The Hexaazidosilicate(IV) Ion, $[\text{Si}(\text{N}_3)_6]^{2-}$: Synthesis, Properties and Molecular Structure

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Supporting Information

1. Experimental Section - General Part.

All experiments were carried out under an atmosphere of argon using Schlenk or glovebox techniques. The glassware was oven-dried (approximately 100 °C), assembled hot and baked in vacuo prior to use. A Teflon-coated spatula was used for all manipulations of **1**. All solvents were dried using standard methods (THF over Na/benzophenone, CH_2Cl_2 over Sicapent (Merck) and then Na/Pb alloy, CH_3CN over Sicapent and then K_2CO_3) and distilled under dinitrogen. CH_3CN and CH_2Cl_2 were stored over CaH_2 and trap-to-trap condensed including one freeze-pump-thaw cycle immediately prior to use. SiCl_4 was freed from HCl upon treatment with K_2CO_3 . It was trap-to-trap condensed and stored in a flask with a Young tap. K_2CO_3 was preheated in an oven at 150 °C. $(\text{PPN})\text{N}_3$ was prepared from $(\text{PPN})\text{Cl}$ and NaN_3 as described previously¹ and shown by elemental analysis to be free of chlorine. Elemental analyses were performed by the Central Analytical Group of the Chemistry Department of the Humboldt-Universität zu Berlin. The C, H, N analyses were obtained on a Leco CHNS-932 elemental analyzer and chlorine was determined using Schöniger's method followed by mercurimetry.² IR spectra of solutions were recorded on a Bruker IFS-55 spectrometer in the spectral range 2300–500 cm^{-1} using a cell of NaCl windows and IR spectra of nujol mulls were recorded in the spectral range 4000–500 cm^{-1} using NaCl windows. Nujol was dried with sodium and stored in the glovebox. The Raman spectra were measured on a Bruker-RFS-100 FT spectrometer using a Nd:YAG laser (power 500 mW). The following abbreviations were used for the intensity and shape of the absorption bands: vs = very strong; s = strong; m = medium;

(1) Martinsen, A.; Songstad, J. *Acta Chem. Scand.* **1977**, A31, 645.

(2) Ehrenberg, C. *Quantitative organische Elementaranalyse*, VCH, Weinheim, **1991**.

w = weak; vw = very weak; br = broad; sh = shoulder. The ^{14}N NMR spectra were recorded on a Bruker AM-300 spectrometer using sample tubes of 10 mm diameter and the ^{29}Si NMR spectrum of **1** on a Bruker ARX-250 spectrometer in dry deoxygenated CH_3CN . The ^{14}N and ^{29}Si NMR chemical shifts were referenced to CH_3NO_2 and SiMe_4 (CH_3CN solutions), respectively. The single-crystal X-ray diffraction study of **1** was performed on a STOE STADI-4 diffractometer (scintillation counter). A suitable colorless single crystal ($0.72 \times 0.60 \times 0.55$ mm) of **1** was obtained upon cooling a saturated CH_3CN solution from +20 to -28 °C. The melting point of **1** was determined several times using a Büchi SMP 530 melting point apparatus (Dr Tottoli, patent 320338) and is corrected. The samples were sealed in capillary tubes under vacuum and heated with a rate of approximately 40 K min^{-1} to a temperature 20 K lower than the expected melting point of **1**. Heating was then continued with a rate of approximately 3 K min^{-1} until the sample melted. Simultaneous thermal analysis (TG-DTA) of **1** was carried out at atmospheric pressure on a Netzsch STA 409 thermoanalyzer, which was coupled via the coupling system Netzsch STA 409 Skimmer[®] ³ with a Balzers QMG 422 quadrupole mass spectrometer for *on line* evolved gas analysis (EGA) (ion current curves). A TG-DTA mini sample carrier system was used equipped with Pt/PtRh10 thermoelements and platinum crucibles. The sample of **1** (39.64 mg) was heated with a rate of 10 K min^{-1} from room temperature to 340 °C and argon was used as purge gas with a flow rate of 40 mL min^{-1} . The characteristic temperatures (T_{on} = onset temperature, $T_{\text{on}}^{\text{ex}}$ = extrapolated onset temperature, T_{p} = peak temperature) were determined on the DTA curves following international recommendations.⁴

(3) Kaisersberger, E.; Post, E. *Thermochim. Acta* **1998**, 324, 197.

(4) *For Better Thermal Analysis*, Special Edition of the International Confederation for Thermal Analysis (ICTA); Hill, J. O. (Ed.), **1991**.

2. Tables of crystal data and structure refinement, atomic coordinates, bond lengths, bond angles, torsion angles and thermal parameters of 1.

Table 1. Crystal data and structure refinement for 1.

Identification code	port18
Empirical formula	C72 H60 N20 P4 Si
Formula weight	1357.37
Temperature	180(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	$a = 11.560(2)$ Å $\alpha = 64.55(2)$ deg. $b = 12.839(3)$ Å $\beta = 71.10(2)$ deg. $c = 13.468(4)$ Å $\gamma = 75.691(18)$ deg.
Volume	$1693.9(7)$ Å ³
Z, Calculated density	1, 1.331 Mg·m ⁻³
Absorption coefficient	0.189 mm ⁻¹
$F(000)$	706
Crystal size	0.72 × 0.60 × 0.55 mm
Theta range for data collection	1.73 to 27.44 deg.
Limiting indices	$-13 \leq h \leq 14$, $-14 \leq k \leq 16$, $0 \leq l \leq 17$
Reflections collected / unique	7721 / 7721 [$R(\text{int}) = 0.0000$]
Completeness to theta = 27.44	99.8 %
Max. and min. transmission	0.9030 and 0.8757
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7721 / 0 / 530
Goodness-of-fit on F^2	1.044
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0330$, $wR_2 = 0.0814$
R indices (all data)	$R_1 = 0.0419$, $wR_2 = 0.0887$
Extinction coefficient	0.0075(8)
Largest diff. peak and hole	0.506 and -0.308 e·Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	8933(1)	5628(1)	2355(1)	18(1)
C(2)	7961(1)	6468(1)	2562(1)	24(1)
C(3)	8154(2)	7627(1)	2091(1)	31(1)
C(4)	9303(2)	7952(1)	1423(1)	32(1)
C(5)	10271(2)	7123(1)	1230(1)	29(1)
C(6)	10093(1)	5959(1)	1697(1)	23(1)
C(7)	10021(1)	3334(1)	2397(1)	19(1)
C(8)	10231(1)	3504(1)	1257(1)	24(1)
C(9)	11256(1)	2913(1)	750(1)	28(1)
C(10)	12078(2)	2151(2)	1372(1)	34(1)
C(11)	11884(2)	1986(2)	2499(1)	38(1)
C(12)	10854(1)	2571(1)	3016(1)	28(1)
C(13)	8512(1)	3676(1)	4483(1)	19(1)
C(14)	9417(1)	3832(1)	4874(1)	23(1)
C(15)	9285(2)	3469(1)	6032(1)	28(1)
C(16)	8253(2)	2959(1)	6800(1)	33(1)
C(17)	7346(2)	2819(2)	6420(1)	34(1)
C(18)	7470(1)	3183(1)	5261(1)	25(1)
C(19)	7847(1)	1676(1)	2998(1)	21(1)
C(20)	8653(2)	1295(1)	2165(1)	31(1)
C(21)	9505(2)	306(2)	2464(2)	41(1)
C(22)	9558(2)	-287(2)	3583(2)	42(1)
C(23)	8751(2)	78(1)	4416(2)	36(1)
C(24)	7886(1)	1053(1)	4134(1)	26(1)
C(25)	5393(1)	2885(1)	3573(1)	22(1)
C(26)	4916(2)	1843(1)	3984(2)	34(1)
C(27)	3711(2)	1745(2)	4646(2)	44(1)
C(28)	2989(2)	2679(2)	4881(2)	43(1)
C(29)	3453(2)	3726(2)	4458(2)	41(1)
C(30)	4661(1)	3832(1)	3806(1)	29(1)
C(31)	6740(1)	3549(1)	1232(1)	21(1)
C(32)	6344(2)	2813(1)	920(1)	28(1)
C(33)	6155(2)	3210(2)	-157(1)	33(1)

C(34)	6345(2)	4335(2)	-915(1)	34(1)
C(35)	6719(1)	5071(1)	-604(1)	30(1)
C(36)	6926(1)	4679(1)	471(1)	24(1)
N(1)	7443(1)	4042(1)	2749(1)	21(1)
N(2)	4016(1)	1334(1)	-715(1)	28(1)
N(3)	4318(1)	2288(1)	-1263(1)	25(1)
N(4)	4523(2)	3226(1)	-1790(1)	44(1)
N(5)	4939(1)	596(1)	1074(1)	30(1)
N(6)	4705(1)	31(1)	2077(1)	39(1)
N(7)	4467(2)	-454(2)	3041(2)	75(1)
N(8)	3579(1)	-695(1)	919(1)	27(1)
N(9)	2728(1)	-608(1)	543(1)	27(1)
N(10)	1892(1)	-572(1)	243(1)	43(1)
P(1)	8662(1)	4131(1)	2985(1)	16(1)
P(2)	6914(1)	3074(1)	2643(1)	17(1)
Si	5000	0	0	19(1)

Table 4. Bond lengths [Å] and angles [deg] for 1.

C(1)-C(6)	1.3979(19)
C(1)-C(2)	1.3992(19)
C(1)-P(1)	1.7988(14)
C(2)-C(3)	1.387(2)
C(3)-C(4)	1.388(3)
C(4)-C(5)	1.383(2)
C(5)-C(6)	1.389(2)
C(7)-C(12)	1.3900(19)
C(7)-C(8)	1.4010(19)
C(7)-P(1)	1.8002(14)
C(8)-C(9)	1.387(2)
C(9)-C(10)	1.383(2)
C(10)-C(11)	1.387(2)
C(11)-C(12)	1.392(2)
C(13)-C(18)	1.392(2)
C(13)-C(14)	1.4008(19)
C(13)-P(1)	1.8028(14)
C(14)-C(15)	1.389(2)
C(15)-C(16)	1.388(2)

C(16)-C(17)	1.383(2)
C(17)-C(18)	1.391(2)
C(19)-C(20)	1.391(2)
C(19)-C(24)	1.399(2)
C(19)-P(2)	1.8035(14)
C(20)-C(21)	1.394(2)
C(21)-C(22)	1.380(3)
C(22)-C(23)	1.381(3)
C(23)-C(24)	1.389(2)
C(25)-C(26)	1.390(2)
C(25)-C(30)	1.393(2)
C(25)-P(2)	1.7999(15)
C(26)-C(27)	1.391(2)
C(27)-C(28)	1.377(3)
C(28)-C(29)	1.385(3)
C(29)-C(30)	1.392(2)
C(31)-C(36)	1.391(2)
C(31)-C(32)	1.399(2)
C(31)-P(2)	1.7936(15)
C(32)-C(33)	1.388(2)
C(33)-C(34)	1.386(3)
C(34)-C(35)	1.385(2)
C(35)-C(36)	1.395(2)
N(1)-P(1)	1.5818(12)
N(1)-P(2)	1.5892(12)
N(2)-N(3)	1.1982(18)
N(2)-Si	1.8662(13)
N(3)-N(4)	1.1438(19)
N(5)-N(6)	1.201(2)
N(5)-Si	1.8811(14)
N(6)-N(7)	1.144(2)
N(8)-N(9)	1.2067(18)
N(8)-Si	1.8673(13)
N(9)-N(10)	1.1463(19)
Si-N(2)#1	1.8662(13)
Si-N(8)#1	1.8673(13)
Si-N(5)#1	1.8811(14)

C(6)-C(1)-C(2)	119.79(13)
C(6)-C(1)-P(1)	121.48(11)
C(2)-C(1)-P(1)	118.70(11)
C(3)-C(2)-C(1)	119.59(14)
C(2)-C(3)-C(4)	120.35(15)
C(5)-C(4)-C(3)	120.27(14)
C(4)-C(5)-C(6)	120.08(15)
C(5)-C(6)-C(1)	119.91(14)
C(12)-C(7)-C(8)	119.40(13)
C(12)-C(7)-P(1)	123.35(11)
C(8)-C(7)-P(1)	117.25(10)
C(9)-C(8)-C(7)	120.34(14)
C(10)-C(9)-C(8)	119.99(14)
C(9)-C(10)-C(11)	120.04(14)
C(10)-C(11)-C(12)	120.38(15)
C(7)-C(12)-C(11)	119.85(14)
C(18)-C(13)-C(14)	119.50(12)
C(18)-C(13)-P(1)	119.48(10)
C(14)-C(13)-P(1)	121.00(10)
C(15)-C(14)-C(13)	119.98(13)
C(14)-C(15)-C(16)	119.94(14)
C(17)-C(16)-C(15)	120.43(14)
C(16)-C(17)-C(18)	119.92(15)
C(17)-C(18)-C(13)	120.20(14)
C(20)-C(19)-C(24)	119.68(14)
C(20)-C(19)-P(2)	121.74(11)
C(24)-C(19)-P(2)	117.85(11)
C(19)-C(20)-C(21)	119.91(16)
C(22)-C(21)-C(20)	120.07(17)
C(23)-C(22)-C(21)	120.34(15)
C(22)-C(23)-C(24)	120.28(16)
C(23)-C(24)-C(19)	119.70(15)
C(26)-C(25)-C(30)	120.09(14)
C(26)-C(25)-P(2)	120.90(12)
C(30)-C(25)-P(2)	118.83(11)
C(25)-C(26)-C(27)	119.66(16)
C(28)-C(27)-C(26)	120.26(17)
C(27)-C(28)-C(29)	120.37(16)
C(28)-C(29)-C(30)	120.01(17)
C(29)-C(30)-C(25)	119.61(16)

C(36)-C(31)-C(32)	120.15(13)
C(36)-C(31)-P(2)	119.54(11)
C(32)-C(31)-P(2)	120.20(11)
C(33)-C(32)-C(31)	119.71(15)
C(34)-C(33)-C(32)	120.06(15)
C(35)-C(34)-C(33)	120.40(14)
C(34)-C(35)-C(36)	120.10(15)
C(31)-C(36)-C(35)	119.57(14)
P(1)-N(1)-P(2)	135.87(8)
N(3)-N(2)-Si	126.45(10)
N(4)-N(3)-N(2)	175.30(15)
N(6)-N(5)-Si	122.55(12)
N(7)-N(6)-N(5)	176.4(2)
N(9)-N(8)-Si	121.88(10)
N(10)-N(9)-N(8)	176.12(16)
N(1)-P(1)-C(1)	109.18(6)
N(1)-P(1)-C(7)	113.94(6)
C(1)-P(1)-C(7)	106.68(7)
N(1)-P(1)-C(13)	111.50(7)
C(1)-P(1)-C(13)	105.85(6)
C(7)-P(1)-C(13)	109.27(6)
N(1)-P(2)-C(31)	109.88(7)
N(1)-P(2)-C(25)	109.44(7)
C(31)-P(2)-C(25)	106.18(7)
N(1)-P(2)-C(19)	113.77(6)
C(31)-P(2)-C(19)	109.37(7)
C(25)-P(2)-C(19)	107.90(7)
N(2)#1-Si-N(2)	180.00(13)
N(2)#1-Si-N(8)	90.68(6)
N(2)-Si-N(8)	89.32(6)
N(2)#1-Si-N(8)#1	89.32(6)
N(2)-Si-N(8)#1	90.68(6)
N(8)-Si-N(8)#1	180.00(9)
N(2)#1-Si-N(5)	89.84(6)
N(2)-Si-N(5)	90.16(6)
N(8)-Si-N(5)	90.30(6)
N(8)#1-Si-N(5)	89.70(6)
N(2)#1-Si-N(5)#1	90.16(6)
N(2)-Si-N(5)#1	89.84(6)
N(8)-Si-N(5)#1	89.70(6)

N(8)#1-Si-N(5)#1 90.30(6)
N(5)-Si-N(5)#1 180.00(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	22(1)	19(1)	16(1)	-6(1)	-9(1)	-3(1)
C(2)	23(1)	25(1)	28(1)	-11(1)	-11(1)	0(1)
C(3)	38(1)	24(1)	40(1)	-14(1)	-23(1)	5(1)
C(4)	50(1)	20(1)	31(1)	-2(1)	-24(1)	-9(1)
C(5)	35(1)	33(1)	21(1)	-4(1)	-10(1)	-16(1)
C(6)	23(1)	28(1)	19(1)	-8(1)	-7(1)	-6(1)
C(7)	19(1)	20(1)	19(1)	-8(1)	-4(1)	-2(1)
C(8)	23(1)	30(1)	20(1)	-11(1)	-6(1)	-3(1)
C(9)	29(1)	36(1)	23(1)	-16(1)	-2(1)	-5(1)
C(10)	30(1)	34(1)	32(1)	-17(1)	0(1)	4(1)
C(11)	33(1)	37(1)	31(1)	-11(1)	-9(1)	16(1)
C(12)	28(1)	29(1)	21(1)	-8(1)	-7(1)	7(1)
C(13)	22(1)	18(1)	16(1)	-7(1)	-6(1)	0(1)
C(14)	25(1)	24(1)	20(1)	-8(1)	-7(1)	-3(1)
C(15)	37(1)	30(1)	23(1)	-11(1)	-14(1)	-2(1)
C(16)	47(1)	34(1)	17(1)	-8(1)	-9(1)	-5(1)
C(17)	36(1)	41(1)	19(1)	-8(1)	1(1)	-13(1)
C(18)	25(1)	30(1)	21(1)	-10(1)	-4(1)	-8(1)
C(19)	20(1)	18(1)	28(1)	-8(1)	-9(1)	-2(1)
C(20)	30(1)	30(1)	34(1)	-16(1)	-8(1)	0(1)
C(21)	34(1)	35(1)	58(1)	-28(1)	-10(1)	6(1)
C(22)	34(1)	24(1)	67(1)	-14(1)	-22(1)	7(1)
C(23)	37(1)	23(1)	43(1)	-1(1)	-20(1)	-2(1)
C(24)	28(1)	21(1)	29(1)	-6(1)	-10(1)	-4(1)
C(25)	19(1)	27(1)	21(1)	-8(1)	-7(1)	-3(1)
C(26)	26(1)	29(1)	45(1)	-12(1)	-7(1)	-6(1)
C(27)	29(1)	44(1)	53(1)	-9(1)	-6(1)	-17(1)

C(28)	23(1)	60(1)	39(1)	-15(1)	-1(1)	-9(1)
C(29)	27(1)	50(1)	41(1)	-23(1)	-2(1)	2(1)
C(30)	26(1)	30(1)	30(1)	-13(1)	-5(1)	-2(1)
C(31)	19(1)	24(1)	21(1)	-10(1)	-7(1)	0(1)
C(32)	33(1)	28(1)	30(1)	-12(1)	-15(1)	-3(1)
C(33)	35(1)	40(1)	37(1)	-21(1)	-20(1)	1(1)
C(34)	30(1)	49(1)	25(1)	-16(1)	-13(1)	4(1)
C(35)	28(1)	33(1)	24(1)	-5(1)	-7(1)	-2(1)
C(36)	22(1)	26(1)	24(1)	-9(1)	-6(1)	-3(1)
N(1)	20(1)	21(1)	26(1)	-10(1)	-10(1)	-1(1)
N(2)	21(1)	24(1)	33(1)	-4(1)	-9(1)	-1(1)
N(3)	22(1)	28(1)	26(1)	-10(1)	-12(1)	2(1)
N(4)	42(1)	27(1)	59(1)	-1(1)	-30(1)	-5(1)
N(5)	30(1)	33(1)	28(1)	-14(1)	-5(1)	-5(1)
N(6)	45(1)	43(1)	32(1)	-19(1)	-14(1)	1(1)
N(7)	116(2)	79(1)	29(1)	-16(1)	-21(1)	-12(1)
N(8)	19(1)	31(1)	25(1)	-5(1)	-5(1)	-5(1)
N(9)	20(1)	22(1)	31(1)	-5(1)	-4(1)	-4(1)
N(10)	29(1)	40(1)	57(1)	-7(1)	-18(1)	-10(1)
P(1)	16(1)	17(1)	15(1)	-6(1)	-5(1)	-1(1)
P(2)	17(1)	18(1)	19(1)	-7(1)	-7(1)	-2(1)
Si	16(1)	21(1)	20(1)	-6(1)	-4(1)	-1(1)

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(2)	7200(17)	6245(15)	3025(15)	29
H(3)	7555(18)	8168(18)	2229(16)	38
H(4)	9425(18)	8718(18)	1105(16)	38
H(5)	11028(18)	7362(16)	783(16)	34
H(6)	10756(17)	5378(15)	1560(14)	28
H(8)	9630(16)	4059(15)	807(15)	28
H(9)	11377(17)	3044(16)	-46(16)	34
H(10)	12780(19)	1718(17)	1042(17)	41
H(11)	12432(19)	1441(18)	2946(17)	45
H(12)	10675(17)	2415(16)	3846(16)	34

H(14)	10150(16)	4198(15)	4339(15)	27
H(15)	9939(17)	3577(16)	6290(16)	34
H(16)	8189(18)	2697(17)	7606(17)	39
H(17)	6630(19)	2461(17)	6929(17)	40
H(18)	6855(17)	3090(16)	4995(15)	30
H(20)	8660(18)	1687(17)	1395(17)	37
H(21)	10060(20)	65(19)	1842(18)	49
H(22)	10170(20)	-955(19)	3778(18)	51
H(23)	8787(19)	-344(18)	5197(18)	44
H(24)	7328(17)	1279(16)	4710(16)	32
H(26)	5402(19)	1197(18)	3819(17)	41
H(27)	3400(20)	1040(20)	4924(19)	53
H(28)	2170(20)	2591(19)	5357(19)	51
H(29)	2940(20)	4402(19)	4616(18)	49
H(30)	4972(17)	4549(17)	3501(16)	35
H(32)	6177(17)	2014(17)	1465(16)	34
H(33)	5903(18)	2678(17)	-340(17)	40
H(34)	6212(18)	4603(17)	-1643(17)	41
H(35)	6837(18)	5836(17)	-1115(16)	36
H(36)	7164(16)	5189(15)	709(15)	29

Table 8. Torsion angles [deg] for 1.

C(6)-C(1)-C(2)-C(3)	1.3(2)
P(1)-C(1)-C(2)-C(3)	179.49(11)
C(1)-C(2)-C(3)-C(4)	-0.3(2)
C(2)-C(3)-C(4)-C(5)	-0.6(2)
C(3)-C(4)-C(5)-C(6)	0.5(2)
C(4)-C(5)-C(6)-C(1)	0.5(2)
C(2)-C(1)-C(6)-C(5)	-1.42(19)
P(1)-C(1)-C(6)-C(5)	-179.55(10)
C(12)-C(7)-C(8)-C(9)	0.3(2)
P(1)-C(7)-C(8)-C(9)	-179.61(11)
C(7)-C(8)-C(9)-C(10)	0.0(2)
C(8)-C(9)-C(10)-C(11)	-0.6(3)
C(9)-C(10)-C(11)-C(12)	0.9(3)
C(8)-C(7)-C(12)-C(11)	0.0(2)
P(1)-C(7)-C(12)-C(11)	179.91(13)

C(10)-C(11)-C(12)-C(7)	-0.6(3)
C(18)-C(13)-C(14)-C(15)	1.7(2)
P(1)-C(13)-C(14)-C(15)	-179.68(11)
C(13)-C(14)-C(15)-C(16)	-0.4(2)
C(14)-C(15)-C(16)-C(17)	-0.6(2)
C(15)-C(16)-C(17)-C(18)	0.4(3)
C(16)-C(17)-C(18)-C(13)	0.8(2)
C(14)-C(13)-C(18)-C(17)	-1.9(2)
P(1)-C(13)-C(18)-C(17)	179.46(12)
C(24)-C(19)-C(20)-C(21)	-0.9(2)
P(2)-C(19)-C(20)-C(21)	169.13(13)
C(19)-C(20)-C(21)-C(22)	-0.7(3)
C(20)-C(21)-C(22)-C(23)	1.5(3)
C(21)-C(22)-C(23)-C(24)	-0.6(3)
C(22)-C(23)-C(24)-C(19)	-0.9(2)
C(20)-C(19)-C(24)-C(23)	1.7(2)
P(2)-C(19)-C(24)-C(23)	-168.70(12)
C(30)-C(25)-C(26)-C(27)	-1.2(2)
P(2)-C(25)-C(26)-C(27)	-176.22(14)
C(25)-C(26)-C(27)-C(28)	0.9(3)
C(26)-C(27)-C(28)-C(29)	0.1(3)
C(27)-C(28)-C(29)-C(30)	-0.9(3)
C(28)-C(29)-C(30)-C(25)	0.6(3)
C(26)-C(25)-C(30)-C(29)	0.4(2)
P(2)-C(25)-C(30)-C(29)	175.53(13)
C(36)-C(31)-C(32)-C(33)	0.8(2)
P(2)-C(31)-C(32)-C(33)	176.87(12)
C(31)-C(32)-C(33)-C(34)	-0.7(2)
C(32)-C(33)-C(34)-C(35)	-0.3(2)
C(33)-C(34)-C(35)-C(36)	1.0(2)
C(32)-C(31)-C(36)-C(35)	-0.1(2)
P(2)-C(31)-C(36)-C(35)	-176.16(11)
C(34)-C(35)-C(36)-C(31)	-0.8(2)
Si-N(2)-N(3)-N(4)	-173.6(19)
Si-N(5)-N(6)-N(7)	-161(3)
Si-N(8)-N(9)-N(10)	170(2)
P(2)-N(1)-P(1)-C(1)	153.59(10)
P(2)-N(1)-P(1)-C(7)	34.45(13)
P(2)-N(1)-P(1)-C(13)	-89.81(12)
C(6)-C(1)-P(1)-N(1)	-132.90(11)

C(2)-C(1)-P(1)-N(1)	48.96(12)
C(6)-C(1)-P(1)-C(7)	-9.34(12)
C(2)-C(1)-P(1)-C(7)	172.51(10)
C(6)-C(1)-P(1)-C(13)	106.96(11)
C(2)-C(1)-P(1)-C(13)	-71.18(12)
C(12)-C(7)-P(1)-N(1)	-130.60(13)
C(8)-C(7)-P(1)-N(1)	49.35(13)
C(12)-C(7)-P(1)-C(1)	108.85(13)
C(8)-C(7)-P(1)-C(1)	-71.20(12)
C(12)-C(7)-P(1)-C(13)	-5.15(14)
C(8)-C(7)-P(1)-C(13)	174.80(10)
C(18)-C(13)-P(1)-N(1)	7.38(13)
C(14)-C(13)-P(1)-N(1)	-171.26(11)
C(18)-C(13)-P(1)-C(1)	125.99(12)
C(14)-C(13)-P(1)-C(1)	-52.65(12)
C(18)-C(13)-P(1)-C(7)	-119.47(12)
C(14)-C(13)-P(1)-C(7)	61.89(12)
P(1)-N(1)-P(2)-C(31)	-116.12(11)
P(1)-N(1)-P(2)-C(25)	127.65(11)
P(1)-N(1)-P(2)-C(19)	6.88(14)
C(36)-C(31)-P(2)-N(1)	-7.13(13)
C(32)-C(31)-P(2)-N(1)	176.83(11)
C(36)-C(31)-P(2)-C(25)	111.13(12)
C(32)-C(31)-P(2)-C(25)	-64.91(13)
C(36)-C(31)-P(2)-C(19)	-132.68(11)
C(32)-C(31)-P(2)-C(19)	51.28(13)
C(26)-C(25)-P(2)-N(1)	-154.94(12)
C(30)-C(25)-P(2)-N(1)	29.98(13)
C(26)-C(25)-P(2)-C(31)	86.51(14)
C(30)-C(25)-P(2)-C(31)	-88.58(13)
C(26)-C(25)-P(2)-C(19)	-30.67(14)
C(30)-C(25)-P(2)-C(19)	154.25(12)
C(20)-C(19)-P(2)-N(1)	-100.93(13)
C(24)-C(19)-P(2)-N(1)	69.27(13)
C(20)-C(19)-P(2)-C(31)	22.35(14)
C(24)-C(19)-P(2)-C(31)	-167.45(11)
C(20)-C(19)-P(2)-C(25)	137.44(12)
C(24)-C(19)-P(2)-C(25)	-52.36(13)
N(3)-N(2)-Si-N(2)#1	-77(100)
N(3)-N(2)-Si-N(8)	161.22(14)

N(3)-N(2)-Si-N(8)#1	-18.78(14)
N(3)-N(2)-Si-N(5)	70.93(14)
N(3)-N(2)-Si-N(5)#1	-109.07(14)
N(9)-N(8)-Si-N(2)#1	-137.51(13)
N(9)-N(8)-Si-N(2)	42.49(13)
N(9)-N(8)-Si-N(8)#1	8(87)
N(9)-N(8)-Si-N(5)	132.65(13)
N(9)-N(8)-Si-N(5)#1	-47.35(13)
N(6)-N(5)-Si-N(2)#1	-48.15(14)
N(6)-N(5)-Si-N(2)	131.85(14)
N(6)-N(5)-Si-N(8)	42.53(14)
N(6)-N(5)-Si-N(8)#1	-137.47(14)
N(6)-N(5)-Si-N(5)#1	123(73)

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4. Experimental and calculated bond lengths and angles of $[\text{Si}(\text{N}_3)_6]^{2-}$.

Methods ^{5,a} / basis sets ⁶	Si–N _α [Å]	N _α –N _β [Å]	N _β –N _γ [Å]	Si–N _α –N _β [°]	N _α –N _β –N _γ [°]	N _α –Si–N _α [°]	N _α –Si–N _α –N _β [°]
X-ray of 1 ^{7,b}	1.871(5)	1.202(3)	1.145(1)	124(1)	175.9(3)	89.9(3) ^c	142 ^d
RI-BP86/DZP ^{e,h}	1.906	1.211	1.169	127.23	174.82	89.36	130
RI-BP86/TZVPP ^{e,h}	1.902	1.205	1.161	127.21	175.30	89.56	130
HF/TZVPP ^f	1.889	1.179	1.108	124.40	176.55	89.64	133
RI-MP2/TZVP ^g	1.876	1.206	1.174	126.08	175.08	90.34	143
RI-MP2/SVP ^g	1.880	1.206	1.178	129.54	175.15	90.59	130
B3LYP/TZVPP ^{e,f}	1.896	1.195	1.146	127.07	175.82	89.57	130

^a RI: resolution of identity. ^b The unweighted mean x_u of the three crystallographically independent bond lengths and angles of **1** is listed. The standard deviation s of x_u is given in parenthesis and was calculated by $s^2 = S(x_i - x_u)^2 / (n^2 - n)$, x_i = individual value, $n = 3$. ^c N_α and N_β denote the atoms N2, N5 and N8 of the azide groups, which are interchanged upon rotation about the pseudo S_6 axis. ^d unweighted mean x_u of the torsion angles N2–Si–N5–N6 131.9(1), N5–Si–N8–N9 132.7(1), N8–Si–N2–N3 161.2(1); the s value is not given due to the large range of values observed. ^e See ref. 5c, 5d and 5e. ^f See ref. 5c. ^g See ref. 5a, 5b and 5c. ^h Calculated with restrained symmetry (S_6).

5. NBO – Analysis, BP86/TZVPP. ⁶

$q(\text{Si})$	$q(\text{N}_\alpha)$	$q(\text{N}_\beta)$	$q(\text{N}_\gamma)$
+1.86	- 0.58	+0.22	- 0.28

6. ²⁹Si and ¹⁴N NMR chemical shift calculations.

²⁹Si NMR chemical shift calculations (BP86/UCTZVPP).

Molecule	calcd. $s_{\text{iso}}(\text{Si})$ ^a	exp. $d(^{29}\text{Si})$ [ppm] ^{b,8}	calcd. $d(^{29}\text{Si})$ of $[\text{Si}(\text{N}_3)_6]^{2-}$ [ppm] ^c
SiMe ₄	332.60878	0	- 198.2
$[\text{SiF}_6]^{2-}$	504.27285	- 187.7 ^d	- 214.2
$[\text{SiF}_6]^{2-}$	504.27285	- 185.3 ^e	- 211.9
$[\text{Si}(\text{N}_3)_6]^{2-}$	530.84732	- 188.7 ^f	./.
$[\text{Si}(\text{ox})_3]^{2-}$ ⁱ	502.46200	- 173.3 ^g	- 201.7
$[\text{Si}(\text{brenzcat})_3]^{2-}$ ^j	459.39308	- 139.3 ^h	- 210.8

^a Isotropic shielding constant. ^b Referenced to SiMe₄. ^c Referenced to the substance listed in the row. ^d (NH₄)₂SiF₆. ^e ZnSiF₆. ^f (PPN)₂[Si(N₃)₆]. ^g (NEt₃H)₂[Si(ox)₃]. ^h (N^tBu)₄[Si(brenzcat)₃]. ⁱ ox: oxalate. ^j brencat: 1,2-benzenediolate.

(5) (a) Weigend, F.; Häser, M.; Patzelt, H.; Ahlrichs, R. *Chem. Phys. Lett.* **1998**, 294, 143. (b) Weigend, F.; Häser, M. *Theor. Chem. Acc.* **1997**, 97, 331. (c) Schäfer, A.; Huber, C.; Ahlrichs, R. *J. Chem. Phys.* **1994**, 100, 5829. (d) Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. *Chem. Phys. Lett.* **1995**, 240, 283. (e) Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc.* **1997**, 97, 119.

(6) For specification of basis sets and lists of cartesian coordinates see below.

(7) See tables of crystal data of **1**, section 2.

(8) Measured chemical shifts of (NH₄)₂SiF₆ and ZnSiF₆: Johannesen, R. B.; Brinckman, F. E.; Coyle, T. D. *J. Phys. Chem.* **1968**, 72, 660; (NEt₃H)₂[Si(ox)₃]: Marssmann, H. C.; Lömer, R. *Chem. Ztg.* **1973**, 79, 660; (N^tBu)₄[Si(brenzcat)₃]: Cella, J.A.; Cargioli, J. D.; Williams, E. A. *J. Organomet. Chem.* **1980**, 186, 13.

¹⁴N NMR chemical shift calculations (BP86/UCTZVPP).

Molecule	$S_{\text{iso}}(\text{N}_\alpha)$	$S_{\text{iso}}(\text{N}_\beta)$	$S_{\text{iso}}(\text{N}_\gamma)$	calcd. $d(^{14}\text{N}_\alpha)^a$	calcd. $d(^{14}\text{N}_\beta)$	calc. $d(^{14}\text{N}_\gamma)$
$[\text{Si}(\text{N}_3)_6]^{2-}$	145.257912 ^b	- 6.187030 ^b	77.226948 ^b	- 284.8 ^b	- 133.3 ^b	- 216.7 ^b
MeNO ₂	- 139.492280	—	—	—	—	—
(N ₃) ⁻	148.967813	- 16.976705	148.967813	- 288.5	- 122.5	- 288.5

^a Values referenced to MeNO₂. ^b Average value of the six ¹⁴N nuclei. Due to symmetry limitations in Turbomole's NMR-shielding module all molecules were calculated in C₁ symmetry.

6. Calculated Vibrational Spectra of $[\text{Si}(\text{N}_3)_6]^{2-}$ (BP86/DZP, effective core potential of Si: Stuttgart RLC ECP).⁹

Observed frequencies ^a [cm ⁻¹]	Unscaled calcd. harmonic frequencies [cm ⁻¹], symmetry, assignment	Rel. Intensities [%]	Raman polarization ratios
<u>Raman spectrum</u>			
2142 (p, w) ^{b,c}	2217, A _g , ν _{as} (NN)	27	p, 0.0415 ^b
2104 (dp, vw, br)	2182, E _g , ν _{as} (NN)	20	dp, 0.7500
2077 – 2080 (p, vw, sh)	1370, A _g , ν _{sym} (NN)	100 ^d	p, 0.0067
1329 (p, m)	1359, E _g , ν _{sym} (NN)	41	dp, 0.7499
1316 (dp, w, sh)	663, E _g , δ(NNN) ^e	1	dp, 0.7367
703 (p, s)	658, A _g , δ(NNN) ^e	6	p, 0.0083
— ^g	596, A _g , δ(NNN) ^f	1	dp, 0.7463
— ^g	589, E _g , δ(NNN) ^f	1	dp, 0.7494
440 (p, vs)	405, A _g , ν _{sym} (SiN)	16	p, 0.0232
— ^h	345, E _g , δ(SiNN) ^e	11	dp, 0.7499
— ^h	306, A _g , δ(SiNN) ^f	3	dp, 0.7239
— ^h	252, E _g , δ(SiNN)	3	dp, 0.7599
<u>IR spectrum</u>			
2109 (vs) ^{a,i}	2190, E _u , ν _{as} (NN)	100 ^j	—
	2186, A _u , ν _{as} (NN)	67	—
1316 (m) ⁱ	1366, E _u , ν _{sym} (NN)	7	—
	1363, A _u , ν _{sym} (NN)	6	—
694 (w) ⁱ	682, E _u , δ(NNN) ^e	11	—
	671, A _u , δ(NNN) ^e	5	—
— ^g	593, A _u , δ(NNN) ^f	4	—
— ^g	591, E _u , δ(NNN) ^f	1	—
— ^h	521, E _u , ν _{as} (SiN)	23	—

^a Solution of **1** in MeCN. ^b p = polarized, dp = depolarized. ^c vs = very strong, s = strong, m = medium, w = weak, vw = very weak, sh = shoulder, br = broad. ^d Corresponds to 141.6 Å⁴ (a.u.)⁻¹.

^e In plane. ^f Out of plane. ^g Not observed. ^h The expected absorption band of $[\text{Si}(\text{N}_3)_6]^{2-}$, the position of which was estimated by calibration of the corresponding calculated frequency, is obscured by absorption bands of the solvent or the PPN cation. ⁱ Solution of $[\text{Na}(\text{MeCN})_n]_2[\text{Si}(\text{N}_3)_6]$ in MeCN. ^j Corresponds to 1580.5 km mol⁻¹.

(9) Bergner, A.; Dolg, M.; Kuechle, W.; Stoll, H.; Preuss, H. *Mol. Phys.* **1993**, *80*, 1431.

6. Isocharge plot of the calculated and experimental electron density.

Isocharge plot of the calculated (left) and experimental (right) electron density (f_o -map) in the $N_\gamma-N_\beta-N_\alpha-Si-N_\alpha'-N_\beta'-N_\gamma'$ surface. The calculated position of an atom center is depicted by a cross. The outermost contour (0.0316 a.u.) of the isocharge plot corresponds roughly to the empirical van der Waals radius. The contour interval amounts 0.05 a. u., the maximum number of contours is 10.

7. Basis set specification.

basis sets^{10,11}

SVP

Si:	(10s7p1d) / [4s3p1d]	{5311/511/1}
N:	(7s4p1d) / [3s2p1d]	{511/31/1}

DZP

Si:	(11s7p1d) / [6s4p1d]	{521111/4111/1}
N:	(8s4p1d) / [4s2p1d]	{5111/31/1}
O:	(8s4p1d) / [4s2p1d]	{5111/31/1}
C:	(8s4p1d) / [4s2p1d]	{5111/31/1}

TZVP

Si:	(14s9p1d) / [5s4p1d]	{73211/6111/1}
N:	(11s6p1d) / [5s3p1d]	{62111/411/1}

TZVPP

Si:	(14s9p2d1f) / [5s5p2d1f]	{73211/51111/11/1}
N:	(11s6p2d1f) / [5s3p2d1f]	{62111/411/11/1}
C:	(11s6p2d1f) / [5s3p2d1f]	{62111/411/11/1}
H:	(5s2p1d) / [3s2p1d]	{311/11/1}

(10) R. Ahlrichs basis sets, SV – split valence, DZ – double zeta valence, TZV – triple zeta valence, P – polarization function.

(11) Schäfer, A.; Horn, H.; Ahlrichs, R. *J. Chem. Phys.* **1992**, 97, 2571.

UCTZVPP¹²

Si:	(14s9p2d1f) / [14s9p2d1f]	{11111111111111/11111111/11/1}
N:	(11s6p2d1f) / [11s6p2d1f]	{1111111111/111111/11/1}
O:	(11s6p2d1f) / [11s6p2d1f]	{1111111111/111111/11/1}
C:	(11s6p2d1f) / [11s6p2d1f]	{1111111111/111111/11/1}
H:	(5s2p1d) / [5s2p1d]	{11111/11/1}
F:	(11s6p2d1f) / [11s6p2d1f]	{1111111111/111111/11/1}

auxiliary basis sets for resolution of identity method

SVP

Si:	(10s7p7d3f) / [8s5p5d2f]	{31111111/31111/31111/12}
N:	(8s6p5d3f) / [6s5p4d1f]	{311111/21111/2111/3}

DZP

Si:	(12s6p5d1f1g) / [5s3p2d1f1g]	{81111/411/41/1/1}
N:	(9s3p3d1f) / [7s3p3d1f]	{3111111/111/111/1}

TZVP

Si:	(10s7p7d3f) / [9s7p6d2f]	{211111111/1111111/211111/12}
N:	(8s6p5d3f) / [7s6p4d1f]	{2111111/111111/2111/3}

TZVPP

Si:	(12s6p5d1f1g) / [5s3p2d1f1g]	{81111/411/41/1/1}
N:	(9s3p3d1f) / [7s3p3d1f]	{3111111/111/111/1}.

(12) Made by decontraction of the CGTO's from a TZVPP-basis set.

8. Cartesian Coordinates

$\text{Si}(\text{N}_3)_6^{2-}$ (B3LYP, TZVPP)

SI	0.0000000	0.0000000	0.0000000
N	-1.5484122	0.1192441	1.0874190
N	-2.0250887	1.1104592	1.5547521
N	-2.5401318	2.0127705	2.0385161
N	0.8774745	1.2813423	1.0874190
N	1.9742302	1.1985486	1.5547521
N	3.0131762	1.1934334	2.0385161
N	0.6709377	-1.4005864	1.0874190
N	0.0508584	-2.3090079	1.5547521
N	-0.4730445	-3.2062039	2.0385161
N	-0.8774745	-1.2813423	-1.0874190
N	-1.9742302	-1.1985486	-1.5547521
N	-3.0131762	-1.1934334	-2.0385161
N	-0.6709377	1.4005864	-1.0874190
N	-0.0508584	2.3090079	-1.5547521
N	0.4730445	3.2062039	-2.0385161
N	1.5484122	-0.1192441	-1.0874190
N	2.0250887	-1.1104592	-1.5547521
N	2.5401318	-2.0127705	-2.0385161

$\text{Si}(\text{N}_3)_6^{2-}$ (RI-MP2, TZVP)

SI	0.0000000	0.0000000	0.0000000
N	-1.5220534	0.1283670	1.0896435
N	-2.0981817	1.1456987	1.3888540
N	-2.7165774	2.0797028	1.7408879
N	0.8721958	1.2539534	1.0896435
N	2.0412951	1.2442293	1.3888540
N	3.1593642	1.3127736	1.7408879
N	0.6498576	-1.3823205	1.0896435
N	0.0568867	-2.3899280	1.3888540
N	-0.4427868	-3.3924765	1.7408879
N	-0.8721958	-1.2539534	-1.0896435
N	-2.0412951	-1.2442293	-1.3888540
N	-3.1593642	-1.3127736	-1.7408879
N	-0.6498576	1.3823205	-1.0896435
N	-0.0568867	2.3899280	-1.3888540
N	0.4427868	3.3924765	-1.7408879
N	1.5220534	-0.1283670	-1.0896435
N	2.0981817	-1.1456987	-1.3888540
N	2.7165774	-2.0797028	-1.7408879

$\text{Si}(\text{N}_3)_6^{2-}$ (HF, TZVPP)

SI	0.0000000	0.0000000	0.0000000
N	-1.5442491	0.0934143	1.0835322
N	-2.0040031	1.0943697	1.5024792
N	-2.4829988	1.9985974	1.9265086
N	0.8530237	1.2906518	1.0835322
N	1.9497535	1.1883327	1.5024792
N	2.9723355	1.1510413	1.9265086
N	0.6912254	-1.3840661	1.0835322
N	0.0542496	-2.2827024	1.5024792
N	-0.4893368	-3.1496387	1.9265086
N	-0.8530237	-1.2906518	-1.0835322
N	-1.9497535	-1.1883327	-1.5024792
N	-2.9723355	-1.1510413	-1.9265086
N	-0.6912254	1.3840661	-1.0835322
N	-0.0542496	2.2827024	-1.5024792
N	0.4893368	3.1496387	-1.9265086
N	1.5442491	-0.0934143	-1.0835322
N	2.0040031	-1.0943697	-1.5024792
N	2.4829988	-1.9985974	-1.9265086

$\text{Si}(\text{N}_3)_6^{2-}$ (BP86, TZVPP)

SI	0.0000000	0.0000000	0.0000000
N	-1.5546412	0.1094243	1.0894864
N	-2.0329192	1.1011087	1.5794045
N	-2.5602830	2.0006805	2.0904457
N	0.8720848	1.2916466	1.0894864
N	1.9700477	1.2100054	1.5794045
N	3.0127817	1.2169298	2.0904457
N	0.6825563	-1.4010709	1.0894864
N	0.0628715	-2.3111140	1.5794045
N	-0.4524987	-3.2176104	2.0904457
N	-0.8720848	-1.2916466	-1.0894864
N	-1.9700477	-1.2100054	-1.5794045
N	-3.0127817	-1.2169298	-2.0904457
N	-0.6825563	1.4010709	-1.0894864
N	-0.0628715	2.3111140	-1.5794045
N	0.4524987	3.2176104	-2.0904457
N	1.5546412	-0.1094243	-1.0894864
N	2.0329192	-1.1011087	-1.5794045
N	2.5602830	-2.0006805	-2.0904457

$\text{Si}(\text{ox})_3^{2-}$ (BP86, UCTZVPP)

Si	-0.0051891	-0.0050067	-0.0015418
O	-1.7048623	-0.5947457	0.2284215
O	-0.1370249	0.9674658	1.5241796
O	1.7263391	0.4663297	-0.2626701
O	0.0136630	-0.9310622	-1.5605420
C	-1.0995570	-1.5802433	-1.8485723
C	-2.1744036	-1.3624056	-0.7374365
C	2.6207766	-0.3275258	0.2965708
O	-0.5422770	1.4799979	-0.8928155
O	0.6123868	-1.4166800	0.9540446
C	-0.7866338	2.5365841	-0.1397399
C	1.9262082	-1.5062742	1.0488500
C	-0.5231471	2.2202133	1.3662897
O	-3.2968789	-1.8463078	-0.7767515
O	-1.2824919	-2.2660850	-2.8442554
O	-1.1696813	3.6240686	-0.5469864
O	-0.6604000	3.0383914	2.2645294
O	3.8332275	-0.1766476	0.2454691
O	2.5356299	-2.3865019	1.6396653

SiF_6^{2-} (BP86, UCTZVPP)

Si	0.0000004	0.0000004	0.0000003
F	-0.0000001	1.7455988	-0.0000001
F	-0.0000001	-1.7455987	-0.0000001
F	-0.0000001	-0.0000001	1.7455977
F	-0.0000001	-0.0000001	-1.7455976
F	1.7455988	-0.0000001	-0.0000001
F	-1.7455987	-0.0000001	-0.0000001

TMS (BP86, UCTZVPP)¹³

Si	-0.0000117	-0.0001129	0.0003354
C	-1.2762166	-1.1851058	-0.7472552
H	-0.8332662	-2.1690035	-0.9578544
H	-1.6784767	-0.7928820	-1.6921068
H	-2.1232683	-1.3409821	-0.0641641
C	-0.8165746	1.6762662	0.3398941
H	-1.6553213	1.5779296	1.0438888
H	-0.0992890	2.3872263	0.7743501
H	-1.2094601	2.1234275	-0.5843498
C	1.4345820	0.2320111	-1.2162138
H	2.1950271	0.9152479	-0.8118900
H	1.9300046	-0.7246524	-1.4352815
H	1.0841195	0.6508915	-2.1702096
C	0.6581105	-0.7230793	1.6240051
H	1.4029959	-0.0579390	2.0838602
H	-0.1519966	-0.8701825	2.3524308
H	1.1389966	-1.6982111	1.4609562

Si(brenzcat)₃²⁻ (BP86, UCTZVPP)

Si	-0.0058697	0.0019642	-0.0001518
O	1.5651235	0.9227849	0.1755971
O	-0.7911474	1.3321583	0.9795733
C	1.4155559	2.0433444	0.8806458
C	0.0792185	2.2755578	1.3364020
C	-0.2139863	3.4182735	2.0868770
C	0.8151118	4.3399994	2.3940276
C	2.1234569	4.1118284	1.9494358
C	2.4275314	2.9577476	1.1886746
H	-1.2481339	3.5815138	2.4282632
H	0.5807331	5.2402048	2.9865153
H	2.9234361	4.8317953	2.1906392
H	3.4506372	2.7624870	0.8310155
O	-1.6431333	-0.7842937	-0.2142558
O	-0.2963816	0.8343355	-1.6030493
C	-2.2352608	-0.4144166	-1.3486706
C	-1.4712492	0.5038495	-2.1364086
C	-1.9798522	0.9730128	-3.3516143
C	-3.2494354	0.5342555	-3.7979860
C	-3.9964350	-0.3659092	-3.0278976
C	-3.4883627	-0.8443544	-1.7963723
H	-1.3787304	1.6802086	-3.9443217
H	-3.6474437	0.9056471	-4.7571476
H	-4.9853611	-0.7062159	-3.3779981
H	-4.0621979	-1.5523237	-1.1780676
O	0.2409198	-0.9618133	1.5354532
O	0.8908790	-1.3309737	-0.8738997
C	0.9101667	-2.0930003	1.3176853
C	1.2589088	-3.0377906	2.2877832
C	1.9736530	-4.2000728	1.9114043
C	2.3319418	-4.4063363	0.5732942
C	1.9832498	-3.4538457	-0.4138364
C	1.2782764	-2.3026509	-0.0491150
H	0.9692621	-2.8594917	3.3352404
H	2.2471099	-4.9436132	2.6787218
H	2.8888627	-5.3127410	0.2824907
H	2.2568917	-3.5995578	-1.4705301.

(13) TMS = SiMe₄.

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