
5	49.7955	0.9213
6	52.9198	0.2356
7	53.9939	0.0307
8	55.2345	0.3568
9	59.5723	2.0931
10	60.47	0.1333
11	75.2163	0.7921
12	84.6144	2.5086
13	91.8956	2.6009
14	127.13	0.0113
15	136.097	0.4525
16	163.437	0.3992
17	171.041	0.2607
18	189.019	1.761
19	207.815	4.8244
20	214.673	0.8195
21	231.378	0.4897
22	241.7	0.609
23	257.301	0.3994
24	266.123	1.2197
25	288.039	0.1163
26	289.089	0
27	300.568	15.7356
28	314.679	6.771
29	328.679	0.5212
30	376.072	16.5745
31	392.297	0.1753
32	403.29	1.9104
33	420.509	77.07
34	432.913	0.0573
35	463.688	0.3908
36	466.002	70.5678
37	490.641	1.3116
38	529.158	251.111
39	559.169	0.2935
40	574.488	273.307
41	574.803	162.845
42	598.296	24.504
43	605.003	37.0476
44	657.743	4.6653
45	668.064	3.2712
46	675.136	14.7653
47	694.674	82.5406
48	708.179	1.0568
49	708.649	143.116
50	711.702	73.6248
51	730.302	1.988
52	730.684	0.1303
53	737.624	1.6313
54	738.242	4.1803
55	754.215	81.8429
56	763.042	0.0278
57	784.104	28.181
58	789.349	1.152
59	823.765	0.0227
60	899.666	0.0305
61	908.333	1.796
62	999.06	0.0028
63	999.748	7.3344
64	1006.85	0.0221
65	1009.98	0.2414
66	1026.78	0.0461
67	1027.99	0.4718
68	1040.28	8.6338
69	1048.66	4.5356
70	1050.35	30.7143
71	1051.97	27.8949
72	1065	5.1289
73	1070.36	2.3617
74	1070.36	1.1113
75	1087.96	57.6819
76	1097.24	2.5441
77	1099.61	0.198
78	1101.37	5.9874
79	1135.74	1.1195
80	1142.95	0.0812
81	1143.34	79.7645
82	1152.57	0.4702
83	1185.75	11.4583
84	1194.53	12.2954
85	1224.65	1.2336
86	1226.61	91.5579
87	1279.76	0.5295
88	1283.85	31.8207
89	1294.33	11.2444
90	1302.51	22.0788
91	1317.93	0.3491
92	1343.24	27.0646
93	1351.12	1.2694
94	1389.03	47.0947
95	1390.07	0.0509
96	1391.11	102.781
97	1395.5	271.747
98	1419.56	0.844
99	1419.61	24.8388
100	1464.51	29.529
101	1479.91	6.7199
102	1479.93	11.328
103	1483.33	69.3824
104	1489.74	40.2797
105	1489.77	1.5565
106	1506.67	36.0596
107	1527.86	7.1628
108	1537.36	109.515
109	1537.62	0.2833
110	1610.69	25.6871
111	1621.87	19.4486
112	1648.3	39.8603
113	1663.4	19.5918
114	2271.87	518.59
115	2292.03	1054.54
116	3042.31	42.4883
117	3042.36	0.0696
118	3095.52	0.2344
119	3095.53	22.4921
120	3129.94	0.0074
121	3129.95	18.3891
122	3189.59	5.3062
123	3190.54	4.7622
124	3210.67	1.4868
125	3213.47	1.2543
126	3215.1	0.472
127	3222.78	1.5335
128	3236.21	0.5014
129	3236.64	43.0153

5.2. *OC-6-24*-[Si(N$_3$)$_2$(*κN*(2)-mtz)(*κN*(1)-mtz)(bpy)] (Table 4 entry b)



Gaussian log file name: Si(N3)2(N4CMe)2(bpy)_b3lyp_6-311G(d,p)_(2,5-1,5)_Xray_freq_355
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]=N)(N=[N]=N)N:2N:NN=C:2C.C:3:C:C:C(:N:C:3)C:4:C:C:C:C:N:4
Formula: $C_{14}H_{14}N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1707.7367263a.u.
Thermal correction to Gibbs Energy (298 K): 0.259756 a.u.

Cartesian Coordinates (*x y z* format)

1	Si1	-0.1235	0.6767	0.0140 Si
2	N2	-0.1296	1.8571	1.3832 N
3	N3	0.8057	2.5401	1.7649 N
4	N4	1.6151	3.2160	2.1832 N
5	N5	0.3339	1.7575	-1.3621 N
6	N6	1.3637	2.3944	-1.5012 N
7	N7	2.2839	3.0225	-1.7158 N
8	N8	-0.6592	-0.8164	1.2844 N
9	N9	-0.2337	-0.9130	-1.2460 N
10	N10	1.6698	0.0803	0.3350 N
11	N11	2.1767	-0.1402	1.5474 N
12	N12	3.4200	-0.5161	1.3925 N
13	N13	2.5725	-0.1518	-0.6279 N
14	N14	-1.9502	0.9458	-0.3068 N
15	N15	-2.7995	-0.1168	-0.4210 N
16	N16	-3.9811	0.3419	-0.6379 N
17	N17	-3.9678	1.6940	-0.6765 N
18	C18	-0.8905	-0.6246	2.5880 C
19	H19	-0.7976	0.3961	2.9293 H
20	C20	-1.2250	-1.6746	3.4320 C
21	H21	-1.4065	-1.4783	4.4801 H
22	C22	-1.3114	-2.9571	2.9064 C
23	H23	-1.5643	-3.7986	3.5399 H
24	C24	-1.0733	-3.1503	1.5507 C
25	H25	-1.1436	-4.1380	1.1179 H
26	C26	-0.7570	-2.0530	0.7586 C
27	C27	-0.5177	-2.1074	-0.6912 C
28	C28	-0.5875	-3.2618	-1.4628 C

29	H29	-0.8147	-4.2145	-1.0060 H
30	C30	-0.3778	-3.1703	-2.8334 C
31	H31	-0.4352	-4.0570	-3.4532 H
32	C32	-0.1017	-1.9298	-3.3945 C
33	H33	0.0617	-1.8125	-4.4574 H
34	C34	-0.0332	-0.8190	-2.5654 C
35	H35	0.1788	0.1753	-2.9307 H
36	C36	3.6504	-0.5149	0.0561 C
37	C37	4.9605	-0.8634	-0.5638 C
38	H38	4.8598	-0.9170	-1.6477 H
39	H39	5.3224	-1.8225	-0.1869 H
40	H40	5.7128	-0.1084	-0.3215 H
41	C41	-2.7128	2.0573	-0.4712 C
42	C42	-2.2614	3.4749	-0.4346 C
43	H43	-3.1244	4.1125	-0.6229 H
44	H44	-1.4981	3.6614	-1.1919 H
45	H45	-1.8326	3.7223	0.5382 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	21.1188	0.2472
2	39.4948	0.406
3	40.4724	0.4637
4	49.8982	1.1062
5	55.0601	0.1726
6	59.3143	5.532
7	59.846	1.4207
8	63.1347	0.0358
9	73.5635	3.1839
10	82.2534	6.6301
11	82.7895	1.5263
12	88.5495	1.3834
13	120.342	0.1537
14	160.069	0.3989
15	161.529	0.3745
16	167.696	0.3922
17	177.231	3.6501
18	187.393	0.2666
19	204.539	2.5899
20	212.414	0.4006
21	240.243	0.2848
22	249.072	0.3309
23	250.342	0.0954
24	276.744	2.1281
25	284.488	0.5258
26	296.676	2.7364
27	305.314	8.3525
28	319.059	4.8738
29	326.901	7.5222
30	374.924	29.0488
31	388.154	15.6692
32	399.733	2.122
33	419.748	26.3087
34	435.845	6.8306
35	461.033	0.2104
36	472.664	31.1932
37	489.392	2.6482
38	536.277	281.246
39	556.384	77.7503
40	559.166	21.1788
41	566.399	322.312
42	600.408	2.634
43	607.867	34.5043
44	657.074	4.6341
45	667.46	0.0479
46	675.778	32.4343
47	690.337	82.3672
48	693.825	108.322
49	699.24	29.6098
50	709.21	34.1046
51	714.929	10.4242
52	729.622	1.5899
53	736.432	0.1054
54	738.175	2.2936
55	753.624	86.2098
56	763.31	0.1786
57	784.37	34.0707
58	789.843	2.2455
59	823.566	0.5814
60	902.208	0.1973
61	909.217	1.3325
62	999.402	4.8593
63	1001.32	7.0085
64	1007.46	0.0267
65	1010.56	0.3163
66	1027.5	0.0196
67	1028.69	0.1897
68	1031.25	8.9924
69	1040.71	7.9391
70	1047.27	12.2795
71	1052.36	36.7267
72	1065.49	5.2542
73	1070.85	1.1916
74	1075.09	3.8637
75	1083.84	22.8497
76	1089.04	73.6599
77	1098.3	1.7512
78	1099.71	1.059
79	1126.57	10.3105
80	1136.56	2.1037
81	1139.48	27.2899
82	1152.3	0.5629
83	1175.78	13.7766
84	1185.76	13.0296
85	1195.03	13.1353
86	1220.45	45.4091
87	1278.26	9.1974
88	1292.62	9.5267
89	1300.58	17.7306
90	1317.85	1.8459
91	1336.17	15.8478
92	1342.05	25.4619
93	1353.69	3.2058
94	1383.92	80.3935
95	1389.97	35.9912
96	1391.61	227.503
97	1398.23	97.738
98	1409.24	71.7175
99	1419.88	11.3048
100	1465.8	18.9931
101	1477.74	8.1616
102	1479.48	8.7821
103	1484.01	73.9614
104	1489.37	21.7236
105	1492.28	15.4339
106	1507.42	35.9072
107	1531.38	13.6243
108	1534.78	41.3327
109	1538.01	53.2228
110	1613.17	23.9952
111	1623.63	25.7887
112	1650.87	37.7446
113	1664.99	23.1697
114	2255.49	212.262
115	2291.35	1124.98
116	3043.89	17.6057
117	3053.7	11.4698
118	3097.84	9.6103
119	3114.06	5.127
120	3132.3	8.3134
121	3139.63	9.1271
122	3190.87	4.7749
123	3191.94	4.4792
124	3211.32	1.6483
125	3213.26	1.0194
126	3216.08	0.0397
127	3225.14	0.8911
128	3233.02	9.0808
129	3233.96	20.9955

3.3. *OC-6-32*-[Si(N$_3$)$_2$(*κN*(2)-mtz)$_2$(bpy)] (Table 4 entry c)

Gaussian log file name: Si(N3)2(CHN4)2(bpy)_b3lyp_6-311G(d,p)_cis-trans-comparison_opt_freq_350_600_1
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]=N)(N=[N]#N)N2N:N:C(C):N2.C:3:C:C:C(:N:C:3)C:4:C:C:C:C:N:4
Formula: $C_{14}H_{14}N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1707.7314632 a.u.
Thermal correction to Gibbs Energy (298 K): 0.257949 a.u.

Cartesian Coordinates (*x y z* format)

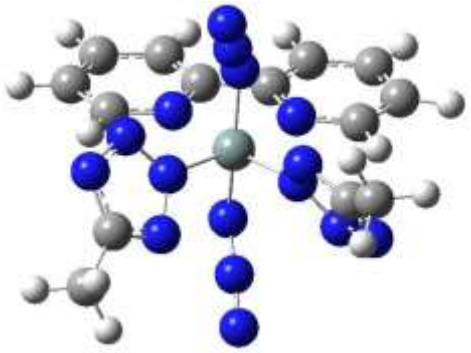
1	Si1	-0.1747	-0.5762	-0.3348 Si
2	C2	-0.2710	2.4002	-0.8553 C
3	H3	-1.3280	2.2419	-0.7119 H
4	C4	0.2457	3.6544	-1.1525 C
5	H5	-0.4241	4.5010	-1.2222 H
6	C6	1.6129	3.7901	-1.3516 C
7	H7	2.0471	4.7554	-1.5823 H
8	C8	2.4215	2.6649	-1.2526 C
9	H9	3.4887	2.7437	-1.4042 H
10	C10	1.8391	1.4360	-0.9560 C
11	N11	-0.2506	-0.7316	-2.1359 N
12	N12	0.5105	1.3182	-0.7598 N
13	C13	0.3898	0.9076	3.2775 C
14	C14	0.2762	1.9322	4.3542 C
15	H15	1.2335	2.0650	4.8628 H
16	H16	-0.4558	1.6205	5.1040 H
17	H17	-0.0452	2.8853	3.9341 H
18	C18	2.3947	-2.0967	-0.3744 C
19	H19	1.7103	-2.8976	-0.1341 H
20	C20	3.7617	-2.2849	-0.5257 C
21	H21	4.1807	-3.2737	-0.3956 H
22	C22	4.5603	-1.1912	-0.8362 C
23	H23	5.6308	-1.3045	-0.9582 H
24	C24	3.9686	0.0571	-0.9880 C
25	H25	4.5714	0.9213	-1.2286 H
26	C26	2.5912	0.1765	-0.8256 C
27	N27	0.2301	-0.1018	1.4616 N
28	N28	0.8460	-0.9296	2.3035 N
29	N29	0.9569	-0.3123	3.4507 N
30	N30	-0.0630	1.0681	2.0412 N
31	N31	-0.4408	-2.3192	-0.0060 N
32	N32	-0.9917	-2.8393	0.9517 N

33	N33	-1.4879	-3.4128	1.7915 N
34	N34	1.8303	-0.8922	-0.5234 N
35	N35	-1.9566	-0.0155	-0.1182 N
36	N36	-2.6581	-0.3236	0.9723 N
37	N37	-2.7365	0.5244	-1.0718 N
38	N38	-1.0178	-1.4709	-2.7248 N
39	N39	-1.7002	-2.1292	-3.3482 N
40	C40	-3.9341	0.5345	-0.5012 C
41	C41	-5.1713	1.0459	-1.1569 C
42	H42	-5.6068	1.8651	-0.5793 H
43	H43	-4.9436	1.3988	-2.1626 H
44	H44	-5.9224	0.2552	-1.2227 H
45	N45	-3.8995	0.0145	0.7517 N

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	28.1858	0.0606	46	675.326	29.4993	91	1316.57	7.1035
2	30.0109	0.5109	47	692.338	112.687	92	1346.84	7.4623
3	34.6461	0.4461	48	700.539	81.9319	93	1354.6	12.5047
4	38.4119	0.0976	49	710.193	46.9754	94	1387.48	119.895
5	51.4998	1.1217	50	714.703	104.753	95	1389.53	26.6904
6	56.9274	0.1979	51	728.161	0.8064	96	1390.42	61.2883
7	58.2035	0.7924	52	730.641	3.8854	97	1395.61	216.248
8	61.5262	0.2799	53	738.153	2.4613	98	1419.76	14.8998
9	66.7372	0.3228	54	739.399	2.0872	99	1420.72	13.7116
10	68.9436	0.4121	55	752.653	95.5871	100	1467.77	28.7008
11	74.5232	2.532	56	763.329	2.423	101	1478.42	8.767
12	88.2835	2.3966	57	784.414	27.4258	102	1480.93	9.2694
13	92.8733	1.3076	58	788.553	0.9403	103	1481.95	72.3737
14	115.944	0.1984	59	824.362	0.4302	104	1487.55	23.0549
15	148.81	0.3044	60	898.924	1.1489	105	1490.64	20.6147
16	165.529	0.3649	61	908.941	2.272	106	1511.86	33.4068
17	169.585	0.5912	62	990.211	2.4709	107	1531.84	4.9941
18	174.214	0.4053	63	998.108	6.3982	108	1539.52	65.6175
19	194.525	1.152	64	999.342	2.6863	109	1539.82	52.9366
20	215.541	2.399	65	1008.39	0.4917	110	1612.32	26.8643
21	236.797	1.3289	66	1021.76	0.2204	111	1623.37	21.5187
22	250.287	0.3731	67	1028.23	0.4781	112	1647.8	35.0349
23	257.325	0.0997	68	1038.94	5.7684	113	1662.62	20.1564
24	265.622	0.8602	69	1043.56	22.9179	114	2275.41	726.812
25	270.854	3.7307	70	1049.1	20.0828	115	2291.84	702.851
26	289.609	0.6538	71	1051.14	21.8259	116	3042.36	19.4543
27	305.673	16.5348	72	1065.83	4.8614	117	3043.06	20.0806
28	321.7	5.1569	73	1069.82	1.982	118	3096.59	10.6441
29	340.61	23.945	74	1071.49	1.5628	119	3096.71	10.0422
30	378.22	4.4732	75	1090.18	44.2131	120	3129.19	9.6579
31	379.439	19.5349	76	1096.97	0.0225	121	3131.84	8.7946
32	401.966	3.771	77	1101.36	2.0894	122	3189.76	4.9632
33	404.747	17.1136	78	1102.05	5.7742	123	3190.79	4.8326
34	430.06	9.9424	79	1127.11	28.2899	124	3210.51	2.1705
35	461.421	0.7184	80	1137.18	1.2729	125	3212.4	1.0917
36	471.007	136.206	81	1146.16	36.0369	126	3214.87	0.2777
37	485.075	0.3914	82	1153	0.6173	127	3224.12	1.3564
38	502.429	198.723	83	1186.59	14.352	128	3229.17	20.5048
39	555.416	0.83	84	1196.41	14.6997	129	3254.42	37.3553
40	561.273	163.854	85	1224.8	40.9908			
41	585.953	209.801	86	1225.54	59.3012			
42	602.232	7.717	87	1281.26	10.4383			
43	604.043	38.4474	88	1284.26	11.673			
44	655.101	6.3087	89	1289.98	13.0155			
45	667.726	3.0055	90	1306.33	17.8356			

5.3. *OC-6-33*-[Si(N_3)$_2$(κN(2)-mtz)$_2$(bpy)] (Table 4 entry d)



Gaussian log file name: Si(ax-N3)2(eq-2,5-N4CMe)(bpy)-b3lyp-6-311g(d,p)_opt_freq
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]#N)(N=[N]#N)N2N:N:C(C):N2.C:3:C:C:C(:N:C:3)C:4:C:C:C:C:N:4
Formula: $C_{14}H_{14}N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1707.7266821 a.u.
Thermal correction to Gibbs Energy (298 K): 0.257668 a.u.

Cartesian Coordinates (*x y z* format)

1	Si1	0.0784	-0.0194	-0.0490 Si
2	C2	0.0019	-0.1296	2.9714 C
3	H3	1.0694	-0.2281	2.8521 H
4	C4	-0.5862	-0.1046	4.2291 C
5	H5	0.0362	-0.2080	5.1079 H
6	C6	-1.9617	0.0577	4.3247 C
7	H7	-2.4523	0.0827	5.2901 H
8	C8	-2.7045	0.1882	3.1581 C
9	H9	-3.7768	0.3120	3.2073 H
10	C10	-2.0521	0.1541	1.9285 C
11	N11	-0.2812	-1.7857	0.0461 N
12	N12	-0.7162	-0.0013	1.8493 N
13	C13	-2.4565	0.2564	-1.6748 C
14	H14	-1.7685	0.1497	-2.4993 H
15	C15	-3.8190	0.4244	-1.8841 C
16	H16	-4.1978	0.4737	-2.8963 H
17	C17	-4.6613	0.5210	-0.7848 C
18	H18	-5.7287	0.6546	-0.9128 H
19	C19	-4.1136	0.4383	0.4891 C
20	H20	-4.7498	0.5066	1.3599 H
21	C21	-2.7390	0.2669	0.6291 C
22	N22	0.0086	1.7809	0.0826 N
23	N23	0.8692	2.6240	-0.0905 N
24	N24	1.5931	3.4846	-0.2293 N
25	N25	-1.9309	0.1844	-0.4459 N
26	N26	1.8497	-0.1815	0.5548 N
27	N27	2.5001	0.6827	1.3385 N
28	N28	2.6409	-1.1852	0.1615 N
29	N29	0.2387	-2.7333	-0.5138 N
30	N30	0.6522	-3.6798	-0.9796 N
31	C31	3.7998	-0.8956	0.7357 C
32	C32	5.0360	-1.7150	0.5877 C
33	H33	5.4616	-1.9501	1.5657 H
34	H34	4.8065	-2.6419	0.0628 H
35	H35	5.7943	-1.1687	0.0206 H
36	N36	3.7247	0.2435	1.4712 N

37	N37	0.5778	-0.0264	-1.8602 N
38	N38	0.1863	-0.9045	-2.7876 N
39	N39	0.8098	-0.6044	-3.8972 N
40	N40	1.4645	0.8467	-2.3492 N
41	C41	1.5981	0.4634	-3.6110 C
42	C42	2.5066	1.1194	-4.5937 C
43	H43	3.3321	0.4538	-4.8593 H
44	H44	1.9689	1.3610	-5.5131 H
45	H45	2.9180	2.0335	-4.1664 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	-11.7304	0.2438	37	487.448	0.8994	73	1071.29	0.6591			
2	27.6141	3.3712	38	493.231	325.087	74	1071.56	3.9266			
3	32.948	0	39	505.994	131.472	75	1095.86	48.1323			
4	33.8309	0.038	40	550.967	1.8286	76	1099.33	0.1523			
5	46.0407	0.353	41	594.044	0.6351	77	1101.45	5.2023			
6	46.4907	0.0077	42	595.179	24.0997	78	1103.6	0.0012			
7	58.8428	0.6532	43	604.049	116.165	79	1134.06	42.336			
8	65.8192	0.2037	44	653.495	10.3574	80	1138.64	0.1494			
9	71.8914	0.0005	45	663.984	87.2295	81	1145.44	27.7773			
10	79.9993	1.2623	46	668.932	11.5134	82	1153.83	0.2617			
11	87.5372	0.7154	47	675.674	45.274	83	1188.08	13.9307			
12	93.3496	3.2004	48	699.727	219.505	84	1198.78	12.3183			
13	98.2265	1.4924	49	709.127	19.3554	85	1222.69	27.077			
14	100.431	2.224	50	709.3	54.7416	86	1222.72	48.9841			
15	150.952	1.2161	51	729.473	0.1404	87	1283.59	9.2053			
16	152.275	0.6177	52	732.498	0.1684	88	1284.76	16.1151			
17	162.479	0.0375	53	739.187	0.0514	89	1288.28	26.4034			
18	170.264	1.0849	54	739.253	3.2751	90	1306.05	2.9817			
19	173.978	0.522	55	749.16	93.4221	91	1321.41	9.4826			
20	213.498	0.2238	56	761.45	0.06	92	1347.52	7.3195			
21	239.718	1.0113	57	783.639	32.9153	93	1354.2	9.9219			
22	252.379	0.2068	58	787.204	0.1736	94	1387.36	6.9423			
23	256.242	3.2746	59	822.687	1.347	95	1388.11	1.1006			
24	263.246	8.5719	60	896.958	0.9589	96	1408.1	65.9917			
25	267.372	0.7881	61	905.295	2.7936	97	1411.48	335.713			
26	289.218	0.3366	62	987.348	2.436	98	1418.11	23.3124			
27	294.521	12.5445	63	989.004	2.0429	99	1418.45	0.052			
28	338.269	2.8662	64	999.88	2.6151	100	1471.98	28.3579			
29	343.82	13.2097	65	1000.01	3.7543	101	1480.13	14.4371			
30	367.48	13.882	66	1019.76	1.0644	102	1480.4	5.4365			
31	389.819	2.9555	67	1022.84	0.417	103	1480.89	78.2418			
32	404.803	6.7799	68	1038.2	2.7477	104	1489.22	23.5934			
33	412.416	14.5163	69	1045.07	31.9482	105	1489.58	14.2459			
34	422.45	8.357	70	1046.93	23.2848	106	1517.21	39.573			
35	451.56	110.381	71	1050.69	14.7136	107	1534.04	10.6075			
36	458.612	2.8928	72	1068.37	2.4128	108	1540.46	44.824			

109	1541.61	73.0114
110	1613.77	29.6723
111	1624.19	21.7185
112	1648.27	30.5276
113	1661.87	17.4368
114	2287.23	1010.53
115	2293.22	363.053
116	3042.83	10.4004
117	3042.92	28.5876
118	3096.88	19.4374
119	3097	3.8188
120	3134.6	0.0405
121	3134.61	12.4982
122	3189.7	4.9678
123	3190.73	4.4142
124	3211.09	1.9559
125	3213.01	0.2926
126	3215.42	0.0727
127	3226.57	2.8142
128	3248.85	0.733
129	3249.19	57.9625

5.4. *OC-6-22*-[$Si(N_3)_2(\kappa^2N,N(1)$-pytz$)_2$] (Table 4 entry e)

Gaussian log file name: Si(N3)2(pytz)2(bpy)_b3lyp_opt_freq_C2_symm
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: N=[N]=N[Si](N=[N]=N)(N:1N:NN=C:1:C:2:C:C:C=C:N:2)N:3N:NN=C:3:C:4:C:C:C=C:N:4
Formula: $C_{12}H_8N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1627.8712204 a.u.
Thermal correction to Gibbs Energy (298 K): 0.189954 a.u.

Cartesian Coordinates (*x y z* format)

1	Si1	0.0000	0.0000	0.4316 Si
2	C2	-1.6291	-1.3824	-1.3270 C
3	C3	1.6291	1.3824	-1.3270 C
4	N4	-2.5876	-1.3392	-2.2351 N
5	N5	2.5876	1.3392	-2.2351 N
6	N6	1.4238	0.6717	2.6356 N
7	N7	-1.4238	-0.6717	2.6356 N
8	N8	-1.3080	-0.1450	-0.9231 N
9	N9	1.3080	0.1450	-0.9231 N
10	N10	-2.0934	0.7003	-1.5995 N
11	N11	2.0934	-0.7003	-1.5995 N
12	N12	-2.8523	-0.0229	-2.3823 N
13	N13	2.8523	0.0229	-2.3823 N
14	N14	0.0000	1.9757	0.2215 N
15	N15	0.0000	-1.9757	0.2215 N
16	N16	1.3442	-0.0584	1.6643 N
17	N17	-1.3442	0.0584	1.6643 N
18	C18	-0.1879	-4.6914	-0.2650 C
19	H19	-0.2570	-5.7565	-0.4514 H
20	C20	-0.7959	2.8315	0.8843 C
21	C21	0.7959	-2.8315	0.8843 C
22	H22	-1.4876	2.3797	1.5816 H
23	H23	1.4876	-2.3797	1.5816 H
24	C24	-1.0050	-3.8086	-0.9598 C
25	H25	-1.7223	-4.1385	-1.6992 H
26	C26	-0.7243	4.1983	0.6662 C
27	C27	0.7243	-4.1983	0.6662 C
28	H28	-1.3795	4.8589	1.2177 H
29	H29	1.3795	-4.8589	1.2177 H
30	N30	1.5650	1.3318	3.5500 N
31	N31	-1.5650	-1.3318	3.5500 N
32	C32	0.8859	2.4510	-0.6969 C
33	C33	-0.8859	-2.4510	-0.6969 C
34	C34	1.0050	3.8086	-0.9598 C
35	H35	1.7223	4.1385	-1.6992 H
36	C36	0.1879	4.6914	-0.2650 C
37	H37	0.2570	5.7565	-0.4514 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	25.4639	1.1455	46	741.684	50.7356	91	1575.12	16.0101
2	39.9466	2.04	47	748.606	55.2564	92	1604.95	15.9155
3	44.4097	7.3376	48	782.947	10.977	93	1605.1	13.9738
4	46.3041	5.0165	49	783.464	8.5324	94	1669.93	4.4389
5	49.8935	0.3776	50	810.948	14.5534	95	1670.14	183.385
6	69.3706	0.2403	51	813.054	12.5461	96	2249.79	452.314
7	80.4626	2.0637	52	923.363	2.39	97	2273.31	946.472
8	100.128	0.9323	53	923.47	3.0415	98	3191.73	9.3187
9	100.166	0.2014	54	1006	9.9956	99	3191.74	0.3812
10	129.172	3.598	55	1009.24	0.019	100	3212.7	0.8116
11	155.882	0.0776	56	1009.44	0.2151	101	3212.7	1.0688
12	167.79	0.0003	57	1012.46	5.7303	102	3219.53	1.2767
13	170.279	1.7642	58	1031.42	11.6815	103	3219.53	2.1921
14	202.445	3.323	59	1031.9	0.5696	104	3227.01	13.2367
15	211.458	0.0489	60	1031.92	0.56	105	3227.02	2.6446
16	232.814	0.0514	61	1033.25	8.8052			
17	237.372	3.6264	62	1061.38	0.7056			
18	271.418	9.7358	63	1063.12	34.5466			
19	277.969	2.812	64	1072.11	49.6955			
20	294.348	0.2542	65	1072.2	7.9249			
21	314.502	0.1599	66	1116.65	24.9259			
22	328.325	5.9038	67	1119.72	11.9363			
23	355.123	0.5092	68	1136.37	6.5416			
24	405.165	15.7592	69	1137.76	9.1016			
25	415.654	2.6684	70	1153.94	23.1933			
26	416.815	6.0896	71	1157.51	11.2288			
27	444.715	119.26	72	1185.33	15.5242			
28	459.221	39.5426	73	1185.57	17.6408			
29	460.045	8.1851	74	1216.37	7.8086			
30	518.607	1.2884	75	1218.78	6.6412			
31	523.462	5.97	76	1269.19	1.2296			
32	528.832	4.6777	77	1271.49	2.7209			
33	538.742	15.1094	78	1305.69	34.5225			
34	573.511	207.724	79	1307.05	11.4994			
35	590.906	254.816	80	1315.68	0.8951			
36	598.784	73.7528	81	1316.01	25.216			
37	603.813	0.6727	82	1379.76	116.217			
38	669.808	0.9	83	1386.05	232.899			
39	677.109	58.2607	84	1426.87	37.9795			
40	685.109	34.1403	85	1431.78	2.2115			
41	689.278	82.8602	86	1483.21	21.7056			
42	727.226	0.9842	87	1485.15	84.9813			
43	728.855	0.3123	88	1498.51	71.8006			
44	738.808	1.0212	89	1498.95	72.086			
45	739.154	26.9899	90	1574.74	35.3394			

5.5. *OC-6-32*-[$Si(N_3)_2(\kappa^2N,N(1)$-pytz$)_2$] (Table 4 entry f)

Gaussian log file name: OC-32-Si(N3)2(pytz)2_b3lyp_6311g(d,p)optfreq7
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: N=[N]=N[Si](N=[N]#N)(N:1N:NN=C:1:C:2:C:C:C:C:N:2)N:3N:NN=C:3:C:4:C:C:C:C:N:4
Formula: $C_{12}H_8N_{16}Si$
Charge, multiplicity: 0, 1

Energy: -1627.8604086 a.u.
Thermal correction to Gibbs Energy (298 K): 0.188055 a.u.

Cartesian Coordinates (*x y z* format)

1	Si1	0.0422	0.7463	0.0308 Si
2	C2	-2.0924	-1.3011	-0.2737 C
3	C3	1.7383	-0.7905	1.6272 C
4	N4	1.8876	-1.4399	2.7648 N
5	N5	0.6670	3.3383	0.2106 N
6	N6	-1.1882	1.3200	-2.3156 N
7	N7	-0.7892	-1.1770	-0.6220 N
8	N8	0.5129	-0.2520	1.5456 N
9	N9	-0.1285	-0.5801	2.6758 N
10	N10	0.6982	-1.2881	3.3952 N
11	N11	1.9245	0.0868	-0.5055 N
12	N12	-1.7236	0.8945	0.5583 N
13	N13	0.7140	2.2327	0.7257 N
14	N14	-0.1483	1.3075	-1.6805 N
15	C15	2.5688	0.3950	-1.6431 C
16	H16	1.9832	0.9349	-2.3747 H
17	C17	3.8941	0.0380	-1.8451 C
18	H18	4.3808	0.3037	-2.7741 H
19	N19	0.6759	4.3962	-0.1938 N
20	N20	-2.1187	1.3523	-2.9643 N
21	C21	2.5870	-0.5740	0.4783 C
22	C22	3.9138	-0.9646	0.3406 C
23	H23	4.3941	-1.4901	1.1550 H
24	C24	4.5736	-0.6518	-0.8410 C
25	H25	5.6100	-0.9368	-0.9775 H
26	N26	-2.4032	1.8909	1.1581 N
27	N27	-3.6214	1.4729	1.3306 N
28	N28	-3.7798	0.2105	0.8597 N
29	C29	-2.5947	-0.1173	0.3910 C
30	C30	-2.8329	-2.4445	-0.5609 C
31	H31	-3.8702	-2.4873	-0.2570 H
32	C32	-0.1957	-2.1813	-1.2805 C
33	H33	0.8419	-2.0371	-1.5511 H
34	C34	-2.2062	-3.4844	-1.2319 C
35	H35	-2.7528	-4.3892	-1.4689 H
36	C36	-0.8676	-3.3512	-1.6023 C
37	H37	-0.3491	-4.1394	-2.1321 H

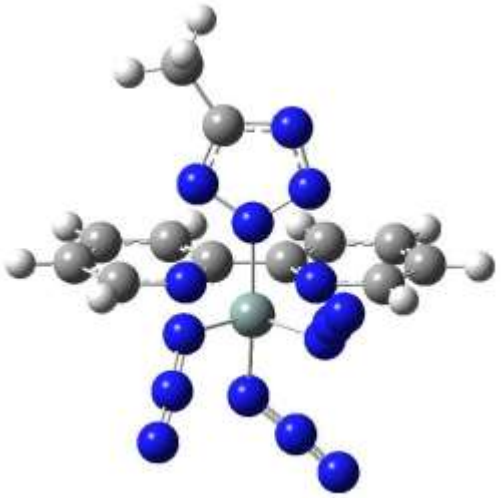
Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	23.8342	0.2917	46	743.611	64.8484			
2	30.9272	0.9664	47	744.673	58.1411			
3	42.7427	3.2703	48	778.094	10.1839			
4	46.7825	0.473	49	783.832	10.6853			
5	53.294	0.2178	50	811.333	11.798			
6	66.7741	1.913	51	815.284	17.5446			
7	84.508	1.2116	52	920.48	3.1585			
8	97.6037	0.4689	53	926.726	1.977			
9	99.637	2.4052	54	987.633	0.1496			
10	115.204	7.1216	55	993.245	2.4095			
11	134.682	0.1788	56	996.241	8.2081			
12	145.612	2.0188	57	1018.46	0.2522			
13	166.9	3.8122	58	1023.13	7.894			
14	192.533	1.8254	59	1026.39	10.8024			
15	209.616	0.2455	60	1029.82	0.1451			
16	226.437	1.4337	61	1032.34	0.1084			
17	231.258	1.7558	62	1054.46	12.278			
18	255.905	1.2961	63	1057.86	17.4573			
19	275.547	4.0878	64	1069.12	16.9333			
20	285.595	1.5584	65	1070.7	9.4379			
21	309.918	13.9436	66	1116.11	26.2658			
22	320.805	20.0104	67	1118.3	18.7244			
23	331.813	2.3543	68	1134.88	11.2391			
24	384.183	24.0111	69	1135.42	18.7279			
25	410.014	7.5294	70	1137.71	7.6167			
26	418.864	3.2618	71	1149.11	20.7707			
27	454.032	10.8859	72	1182.54	12.9204			
28	457.46	10.8892	73	1183.27	16.0789			
29	481.671	140.326	74	1224.43	7.7956			
30	518.565	1.4098	75	1232.38	12.3197			
31	523.466	11.3142	76	1276.82	0.7365	91	1581.09	12.0203
32	527.767	5.9965	77	1282.29	1.9487	92	1604.74	15.4756
33	539.033	25.9932	78	1302.35	29.1605	93	1606.96	10.0264
34	578.972	167.604	79	1305.66	1.8306	94	1662.02	90.2337
35	587.873	192.232	80	1309.73	22.2311	95	1665.35	87.2075
36	595.042	16.8713	81	1315.03	13.3543	96	2270.2	555.502
37	601.553	13.0575	82	1386.06	168.228	97	2286.56	879.028
38	654.211	10.3566	83	1393.38	259.508	98	3190.23	3.3124
39	662.146	16.9984	84	1426.2	38.1257	99	3190.62	4.4682
40	691.311	92.4182	85	1433.08	2.6498	100	3203.57	0.8995
41	707.769	155.26	86	1482.84	49.2072	101	3209.34	1.0279
42	727.345	0.3912	87	1486.89	52.1975	102	3216.07	2.52
43	728.134	2.1646	88	1497.5	60.1476	103	3217.37	2.2562
44	736.631	8.5354	89	1498.97	83.0785	104	3219.07	2.7871
45	740.127	15.726	90	1579.71	27.5635	105	3222.72	8.8884

5.6. *OC-6-13*-[$Si(N_3)_2(\kappa^2N,N(1)$-pytz$)_2$] (Table 4 entry g)

Gaussian log file name: OC-6-13-Si(N3)2(pyttz)2_b3lyp_6311g(d,p)goptfreq_C1
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: N=[N]=N[Si](N=[N]=N)(N:1NNN:C:1:C:2:C:C:C:C:N:2)N:3NNN:C:3:C:4:C:C:C:C:N:4
Formula: $C_{12}H_8N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1627.8620308 a.u.
Thermal correction to Gibbs Energy (298 K): 0.190622706771708 a.u.

5.7. *OC-6-23*-[Si(N$_3$)$_3$(*κN*(2)-mtz)(bpy)] (Table 4 entry h)



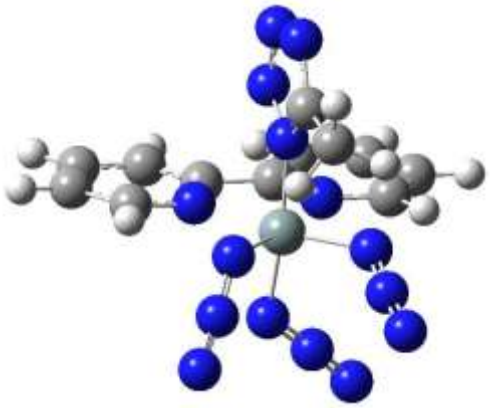
Gaussian log file name: eq-Si(N3)3(2,5-N4CMe)(bpy)_hf_6-311g(d,p)_opt_freq_355@2011-09-22T03;01;12
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]=N)(N=[N]=N)N=[N]#N.C:2:C:C:C(:N:C:2)C:3:C:C:C:C:N:3
Formula: $C_{12}H_{11}N_{15}Si$
Charge, multiplicity: 0, 1
Energy: -1574.91621248 a.u.
Thermal correction to Gibbs Energy (298 K): 0.210567 a.u.

Cartesian Coordinates (*x y z* format)

1	Si1	0.6307	-0.5106	0.3497 Si
2	C2	-0.6272	1.3726	2.2917 C
3	H3	0.3975	1.4129	2.6326 H
4	C4	-1.6586	2.0746	2.9006 C
5	H5	-1.4480	2.6867	3.7674 H
6	C6	-2.9406	1.9765	2.3740 C
7	H7	-3.7671	2.5109	2.8270 H
8	C8	-3.1519	1.1886	1.2490 C
9	H9	-4.1388	1.1071	0.8157 H
10	C10	-2.0744	0.5093	0.6873 C
11	N11	-0.0330	-1.8691	1.3986 N
12	N12	1.8436	0.0739	1.5546 N
13	N13	2.4191	-0.6689	2.3317 N
14	N14	3.0007	-1.2896	3.0830 N
15	N15	-0.8400	0.6005	1.2199 N
16	C16	1.2020	2.9920	-1.3877 C
17	C17	1.3894	4.4709	-1.4222 C
18	H18	0.7356	4.9258	-2.1696 H
19	H19	2.4192	4.7229	-1.6889 H
20	H20	1.1704	4.8995	-0.4441 H
21	C21	-0.9082	-1.6365	-1.9895 C
22	H22	0.0751	-2.0187	-2.2240 H
23	C23	-2.0330	-1.9118	-2.7570 C
24	H24	-1.9384	-2.5370	-3.6346 H
25	C25	-3.2548	-1.3708	-2.3778 C
26	H26	-4.1496	-1.5658	-2.9566 H
27	C27	-3.3177	-0.5682	-1.2440 C
28	H28	-4.2570	-0.1318	-0.9348 H
29	C29	-2.1546	-0.3346	-0.5167 C

30	N30	0.9089	1.0347	-0.7327 N
31	N31	1.0570	0.9760	-2.0547 N
32	N32	1.2426	2.1979	-2.4854 N
33	N33	0.9877	2.2915	-0.2808 N
34	N34	1.6485	-1.5980	-0.6722 N
35	N35	2.7624	-1.3268	-1.0865 N
36	N36	3.8040	-1.1487	-1.4972 N
37	N37	-0.9759	-0.8710	-0.8928 N
38	N38	-0.0700	-3.0368	1.0608 N
39	N39	-0.1488	-4.1428	0.8061 N

5.8. *OC-6-23*-[Si(N$_3$)$_3$(*κN*(1)-mtz)(bpy)] (Table 4 entry i)



Gaussian log file name: ax-Si(N3)3(1,5-N4CMe)2(bpy)_b3lyp_6-311G(d,p)_opt_freq
Route: opt freq b3lyp/6-311g(d,p) geom=connectivity
SMILES: CC:1:NN:NN:1[Si](N=[N]=N)(N=[N]=N)N=[N]#N.C:2:C:C:C(:N:C:2)C:3:C:C:C:C:N:3
Formula: $C_{12}H_{11}N_{15}Si$
Charge, multiplicity: 0, 1
Energy: -1574.9141127 a.u.
Thermal correction to Gibbs Energy (298 K): 0.212537 a.u.

Cartesian Coordinates (*x y z* format)

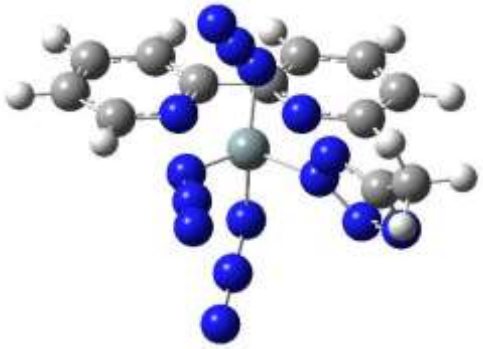
1	Si1	0.6510	0.0714	-0.2402 Si
2	C2	-0.7844	-2.3015	-1.3511 C
3	H3	0.2338	-2.6435	-1.4718 H
4	C4	-1.8806	-3.0546	-1.7497 C
5	H5	-1.7257	-4.0217	-2.2090 H
6	C6	-3.1554	-2.5431	-1.5422 C
7	H7	-4.0321	-3.1039	-1.8429 H
8	C8	-3.2954	-1.3029	-0.9305 C
9	H9	-4.2782	-0.8939	-0.7438 H
10	C10	-2.1551	-0.6059	-0.5472 C
11	N11	0.3654	0.8843	-1.8881 N
12	N12	1.8493	-1.1130	-0.9103 N
13	N13	2.4037	-1.0148	-1.9947 N
14	N14	2.9564	-1.0118	-2.9849 N
15	N15	-0.9248	-1.1030	-0.7762 N
16	C16	-0.8067	2.3158	1.1195 C
17	H17	0.2095	2.6211	1.3263 H
18	C18	-1.9136	3.0580	1.5112 C
19	H19	-1.7689	3.9849	2.0498 H
20	C20	-3.1820	2.5891	1.1971 C
21	H21	-4.0653	3.1453	1.4868 H
22	C22	-3.3071	1.3889	0.5064 C
23	H23	-4.2849	1.0009	0.2586 H

24	C24	-2.1602	0.6892	0.1508 C
25	N25	0.6116	-0.8453	1.4083 N
26	N26	-0.5755	-1.2093	1.9736 N
27	N27	1.7682	1.3532	0.4214 N
28	N28	2.8856	1.5829	-0.0034 N
29	N29	3.9411	1.8400	-0.3358 N
30	N30	-0.9321	1.1609	0.4520 N
31	N31	0.2730	2.0826	-2.0588 N
32	N32	0.1677	3.1969	-2.2732 N
33	N33	1.0142	-1.8661	3.2966 N
34	N34	-0.3199	-1.8077	3.0839 N
35	C35	1.5795	-1.2673	2.2610 C
36	C36	3.0510	-1.1021	2.1081 C
37	H37	3.5437	-1.7085	2.8672 H
38	H38	3.3817	-1.4117	1.1162 H
39	H39	3.3446	-0.0594	2.2512 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	30.3532	0.6405	46	699.407	19.1782			
2	40.087	0.2204	47	700.846	121.355			
3	41.0717	0.342	48	717.331	16.8402			
4	47.1898	0.5085	49	736.754	0.2146			
5	58.391	5.5946	50	754.088	73.1658			
6	63.2532	1.8449	51	763.668	0.2941			
7	67.9118	2.0061	52	784.13	39.8216			
8	82.0148	4.8669	53	789.217	1.6623			
9	85.8697	2.2573	54	824.118	1.1506			
10	89.2287	1.2562	55	904.376	0.1578			
11	118.803	0.2257	56	911.921	1.3893			
12	148.534	3.0414	57	1003.99	7.1754			
13	161.209	0.2949	58	1006.34	0.2385			
14	165.037	0.594	59	1010.13	0.2436			
15	178.292	2.5944	60	1026.7	0.2126			
16	187.667	0.2207	61	1028.68	0.0617			
17	206.486	0.4701	62	1032.52	8.7687			
18	229.174	1.6713	63	1038.92	6.7957			
19	249.756	0.1034	64	1050.28	32.2972			
20	253.571	0.8335	65	1064.46	5.2964			
21	275.184	0.5209	66	1070.67	7.4537			
22	281.576	1.8883	67	1084.83	14.1971			
23	285.257	0.7125	68	1088.64	72.8912			
24	314.155	3.1919	69	1099.06	1.7467			
25	337.649	17.4083	70	1127.3	9.3981	91	1507.07	43.476
26	347.138	22.7608	71	1134.94	2.904	92	1529.57	13.0327
27	378.287	3.7143	72	1150.63	1.105	93	1533.11	41.6372
28	410.503	40.532	73	1171.48	12.8727	94	1611.41	21.5464
29	418.54	25.2765	74	1185.76	11.5172	95	1622.36	23.5137
30	437.487	10.658	75	1195.2	12.5848	96	1649.1	32.9022
31	463.426	0.7792	76	1291.86	7.1333	97	1662.41	19.0515
32	485.651	4.3879	77	1300.16	10.7051	98	2240.2	512.234
33	486.919	1.934	78	1316.76	2.2483	99	2256.01	361.57
34	543.926	189.163	79	1332.57	14.2057	100	2283.94	1238.13
35	548.597	171.658	80	1342.99	17.9489	101	3051.41	11.5174
36	560.529	283.512	81	1351.06	2.1795	102	3112.24	6.7387
37	561.683	31.8751	82	1369.57	162.864	103	3141.3	6.0976
38	597.805	16.8354	83	1379.1	111.345	104	3190.84	4.3932
39	608.58	6.0696	84	1388.43	235.789	105	3191.84	4.2029
40	612.309	26.4707	85	1395.67	63.116	106	3210.52	1.2193
41	654.907	5.93	86	1411.71	59.6073	107	3212.01	2.919
42	667.604	0.8669	87	1464.54	21.8454	108	3215.36	0.3743
43	674.419	24.1296	88	1482.33	37.4152	109	3224.05	5.1513
44	680.015	14.8569	89	1482.86	40.2585	110	3225.48	8.5731
45	692.479	106.254	90	1494.6	11.4719	111	3227.74	13.3772

5.9. *OC-6-33*-[Si(N$_3$)$_3$(*κN*(2)-mtz)(bpy)] (Table 4 entry j)



Gaussian log file name: eq-Si(N3)3(2-5-eq-CN4CH3)(bpy)_b3lyp_opt_freq
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]=N)(N=[N]=N)N=[N]=N.C:2:C:C:C(:N:C:2)C:3:C:C:C:C:N:3
Formula: $C_{12}H_{11}N_{15}Si$
Charge, multiplicity: 0, 1
Energy: -1574.9099754 a.u.
Thermal correction to Gibbs Energy (298 K): 0.209359 a.u.

Cartesian Coordinates (*x y z* format)

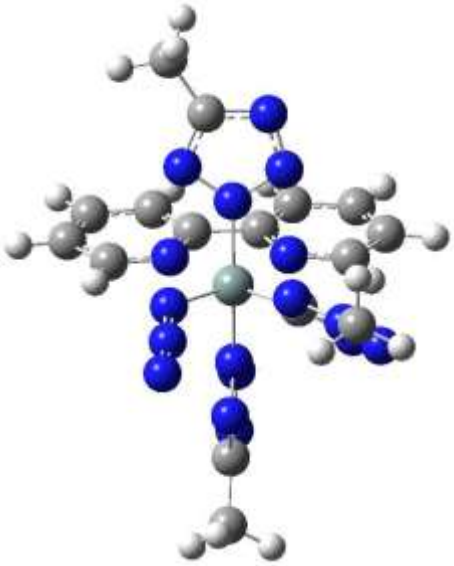
1	Si1	-0.1102	-0.3169	0.0946 Si
2	C2	0.3185	2.6670	0.0790 C
3	H3	-0.7508	2.6734	0.2300 H
4	C4	1.0505	3.8439	-0.0164 C
5	H5	0.5368	4.7946	0.0356 H
6	C6	2.4281	3.7678	-0.1716 C
7	H7	3.0276	4.6665	-0.2520 H
8	C8	3.0329	2.5175	-0.2135 C
9	H9	4.1049	2.4339	-0.3226 H
10	C10	2.2411	1.3771	-0.1103 C
11	N11	0.0142	-0.1573	-1.7264 N
12	N12	0.9035	1.4660	0.0213 N
13	C13	2.1890	-2.2472	0.0381 C
14	H14	1.3712	-2.9480	0.1382 H
15	C15	3.5180	-2.6382	-0.0601 C
16	H16	3.7674	-3.6907	-0.0328 H
17	C17	4.4976	-1.6617	-0.1918 C
18	H18	5.5432	-1.9332	-0.2722 H
19	C19	4.1188	-0.3246	-0.2175 C
20	H20	4.8651	0.4511	-0.3150 H
21	C21	2.7690	0.0004	-0.1143 C
22	N22	0.1729	-0.1186	1.8870 N
23	N23	-0.4400	-0.7076	2.7566 N
24	N24	-0.9648	-1.2220	3.6236 N
25	N25	-0.6393	-2.0547	0.1348 N
26	N26	-1.7683	-2.5037	0.2148 N
27	N27	-2.7871	-2.9975	0.2886 N
28	N28	1.8298	-0.9576	0.0076 N
29	N29	-1.8224	0.4726	0.1385 N
30	N30	-2.3176	1.2729	1.0887 N
31	N31	-2.7380	0.1944	-0.7985 N
32	N32	-0.4506	-0.9448	-2.5279 N
33	N33	-0.8477	-1.6353	-3.3380 N
34	C34	-3.8079	0.8546	-0.3788 C
35	C35	-5.1258	0.8437	-1.0744 C
36	H36	-5.5042	1.8608	-1.1970 H

37 H37	-5.0265	0.3745	-2.0529 H
38 H38	-5.8626	0.2835	-0.4927 H
39 N39	-3.5601	1.5312	0.7719 N

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	25.2098	0.1688	46	702.222	169.635	91	1511.39	42.4625
2	31.519	0.3368	47	708.303	33.8467	92	1531.27	7.4894
3	34.4111	1.0667	48	729.972	0.4563	93	1541.36	58.5552
4	37.0615	1.1583	49	737.721	2.4782	94	1611.5	27.3052
5	40.1242	0.1426	50	754.02	81.731	95	1623.15	21.4506
6	40.6728	0.6978	51	764.13	2.1178	96	1646.61	26.2038
7	51.4997	0.0508	52	785.113	39.4	97	1661.26	20.4925
8	63.4453	0.4009	53	787.932	0.5911	98	2257.07	109.659
9	76.792	2.3789	54	827.779	0.5063	99	2263.27	932.735
10	88.2775	3.2698	55	903.222	0.5216	100	2292.96	1092.04
11	98.5884	0.8789	56	912.049	1.3349	101	3043.4	18.7641
12	107.146	0.144	57	995.927	1.7489	102	3097.8	11.0563
13	145.736	0.3533	58	1001.1	3.6195	103	3134.73	6.9169
14	153.755	0.439	59	1008.85	0.0489	104	3189.47	4.8097
15	162.525	1.1181	60	1024.14	1.1042	105	3190.61	5.4057
16	181.7	0.3612	61	1029.44	0.0874	106	3207.98	4.3396
17	186.298	0.1994	62	1039.23	3.0268	107	3211	3.3494
18	234.652	2.6841	63	1043.13	25.1764	108	3213.82	0.0941
19	245.544	1.8047	64	1051.1	29.4543	109	3218.91	14.634
20	254.783	1.1874	65	1065.05	5.0771	110	3223.78	4.8917
21	268.964	0.6486	66	1071.38	1.8449	111	3236.46	35.5552
22	275.3	1.7102	67	1090.46	49.9695			
23	288.75	7.2152	68	1099.36	3.7001			
24	305.507	15.8465	69	1101.81	2.1553			
25	343.924	25.453	70	1131.91	25.8678			
26	360.776	17.7012	71	1136	6.5596			
27	378.663	7.7089	72	1151.83	0.6609			
28	400.866	2.8649	73	1185.93	11.738			
29	422.032	21.0287	74	1196.26	12.8637			
30	430.536	6.3532	75	1217.13	45.6969			
31	463.971	3.0054	76	1279.22	12.4388			
32	468.612	115.325	77	1289.25	14.5452			
33	488.615	0.9262	78	1304.4	9.8979			
34	498.025	195.789	79	1316.05	10.4074			
35	544.712	181.374	80	1345.91	6.4185			
36	558.248	1.4059	81	1351.51	16.3458			
37	586.961	26.1858	82	1385.51	13.8456			
38	598.322	175.015	83	1386.45	51.764			
39	603.041	7.4419	84	1389.53	237.117			
40	606.59	17.1357	85	1400.5	215.32			
41	653.997	6.0278	86	1418.89	10.2688			
42	667.248	0.6155	87	1466.81	32.724			
43	674.847	21.9686	88	1479.62	9.75			
44	676.748	57.3337	89	1481.47	72.2376			
45	685.076	142.982	90	1489.28	18.939			

5.10. *OC-6-31*-[Si(N_3)(κN(2)-mtz)$_3$(bpy)] (Table 4 entry k)



Gaussian log file name: OC-6-13-Si(N3)(N4CMe)3(bpy)(2,5,2,5,2,5)_b3lyp-6-311g(d,p)2.out
Route: opt freq b3lyp/6-311g(d,p) geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]=N)(C:2:N:NN(C)N:2)N3N:C(C):NN3.C:4:C:C:C(:N:C:4)C:5:C:C:C:C:N:5
Formula: $C_{16}H_{17}N_{17}Si$
Charge, multiplicity: 0, 1
Energy: -1840.5219035 a.u.
Thermal correction to Gibbs Energy (298 K): 0.306058 a.u.

Cartesian Coordinates (*x y z* format)

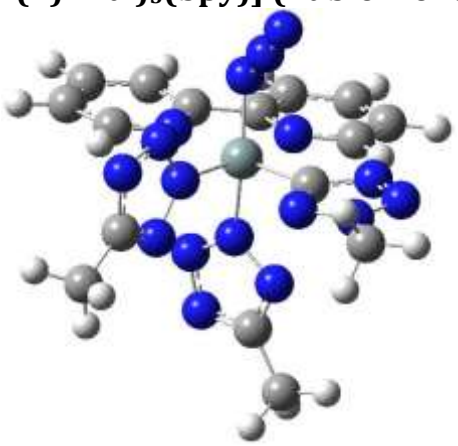
1	Si1	-0.2111	0.0478	-0.2909 Si
2	C2	-1.9346	-3.4758	-0.4771 C
3	C3	-3.0505	-4.3913	-0.8505 C
4	H4	-3.5606	-4.7650	0.0415 H
5	H5	-2.6721	-5.2554	-1.4011 H
6	H6	-3.7745	-3.8610	-1.4687 H
7	C7	1.9169	-0.8096	-2.2196 C
8	H8	1.1379	-0.5331	-2.9151 H
9	C9	3.1622	-1.2741	-2.6185 C
10	H10	3.3766	-1.3821	-3.6734 H
11	C11	4.1065	-1.5838	-1.6483 C
12	H12	5.0882	-1.9483	-1.9266 H
13	C13	3.7767	-1.4196	-0.3094 C
14	H14	4.4940	-1.6571	0.4629 H
15	C15	2.5071	-0.9569	0.0239 C
16	N16	-0.7671	-1.7728	-0.1990 N
17	N17	-0.0804	-2.7908	0.3134 N
18	N18	-0.7991	-3.8737	0.1474 N
19	N19	-1.9350	-2.1687	-0.7088 N
20	N20	-0.6543	0.2315	-2.0285 N
21	N21	-1.7562	0.3221	-2.5282 N
22	N22	-2.7451	0.4170	-3.0763 N
23	N23	1.5995	-0.6626	-0.9263 N
24	C24	1.8040	3.4317	-0.6632 C
25	C25	2.6510	4.4330	-1.3730 C

26	H26	3.4967	4.7359	-0.7511 H
27	H27	2.0747	5.3328	-1.6043 H
28	H28	3.0251	4.0114	-2.3060 H
29	C29	0.2029	-0.1709	2.7055 C
30	H30	-0.8381	0.1203	2.7225 H
31	C31	0.9190	-0.3953	3.8745 C
32	H32	0.4309	-0.2493	4.8289 H
33	C33	2.2428	-0.8006	3.7881 C
34	H34	2.8295	-0.9775	4.6815 H
35	C35	2.8071	-0.9875	2.5323 C
36	H36	3.8322	-1.3159	2.4377 H
37	C37	2.0323	-0.7572	1.4012 C
38	N38	0.6933	1.7289	-0.2068 N
39	N39	0.6085	2.5321	0.8497 N
40	N40	1.2993	3.6119	0.5823 N
41	N41	1.4457	2.2611	-1.1761 N
42	N42	0.7543	-0.3379	1.4962 N
43	C43	-1.8299	0.7416	0.4815 C
44	N44	-2.5427	0.2898	1.5543 N
45	N45	-2.4721	1.7546	-0.1047 N
46	N46	-3.5585	1.8825	0.6403 N
47	N47	-3.6232	1.0207	1.6448 N
48	C48	-4.5976	2.8613	0.3699 C
49	H49	-5.0186	2.6768	-0.6186 H
50	H50	-5.3609	2.7456	1.1357 H
51	H51	-4.1704	3.8633	0.4060 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	28.9738	0.5641
2	32.8118	0.0656
3	37.6897	1.4346
4	42.2998	0.3266
5	46.7032	0.6062
6	51.4482	1.2365
7	52.3161	0.3619
8	56.7744	3.3857
9	59.5714	2.0371
10	60.5823	1.2745
11	69.1476	0.3949
12	80.2934	3.1296
13	84.6577	5.5875
14	91.7375	0.0506
15	114.007	0.1125
16	119.032	1.6634
17	143.008	1.2449
18	155.604	0.1924
19	165.483	0.2521
20	171.714	0.0921
21	187.847	1.9466
22	198.747	3.2654
23	216.097	3.6331
24	218.688	2.61
25	235.486	1.4002
26	249.733	1.7085
27	262.309	0.6459
28	270.8	1.0358
29	282.832	1.0413
30	294.039	8.9811
31	323.277	0.3226
32	331.124	2.1199
33	358.665	28.6222
34	378.034	0.8542
35	385.941	4.4021
36	401.833	7.1762
37	414.834	8.283
38	430.156	0.4307
39	458.703	6.1013
40	462.041	60.4874
41	480.81	19.765
42	528.836	259.915
43	530.549	269.104
44	556.003	2.1555
45	560.346	177.492
46	597.476	18.7661
47	654.95	5.9189
48	668.23	0.7895
49	676.396	43.1157
50	688.808	89.9576
51	700.281	1.7727
52	708.352	3.4744
53	711.35	74.5504
54	729.762	37.3146
55	730.121	18.9889
56	731.16	4.1555
57	737.515	0.7506
58	739.89	2.3177
59	753.976	76.5772
60	762.445	1.744
61	771.967	6.1011
62	784.869	32.6541
63	790.002	0.3176
64	824.292	0.6033
65	900.026	0.3651
66	909.416	1.6122
67	998.688	2.6859
68	1000.78	3.0278
69	1007.89	1.0003
70	1011.53	1.5792
71	1027.61	0.7198
72	1029.58	18.9674
73	1032.57	20.8201
74	1038.38	9.0822
75	1048.43	21.6773
76	1049.54	6.9741
77	1052.34	14.9424
78	1054.09	18.4709
79	1066.6	4.3234
80	1069.93	1.7433
81	1071.51	1.9701
82	1088.69	10.7444
83	1095.34	36.084
84	1099.76	1.9467
85	1101.57	4.4932
86	1102.17	12.078
87	1137.42	1.6467
88	1146.61	30.463
89	1147.77	0.1261
90	1150.81	37.9453
91	1153.99	0.2723
92	1187.23	13.424
93	1197.63	15.2501
94	1223.32	41.3351
95	1226.26	7.4322
96	1228.16	45.3295
97	1266.55	10.6468
98	1278.5	4.2253
99	1283.8	31.5997
100	1289.34	12.8953
100	1289.34	12.8953
101	1310.29	14.7922
102	1318.74	15.736
103	1336.57	11.2671
104	1350.02	5.3088
105	1362.58	13.8484
106	1390	6.5587
107	1390.43	5.9301
108	1408.97	7.3397
109	1417.16	22.8257
110	1417.95	12.3647
111	1419.85	161.656
112	1433.19	17.4864
113	1449.79	0.843
114	1470.17	36.7429
115	1479.57	10.8316
116	1480.39	8.1968
117	1481.31	4.0159
118	1481.91	75.5944
119	1489.92	24.1025
120	1490.09	15.5203
121	1508.87	6.5096
122	1516.12	39.4492
123	1536.06	83.1405
124	1536.69	27.6109
125	1539.44	9.8996
126	1613.27	31.8856
127	1623.76	21.9754
128	1651.08	37.7282
129	1665.91	20.5816
130	2293.07	789.604
131	3040.37	25.8727
132	3041.21	22.202
133	3063.12	23.3544
134	3092.82	12.56
135	3094.5	12.7455
136	3128.46	9.5651
137	3132.72	7.4226
138	3134.98	5.9383
139	3169.04	1.5576
140	3188.59	5.3543
141	3189.42	12.5295
142	3203.49	80.4175
143	3210.85	4.7975
144	3213.56	8.8823
145	3216.31	9.3545
146	3226.72	1.4718
147	3230.54	29.4123

5.11. *OC-6-33*-[Si(N_3)(κN(2)-mtz)$_3$(bpy)] (Table 4 entry k)



Gaussian log file name: OC-6-33-Si(N3)(N4CMe)3(bpy)(2,5,2,5,2,5)_stereoisomer_b3lyp-6-311g(d,p)4

Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:N:NN(N:1)[Si](N=[N]=N)(C:2:N:NN(C)N:2)N3N:N:C(C):N3.C:4:C:C:C(:N:C:4)C:5:C:C:C:C:N:5
Formula: $C_{16}H_{17}N_{17}Si$
Charge, multiplicity: 0, 1
Energy: -1840.5132808 a.u.
Thermal correction to Gibbs Energy (298 K): 0.303454 a.u.

Cartesian Coordinates (*x y z* format)

1	Si1	0.0003	-0.0318	-0.4412 Si
2	C2	0.0335	-0.5368	3.4555 C
3	C3	0.5042	-1.1871	4.7120 C
4	H4	-0.3421	-1.4529	5.3491 H
5	H5	1.1463	-0.5094	5.2815 H
6	H6	1.0734	-2.0864	4.4765 H
7	C7	-1.4519	2.6046	-0.5235 C
8	H8	-0.4437	2.9844	-0.5266 H
9	C9	-2.5440	3.4580	-0.5836 C
10	H10	-2.3815	4.5265	-0.6278 H
11	C11	-3.8212	2.9140	-0.5827 C
12	H12	-4.6961	3.5514	-0.6269 H
13	C13	-3.9627	1.5343	-0.5262 C
14	H14	-4.9464	1.0875	-0.5284 H
15	C15	-2.8233	0.7365	-0.4662 C
16	N16	-0.2095	-0.0246	1.4507 N
17	N17	-1.0092	0.7793	2.1486 N
18	N18	-0.8690	0.4717	3.4138 N
19	N19	0.4548	-0.8702	2.2417 N
20	N20	-0.2534	0.0001	-2.2436 N
21	N21	0.5796	-0.2764	-3.0864 N
22	N22	1.2966	-0.5246	-3.9308 N
23	N23	-1.5912	1.2757	-0.4642 N
24	C24	2.5925	2.8124	0.2964 C
25	C25	3.4663	3.6506	1.1666 C
26	H26	3.3503	4.7102	0.9273 H
27	H27	4.5184	3.3938	1.0177 H
28	H28	3.2112	3.4901	2.2139 H
29	C29	-1.5584	-2.6632	-0.3151 C
30	H30	-0.5573	-3.0819	-0.3232 H
31	C31	-2.6936	-3.4640	-0.2639 C
32	H32	-2.5781	-4.5387	-0.2138 H
33	C33	-3.9455	-2.8663	-0.2789 C
34	H34	-4.8488	-3.4632	-0.2377 H
35	C35	-4.0247	-1.4810	-0.3468 C
36	H36	-4.9875	-0.9905	-0.3544 H
37	C37	-2.8517	-0.7336	-0.3979 C
38	N38	1.1911	1.4227	-0.3709 N
39	N39	1.7143	1.9894	-1.4619 N
40	N40	2.5930	2.8694	-1.0608 N
41	N41	1.7255	1.9207	0.7520 N
42	N42	-1.6386	-1.3251	-0.3816 N
43	C43	1.4235	-1.3428	-0.4250 C
44	N44	1.3658	-2.6980	-0.5809 N
45	N45	2.6986	-0.9483	-0.3614 N
46	N46	3.3648	-2.0880	-0.4654 N
47	N47	2.5909	-3.1527	-0.5981 N
48	C48	4.8157	-2.1633	-0.4641 C
49	H49	5.1996	-1.7418	0.4647 H
50	H50	5.0873	-3.2131	-0.5460 H

51 H51 5.2088 -1.6020 -1.3118 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	18.1206	3.0111	50	685.258	101.591	100	1286.7	19.8123
2	23.9782	1.5829	51	698.008	0.3675	101	1310.58	6.4135
3	31.9392	0.1311	52	709.943	38.6382	102	1322.95	14.4152
4	34.0004	0.1223	53	711.715	62.5566	103	1334.7	10.4026
5	38.3833	0.2202	54	730.926	15.1189	104	1347.3	4.1193
6	40.1753	0.9474	55	731.13	3.0713	105	1369.4	17.3225
7	42.8252	0.1267	56	732.33	43.5307	106	1388.07	1.6069
8	47.3032	0.4292	57	739.391	3.3892	107	1391.93	96.9834
9	52.423	0.5865	58	742.038	5.452	108	1392.25	99.3528
10	57.2865	0.3552	59	751.92	70.6636	109	1413.34	8.3923
11	67.677	1.2482	60	760.686	0.8718	110	1418.11	11.4817
12	76.3231	4.2543	61	770.295	4.419	111	1419.2	12.4764
13	81.5008	1.9476	62	783.453	32.5434	112	1425.79	12.2448
14	84.1439	2.4785	63	788.591	0.4819	113	1449.52	0.9443
15	96.1774	3.0364	64	824.635	2.0551	114	1473.14	43.8526
16	108.012	0.5306	65	893.505	1.5149	115	1479.3	10.4633
17	148.788	0.1488	66	911.892	0.9813	116	1480.02	7.4096
18	156.465	0.5741	67	980.936	0.6068	117	1480.87	8.3204
19	166.25	0.2108	68	997.843	5.5578	118	1482.19	61.3469
20	168.874	0.967	69	1001.36	2.1501	119	1488.67	18.4998
21	188.436	0.8899	70	1014.04	0.186	120	1491.47	20.2403
22	202.522	2.7808	71	1020.68	0.2255	121	1508.67	7.8223
23	211.385	1.5652	72	1035.35	5.2536	122	1522.31	40.5989
24	224.985	1.9326	73	1037.78	42.262	123	1536.05	54.1589
25	236.553	2.9165	74	1043.22	31.7411	124	1542.35	53.0352
26	240.565	2.4037	75	1048.39	13.0382	125	1543.16	16.3099
27	256.83	0.2094	76	1048.81	14.3314	126	1613.11	33.498
28	260.866	1.6704	77	1053.31	13.7312	127	1625.33	20.6133
29	283.081	0.7623	78	1057.56	0.7864	128	1650.71	33.5769
30	298.855	13.142	79	1067.82	1.5103	129	1664.63	19.664
31	337.058	1.8389	80	1070.11	2.0458	130	2272.31	743.753
32	346.13	2.4012	81	1070.96	1.8467	131	3040.17	22.754
33	366.379	10.8063	82	1091	7.9613	132	3041.08	24.7802
34	373.75	5.9495	83	1098.72	15.8276	133	3063.64	23.5521
35	390.459	8.8132	84	1101.8	2.9854	134	3093.06	12.8121
36	403.355	9.1521	85	1103	28.1647	135	3093.81	12.462
37	408.387	20.2539	86	1103.33	2.7568	136	3129.53	8.5713
38	426.145	5.8588	87	1130.71	32.919	137	3131.89	8.2639
39	456.524	15.4513	88	1138.75	2.2229	138	3135.28	6.1396
40	457.352	68.2813	89	1144.23	29.9719	139	3140.07	246.464
41	481.075	7.1956	90	1147.59	0.3145	140	3168.99	1.5912
42	497.565	214.792	91	1154.77	0.7918	141	3187.76	4.1642
43	524.702	158.907	92	1188.8	15.0842	142	3190	4.442
44	553.663	0.1959	93	1199.65	15.9049	143	3209.85	4.013
45	576.324	262.258	94	1221.63	54.3921	144	3212.96	0.8054
46	599.241	11.1671	95	1226.82	11.3847	145	3216.03	0.1302
47	652.589	8.9159	96	1228.91	30.5769	146	3227.77	4.1967
48	668.754	9.7038	97	1272.41	16.4139	147	3269.76	10.6796
49	674.069	23.7897	98	1282.33	17.3869			
			99	1283.41	9.457			

5.12. Transition state 4a / 4b

Gaussian log file name: Si(N3)2(N4CMe)2(bpy)_b3lyp_6-311G(d,p)_(2,5-1,5)_Xray_TS_search_no_restrictions_2
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: CC:1:NN:NN:1.CC:2:N:NN(N:2)[Si](N=[N]=N)(N=[N]#N)N:3:C:C:C:C:C:3C:4:C:C:C:C:N:4

Formula: $C_{14}H_{14}N_{16}Si$
Charge, multiplicity: 0, 1
Energy: -1707.6830073 a.u.
Thermal correction to Gibbs Energy (298 K): 0.255555 a.u.

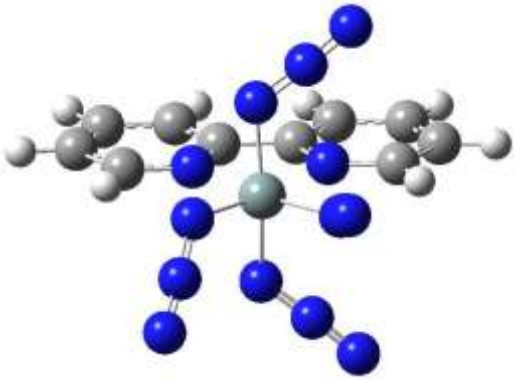
Cartesian Coordinates (*x y z* format)

1	Si1	0.0967	-0.5420	0.0286 Si
2	C2	3.7858	-0.2300	-0.2800 C
3	C3	4.7579	-1.2664	0.1753 C
4	H4	5.7601	-1.0104	-0.1704 H
5	H5	4.5000	-2.2490	-0.2316 H
6	H6	4.7608	-1.3461	1.2640 H
7	C7	-0.7618	0.9342	-2.4088 C
8	H8	-0.5628	-0.0179	-2.8762 H
9	C9	-1.2182	2.0425	-3.1105 C
10	H10	-1.3849	1.9630	-4.1763 H
11	C11	-1.4471	3.2294	-2.4271 C
12	H12	-1.8021	4.1087	-2.9504 H
13	C13	-1.2074	3.2804	-1.0579 C
14	H14	-1.3696	4.1947	-0.5046 H
15	C15	-0.7396	2.1401	-0.4185 C
16	N16	2.0652	1.0056	-0.4534 N
17	N17	2.8738	1.3164	-1.4400 N
18	N18	3.9790	0.5732	-1.3363 N
19	N19	2.6049	0.0225	0.3019 N
20	N20	0.5217	-1.3790	-1.4692 N
21	N21	1.3530	-2.2699	-1.5511 N
22	N22	2.0998	-3.1044	-1.7116 N
23	N23	-0.5286	0.9942	-1.0931 N
24	C24	-3.7261	-1.3757	-0.2053 C
25	C25	-5.0069	-1.6820	-0.9029 C
26	H26	-5.8068	-1.0317	-0.5418 H
27	H27	-5.3107	-2.7144	-0.7120 H
28	H28	-4.8906	-1.5459	-1.9778 H
29	C29	0.5051	0.6276	2.6306 C
30	H30	0.8797	-0.3648	2.8312 H
31	C31	0.4624	1.6372	3.5794 C
32	H32	0.8182	1.4370	4.5809 H
33	C33	-0.0361	2.8829	3.2193 C
34	H34	-0.0841	3.6884	3.9421 H
35	C35	-0.4643	3.0917	1.9136 C
36	H36	-0.8400	4.0568	1.6054 H
37	C37	-0.3863	2.0480	1.0016 C
38	N38	-1.7295	-0.9357	0.1954 N
39	N39	-2.3350	-1.0637	1.3791 N
40	N40	-3.5898	-1.3368	1.1455 N
41	N41	-2.5802	-1.1195	-0.8226 N
42	N42	0.6046	-1.7824	1.2344 N
43	N43	0.1211	-2.9007	1.2949 N
44	N44	-0.2687	-3.9594	1.4169 N
45	N45	0.0763	0.8339	1.3756 N

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	-178.456	8.0465	34	423.893	74.4818	67	1026.7	0.24			
2	21.2954	2.2467	35	436.374	92.0291	68	1036.56	22.3195			
3	32.4162	0.4663	36	456.612	16.3834	69	1040.54	23.5409			
4	37.335	0.9283	37	488.126	83.4313	70	1042.56	2.4803	100	1437.62	64.4789
5	40.5057	1.3357	38	499.125	2.5224	71	1044.34	6.2274	101	1466.73	28.508
6	43.6463	0.1099	39	554.342	30.0981	72	1058.72	27.2821	102	1476.68	7.1963
7	49.794	0.3408	40	555.561	102.09	73	1064.62	0.9478	103	1479.94	13.1616
8	56.8152	0.503	41	588.436	13.9539	74	1068.69	9.8767	104	1485.47	64.9079
9	57.3958	0.0991	42	591.615	29.2705	75	1078.8	4.017	105	1497.55	10.957
10	66.9173	1.1588	43	601.407	130.251	76	1090.54	52.2197	106	1498.83	65.0492
11	72.4036	1.1057	44	662.227	0.9474	77	1091.74	10.5423	107	1501.89	4.2946
12	76.0256	0.6785	45	668.408	1.6124	78	1099.66	6.9405	108	1509.08	41.3919
13	77.8964	0.6832	46	680.575	36.8022	79	1111.18	9.8856	109	1530.75	9.5094
14	89.6361	4.3397	47	681.912	22.7873	80	1132.29	42.8476	110	1609.91	20.9903
15	96.7061	13.542	48	692.118	54.4208	81	1137.81	1.8561	111	1620.95	18.0733
16	117.313	55.0371	49	696.399	41.1407	82	1152.6	6.903	112	1652.7	38.6977
17	126.523	5.3047	50	709.37	0.7607	83	1154.93	1.1526	113	1667.14	17.6525
18	160.415	8.3054	51	731.084	1.0817	84	1187.87	10.5822	114	2264.64	459.3
19	180.479	5.0935	52	732.592	25.0706	85	1195.25	11.2183	115	2292.82	880.219
20	198.26	2.2493	53	735.188	111.882	86	1222.43	38.6073	116	3034.82	22.3744
21	215.059	1.6211	54	741.741	59.0095	87	1228.08	5.2324	117	3037.84	17.3429
22	236.14	1.9075	55	749.502	11.2188	88	1276.81	34.6455	118	3078.23	9.2698
23	242.053	0.7166	56	762.524	0.8161	89	1294.33	9.8791	119	3091.62	17.0735
24	251.628	1.5553	57	783.289	44.9885	90	1303.97	14.98	120	3112.36	7.7177
25	272.897	1.4061	58	791.538	3.1766	91	1321.03	0.2112	121	3124.58	12.6608
26	283.938	4.1565	59	814.232	0.9269	92	1344.57	10.2749	122	3192.73	4.0353
27	296.494	5.196	60	897.957	0.164	93	1347.31	33.8329	123	3193.53	3.7408
28	299.774	3.1722	61	906.444	1.6546	94	1354.82	0.8451	124	3213.69	1.4485
29	318.108	8.1808	62	981.627	5.4467	95	1378.81	176.311	125	3216.27	0.5464
30	341.791	13.1244	63	987.607	3.8498	96	1386.16	9.191	126	3218.5	0.6022
31	385.519	30.4308	64	996.994	0.6234	97	1392.49	207.497	127	3226.24	0.876
32	390.342	2.7459	65	1006.53	0.2117	98	1396.29	8.4809	128	3239.35	25.2129
33	406.929	139.441	66	1021.03	0.38	99	1405.5	24.409	129	3246.2	11.3585

5.13. *OC-6-22*-[$Si(N_3)_4$(bpy)] (1)



Gaussian log file name: Si(N3)4(bpy)_b3lyp-6-311G(d,p)
Route: opt freq b3lyp/6-311g(d,p) nosymm geom=connectivity
SMILES: N=[N]=N[Si](N=[N]=N)(N=[N]=N)N=[N]=N.C:1:C:C:C(:N:C:1)C:2:C:C:C:C:N:2
Formula: $C_{10}H_{18}N_{14}Si$
Charge, multiplicity: 0, 1
Energy: -1442.0 923545 a.u.
Thermal correction to Gibbs Energy (298 K): 0.162571 a.u.

Cartesian Coordinates (*x y z* format)

1 C1	-2.8362	-2.9089	0.5743	C
2 C2	-0.4944	-2.4913	0.3155	C
3 C3	-1.5337	-3.3882	0.5330	C
4 H4	-3.6684	-3.5815	0.7430	H
5 H5	0.5441	-2.7906	0.2765	H
6 H6	-1.3117	-4.4386	0.6662	H
7 N7	-0.7165	-1.1803	0.1453	N
8 Si8	0.7927	0.2346	-0.1343	Si
9 N9	1.8467	1.6755	-0.4153	N
10 N10	2.6026	2.1346	0.4257	N
11 N11	3.3348	2.6237	1.1417	N

12	N12	0.4937	0.0541	-1.9468 N
13	N13	0.4909	-1.0042	-2.5379 N
14	N14	0.4653	-1.9674	-3.1486 N
15	N15	0.6502	0.5123	1.6912 N
16	N16	0.8864	-0.3334	2.5305 N
17	N17	1.0791	-1.0845	3.3645 N
18	C18	-1.9786	-0.7023	0.1818 C
19	C19	-2.0851	0.7520	-0.0290 C
20	C20	-0.8794	2.6968	-0.4425 C
21	H21	0.1052	3.1152	-0.6008 H
22	C22	-2.0405	3.4570	-0.4874 C
23	H23	-1.9761	4.5202	-0.6770 H
24	C24	-3.2628	2.8265	-0.2881 C
25	H25	-4.1875	3.3902	-0.3147 H
26	N26	-0.9070	1.3799	-0.2107 N
27	N27	2.0097	-1.1151	0.0171 N
28	N28	3.1089	-1.1150	-0.5087 N
29	N29	4.1484	-1.1780	-0.9610 N
30	C30	-3.0627	-1.5483	0.3962 C
31	C31	-3.2865	1.4561	-0.0597 C
32	H32	-4.0694	-1.1557	0.4251 H
33	H33	-4.2270	0.9444	0.0889 H

Frequencies (mode, wavenumber / cm^{-1}, intensity / km mol^{-1})

1	23.461	0.6681
2	35.351	1.1854
3	37.1827	0.3161
4	39.6294	0.141
5	45.0322	0.2741
6	66.5861	0.43
7	71.2464	0.7311
8	82.831	1.0029
9	91.2418	1.6639
10	115.388	1.5698
11	118.754	0.0442
12	157.293	0.8187
13	174.355	0.3316
14	181.286	0.359
15	201.82	0.4948
16	238.007	3.3562
17	261.787	0.4843
18	264.514	1.2604
19	277.705	1.284
20	289.171	1.9677
21	317.08	14.2526
22	347.754	36.9169
23	363.526	27.2865
24	392.631	24.7422
25	430.401	57.3463
26	437.228	6.3632
27	463.529	1.4318
28	481.926	3.732
29	490.286	1.8964
30	542.409	250.234
31	548.885	133.261
32	563.813	1.2692
33	577.853	253.082
34	598.254	28.1629
35	604.519	13.5009
36	607.042	3.1132
37	610.985	42.9052
38	650.179	7.8911
39	667.115	1.4403
40	669.572	13.362
41	677.051	4.7293
42	684.302	56.0669
43	697.301	120.203
44	708.941	153.88
45	755.763	54.2194
46	763.871	0.0655
47	784.519	43.8362
48	787.791	0.6324
49	825.522	0.0682
50	904.528	0.0777
51	914.479	1.487
52	1006.66	0.2276
53	1010.36	0.1201
54	1028.95	0.4278
55	1029.64	0.3707
56	1033.85	5.8493
57	1045.2	23.6892
58	1062.38	4.5762
59	1085.61	44.7778
60	1097.96	1.6862
61	1132.1	1.0694
62	1148.9	1.6942
63	1185.34	9.1124
64	1194.33	10.2063
65	1291.5	5.4946
66	1298.99	12.9338
67	1313.11	0.4226
68	1342.32	15.5669
69	1344.5	0.5095
70	1371.05	242.006
71	1379.07	170.666
72	1384.45	153.144
73	1393.89	111.849
74	1461.05	33.1076
75	1479.97	60.7225
76	1504.86	45.419
77	1522.9	3.248
78	1607.44	19.5175
79	1619.9	18.4209
80	1644.1	24.6281
81	1657.11	13.7412
82	2239.67	737.539
83	2247.01	598.398
84	2260.69	639.617
85	2284.62	1044.25
86	3189.58	4.7693
87	3191.18	4.4308
88	3208.39	1.6685
89	3210.25	6.1283
90	3212.81	0.3099
91	3220.56	12.0166
92	3221.33	2.1548
93	3223.32	17.3356

5.14. Calculated stick spectra

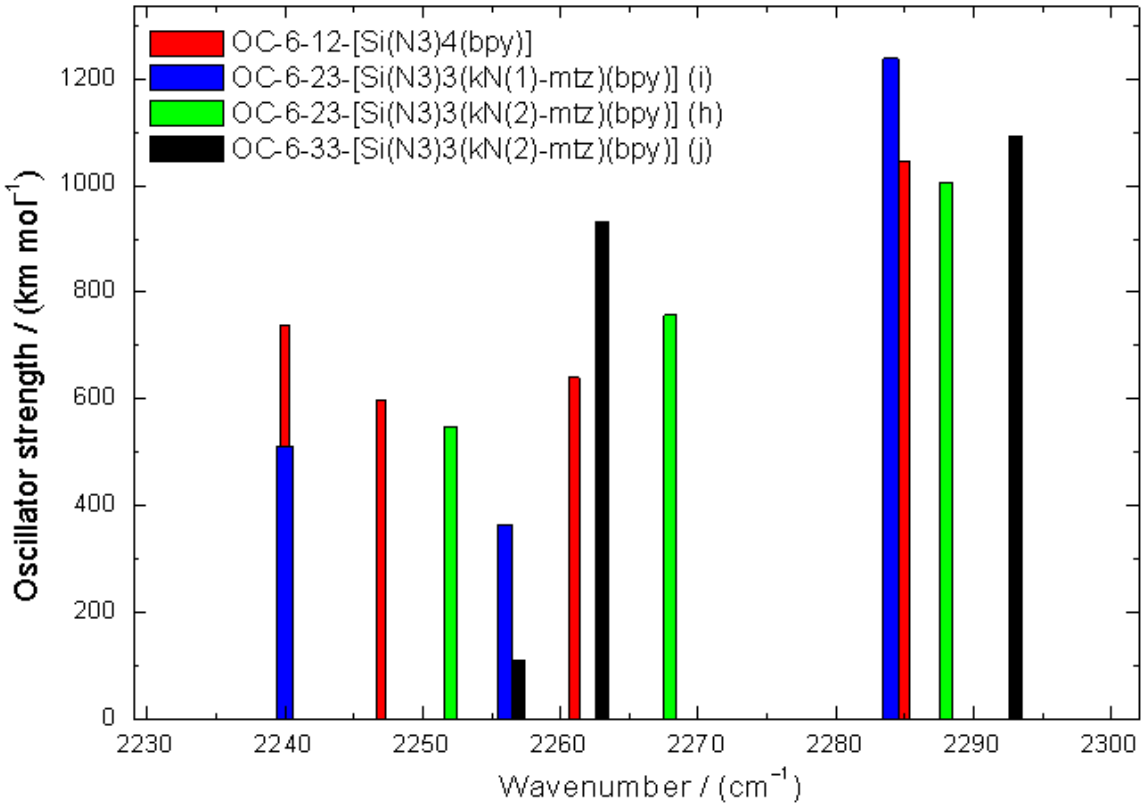


Fig. S12. Calculated stick spectra of *OC-6-12*-[Si(N_3)$_4$(bpy)], *OC-6-23*-[Si(N_3)$_3$(*κN(1)*-mtz)(bpy)] (**i**), *OC-6-23*-[Si(N_3)$_3$(*κN(2)*-mtz)(bpy)] (**h**) and *OC-6-33*-[Si(N_3)$_3$(*κN(2)*-mtz)(bpy)] (**j**)

6. References

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(3) *V2.1 Bruker Nonius Madison*, Apex II software.

(4) *SHELXTL, An integrated system for solving and refining crystal structures from diffraction data (Revision 5.1), Bruker AXS LTD.*