Thomas Henneberger, Wilhelm Klein and Thomas F. Fässler* **Crystal structure of [(1,2-\eta)-1,2,3,4,5-pentamethyl-cyclopenta-2,4-dien-1yl] (1,4,10,13-tetraoxa-7,16-diazacyclooctadecane-\kappa^6 N_2,O_4) rubidium (I), [Rb(diaza-18-crown-6)]Cp*, C₂₂H₄₁N₂O₄Rb**



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Abstract

C₂₂H₄₁N₂O₄Rb, monoclinic, P_{21}/n (no. 14), a = 10.8160(9) Å, b = 17.7253(16) Å, c = 13.2179(12) Å, $\beta = 93.961(8)^{\circ}$, V = 2528.0(4) Å³, Z = 4, $R_{gt}(F) = 0.0376$, $wR_{ref}(F^2) = 0.0694$, T = 120(2) K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The Zintl phase $Rb_{12}Si_{17}$ [5] was prepared from stoichiometric mixtures of the elements in sealed tantalum containers, which were encapsulated in an evacuated fused Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	$0.20\times0.15\times0.15~\text{mm}$
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	1.99 mm ⁻¹
Diffractometer, scan mode:	Oxford Xcalibur 3, ω and π
θ_{\max} , completeness:	26.0°, >99%
N(hkl) _{measured} , N(hkl) _{unique} , R _{int} :	26792, 4963, 0.100
Criterion for I _{obs} , N(hkl) _{gt} :	$I_{\rm obs} > 2 \; \sigma(I_{\rm obs})$, 2435
N(param) _{refined} :	272
Programs:	CrysAlis [1], SHELX [2, 3],
	Diamond [4]

silica tube. The mixture was heated to 800 °C for 15 h and slowly cooled to room temperature with a rate of 0.5 °C/min. Bis(pentamethylcyclopentadienyl)zinc (ZnCp*₂) was prepared as described in literature [6]. 113 mg Rb₁₂Si₁₇, 35 mg 1,4,10,13-tetraoxa-7,16-diazacyclooctadecane (diaza-18-crown-6; Merck, p. a.), and 25 mg Zn₂Cp*₂ were placed in into a dry Schlenk vessel and *ca* 2 mL NH₃ (Westfalen, 99.999%, stored over elemental Na) were condensed on this. The obtained light yellow solution was stored at -70 °C for 11 months, after this time yellow crystals of the title compound were found. An appropriate crystal was selected under perfluoroalkylether in a stream of cold nitrogen gas.

Experimental details

The methylene and methyl H atoms have been refined using a riding model with U_{iso} set to 1.2 and 1.5 $U_{eq}(C)$, respectively. The H atoms bound to N Atoms have been located from the difference Fourier map and refined with free atomic coordinates and an U_{iso} of 1.2 $U_{eq}(N)$ [3].

Comment

During our investigations of the behaviour and reactivity of Si containing Zintl compounds in solution with the goal to synthesize transition metal complexes with Si clusters as ligands analogously to the known Ge compounds [7], liquid ammonia has been found to be a highly suitable solvent [8, 9]. For supporting the dissolution of the solid Zintl compounds often sequestering agents like crown ethers or cryptands are necessary. In the present experiment, diaza-18-crown-6 has been used to dissolve Rb₁₂Si₁₇ in liquid ammonia in presence

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Rb 0.44660(3) 0.33795(2) 0.34703(3) 0.03586(11) 01 0.7034(2) 0.30542(13) 0.30666(16) 0.0386(6) C1 0.7869(3) 0.3673(2) 0.3013(3) 0.0477(11) H1A 0.8607 0.3515 0.2664 0.057* C2 0.7224(3) 0.4307(2) 0.2443(3) 0.0465(11) H2A 0.7828 0.4707 0.2304 0.056* O2 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3B 0.6159 0.5573 0.2262 0.064* H3B 0.6159 0.5573 0.2262 0.064* N1 0.3790(3) 0.4984(17) 0.3511(1) 0.40430(9) H4B 0.4288 0.5971 0.2870 0.064* N1 0.37906 0.5347 0.4954 0.070* H5A 0.2661 0.5799 0.4185 0.070* H5A 0.2	Atom	X	у	Z	U _{iso} */U _{eq}
01 0.7034(2) 0.30542(13) 0.30666(16) 0.0386(6) C1 0.7869(3) 0.3673(2) 0.3013(3) 0.0477(11) HA 0.8607 0.3515 0.2664 0.057* C2 0.7224(3) 0.4307(2) 0.2443(3) 0.0465(11) H2A 0.7828 0.4707 0.2304 0.056* O2 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3A 0.5114 0.4968 0.1906 0.064* H3B 0.6159 0.5573 0.2262 0.064* H4B 0.4288 0.5971 0.2870 0.064* H4B 0.4288 0.5971 0.2870 0.064* N1 0.3790(3) 0.4984(17) 0.311(2) 0.0430(9) H4B 0.4288 0.5971 0.2870 0.064* N1 0.37906 0.5347 0.4984 0.070* H5B 0.3706 <t< td=""><td>Rb</td><td>0.44660(3)</td><td>0.33795(2)</td><td>0.34703(3)</td><td>0.03586(11)</td></t<>	Rb	0.44660(3)	0.33795(2)	0.34703(3)	0.03586(11)
C1 0.7869(3) 0.3673(2) 0.3013(3) 0.0477(11) H1A 0.8607 0.3515 0.2664 0.057* C2 0.7224(3) 0.4307(2) 0.2443(3) 0.0465(11) H2A 0.7828 0.4707 0.2304 0.056* H2B 0.6847 0.4121 0.1786 0.056* O2 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5514(0.5184(2) 0.2503(3) 0.0531(12) H3B 0.6159 0.5573 0.2262 0.064* H4A 0.5196 0.5727 0.3823 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5234(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.0576(12) H6A 0.172	01	0.7034(2)	0.30542(13)	0.30666(16)	0.0386(6)
H1A 0.8607 0.3515 0.2664 0.057* H1B 0.8147 0.3841 0.3706 0.057* C2 0.7224(3) 0.4307(2) 0.2443(3) 0.0465(1) H2A 0.7828 0.4707 0.2304 0.056* H2B 0.6887 0.4121 0.1786 0.0505* O2 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) G3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3A 0.5114 0.4968 0.1906 0.064* H4B 0.4288 0.5971 0.2870 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5790 0.4185 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.057* H5B 0.3706	C1	0.7869(3)	0.3673(2)	0.3013(3)	0.0477(11)
H1B 0.8147 0.3841 0.3706 0.057* C2 0.7224(3) 0.4307(2) 0.2443(3) 0.0465(1) H2A 0.7828 0.4707 0.2304 0.056* H2B 0.6847 0.4121 0.1786 0.0557 O2 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3B 0.6159 0.5573 0.2262 0.064* H3B 0.6159 0.5727 0.3823 0.064* H4A 0.5196 0.5727 0.3823 0.064* N1 0.3790(3) 0.4984(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5234(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.579 0.4185 0.070* C6 0.2197(4) 0.4863 0.5239 0.069* H3B 0.6203 0.43	H1A	0.8607	0.3515	0.2664	0.057*
C2 0.7224(3) 0.4307(2) 0.243(3) 0.0465(11) H2A 0.7828 0.4707 0.2304 0.056* H2B 0.6847 0.4121 0.1786 0.056* O2 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5573 0.2262 0.064* H3B 0.6159 0.5573 0.2262 0.064* H4 0.5196 0.5727 0.3823 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.0576(12) H6A 0.1724 0.4863 0.5239 0.069* H6B 0.1603 0.4382 0.57* 0.3042(2) 0.5397(2) 0.0475(10)	H1B	0.8147	0.3841	0.3706	0.057*
H2A 0.7828 0.4707 0.2304 0.056* H2B 0.6847 0.4121 0.1786 0.055* 02 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3A 0.5114 0.4968 0.1906 0.064* H3B 0.6159 0.5573 0.2262 0.064* H4A 0.5196 0.5727 0.3823 0.066* H4B 0.4293(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4685(3) 0.070* H5B 0.3706 0.5347 0.4954 0.070* H5B 0.3706 0.5347 0.4954 0.070* H6A 0.1724 0.4863 0.5239 0.669* O3 0.2834(2) 0.3942(2) 0.539(2) 0.0475(10) H7A 0.1413 0.3280<	C2	0.7224(3)	0.4307(2)	0.2443(3)	0.0465(11)
H2B 0.6847 0.4121 0.1786 0.056* 02 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3A 0.6159 0.5573 0.2262 0.064* C4 0.4717(4) 0.5537(2) 0.3211(3) 0.0531(11) H4A 0.5196 0.5727 0.3823 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.057(12) H5A 0.2661 0.5799 0.4185 0.070* C6 0.2197(4) 0.4863 0.5239 0.069* H6B 0.1603 0.4538 0.4105 0.057* C8 0.2770(3) 0.3783(2) 0.5783(3) 0.0445(10) H7B 0.1572 0.3661 0.5954 0.057* C8 0.2770(3)	H2A	0.7828	0.4707	0.2304	0.056*
02 0.6287(2) 0.46052(12) 0.30345(16) 0.0404(6) C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3A 0.6119 0.5573 0.2262 0.064* H3B 0.6159 0.5573 0.2262 0.064* H4A 0.5196 0.5727 0.3823 0.064* H4B 0.4288 0.5971 0.2870 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.0576(12) H6A 0.1724 0.4863 0.5239 0.069* 03 0.2834(2) 0.3992(3) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3478(2) 0.5783(3) 0.04475(10) H7B 0	H2B	0.6847	0.4121	0.1786	0.056*
C3 0.5591(4) 0.5184(2) 0.2503(3) 0.0531(12) H3A 0.5114 0.4968 0.1906 0.064* H3B 0.6159 0.5573 0.2262 0.064* C4 0.4717(4) 0.5537(2) 0.3211(3) 0.0531(11) H4A 0.5196 0.5727 0.3823 0.064* H4B 0.4288 0.5971 0.2870 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* H5B 0.3706 0.5347 0.4954 0.070* H6A 0.1724 0.4863 0.5239 0.669* O3 0.2834(2) 0.3922(13) 0.50214(17) 0.046(6) C7 0.2026(3) 0.2783(2) 0.5783(3) 0.0475(10) H7B 0.1572	02	0.6287(2)	0.46052(12)	0.30345(16)	0.0404(6)
H3A 0.5114 0.4968 0.1906 0.064* H3B 0.6159 0.5573 0.2262 0.064* H4A 0.5196 0.5727 0.3823 0.064* H4B 0.4288 0.5971 0.2870 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4185 0.070* H5B 0.3706 0.5347 0.4954 0.070* C6 0.2197(4) 0.4683 0.5239 0.069* H6B 0.1603 0.4538 0.4105 0.069* G3 0.2834(2) 0.39923(13) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3442(2) 0.5399(2) 0.0475(10) H7A 0.1413 0.3283 0.6302 0.057* C8 0.2770(3) 0.2783(2) 0.5783(3) 0.0445(10) H8A 0.3341 0.2953 </td <td>С3</td> <td>0.5591(4)</td> <td>0.5184(2)</td> <td>0.2503(3)</td> <td>0.0531(12)</td>	С3	0.5591(4)	0.5184(2)	0.2503(3)	0.0531(12)
H3B 0.6159 0.5573 0.2262 0.064* C4 0.4717(4) 0.5537(2) 0.3211(3) 0.0531(11) H4A 0.5196 0.5727 0.3823 0.064* H4B 0.4288 0.5971 0.2870 0.064* N1 0.329(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.49852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* C6 0.2197(4) 0.44652 0.4685(3) 0.0576(12) H6B 0.1603 0.4538 0.4105 0.069* O3 0.2834(2) 0.39923(13) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3442(2) 0.5399(2) 0.0475(10) H7A 0.1413 0.3280 0.4852 0.057* C8 0.2770(3) 0.2783(2) 0.5783(3) 0.0445(10) M8 0.2225	H3A	0.5114	0.4968	0.1906	0.064*
C4 0.4717(4) 0.5537(2) 0.3211(3) 0.0531(11) H4A 0.5196 0.5727 0.3823 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.0576(12) H6A 0.1724 0.4863 0.5239 0.069* 03 0.2834(2) 0.39923(13) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3442(2) 0.5399(2) 0.0475(10) H7B 0.1572 0.3661 0.5954 0.057* C8 0.2770(3) 0.2783(2) 0.5783(3) 0.0445(10) H8A 0.3414 0.2953 0.6302 0.053* O4 0.3341(2) 0.24242(13) 0.49762(16) 0.0392(6) C9	H3B	0.6159	0.5573	0.2262	0.064*
H4A0.51960.57270.38230.064*H4B0.42880.59710.28700.0064*N10.379030.49846(17)0.3511(2)0.0430(9)H10.329(3)0.4852(19)0.295(2)0.052*C50.3108(4)0.5236(2)0.4372(3)0.0581(12)H5A0.26610.57090.41850.070*C60.2197(4)0.4658(2)0.4685(3)0.0576(12)H6A0.17240.48630.52390.069*H6B0.16030.45380.41050.069*O30.2834(2)0.39923(13)0.50214(17)0.0406(6)C70.2026(3)0.3442(2)0.5399(2)0.0475(10)H7A0.14130.32800.48520.057*C80.2770(3)0.2783(2)0.5783(3)0.0445(10)H8A0.34140.29530.63020.053*H8B0.22250.24190.61060.0392(6)C90.3971(3)0.1748(2)0.5307(3)0.0437(10)H9A0.33590.13470.54230.052*H9B0.44630.18430.59540.052*H0B0.43360.14650.38430.049*H10A0.51490.09910.46810.049*H10B0.43360.14650.38430.049*H10B0.43360.14650.38430.049*H10B0.436(3)0.1901(18)0.500(2)0.044*C110.6684(3)0.18081(19)0.3656(3	C4	0.4717(4)	0.5537(2)	0.3211(3)	0.0531(11)
H4B 0.4288 0.5971 0.2870 0.064* N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.0576(12) H6A 0.1724 0.4863 0.5239 0.069* G3 0.2834(2) 0.39923(13) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3442(2) 0.5399(2) 0.0475(10) H7A 0.1413 0.3280 0.4852 0.057* K8 0.2770(3) 0.2783(2) 0.5783(3) 0.0445(10) H8A 0.3414 0.2953 0.6302 0.053* H8B 0.2225 0.2419 0.6106 0.0392(6) C9 0.3971(3) 0.1748(2) 0.5307(3) 0.04411(9) H9A	H4A	0.5196	0.5727	0.3823	0.064*
N1 0.3790(3) 0.49846(17) 0.3511(2) 0.0430(9) H1 0.329(3) 0.4852(19) 0.295(2) 0.052* C5 0.3108(4) 0.5236(2) 0.4372(3) 0.0581(12) H5A 0.2661 0.5709 0.4185 0.070* H5B 0.3706 0.5347 0.4954 0.070* C6 0.2197(4) 0.4658(2) 0.4685(3) 0.0576(12) H6A 0.1724 0.4863 0.5239 0.069* H6B 0.1603 0.4538 0.4105 0.069* O3 0.2834(2) 0.39923(13) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3442(2) 0.5399(2) 0.0475(10) H7A 0.1413 0.3280 0.4852 0.057* C8 0.2770(3) 0.2783(2) 0.5783(3) 0.0445(10) H8A 0.3414 0.2953 0.6302 0.052* C4 0.3341(2) 0.24242(13) 0.49762(16) 0.0392(6) C9 0	H4B	0.4288	0.5971	0.2870	0.064*
H1 $0.329(3)$ $0.4852(19)$ $0.295(2)$ $0.052*$ C5 $0.3108(4)$ $0.5236(2)$ $0.4372(3)$ $0.0581(12)$ H5A 0.2661 0.5709 0.4185 $0.070*$ H5B 0.3706 0.5347 0.4954 $0.070*$ C6 $0.2197(4)$ $0.4658(2)$ $0.4685(3)$ $0.0576(12)$ H6A 0.1724 0.4863 0.5239 $0.069*$ H6B 0.1603 0.4538 0.4105 $0.0406(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 $0.057*$ C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 $0.053*$ O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 $0.052*$ H9B 0.4463 0.1843 0.5954 $0.052*$ C10 $0.4814(3)$ $0.14978(19)$ 0.4681 $0.049*$ H10B 0.4336 0.1465 0.3843 $0.049*$ H11A 0.6215 $0.278(19)$ $0.3656(3)$ <	N1	0.3790(3)	0.49846(17)	0.3511(2)	0.0430(9)
C5 $0.3108(4)$ $0.5236(2)$ $0.4372(3)$ $0.0581(12)$ H5A 0.2661 0.5709 0.4185 $0.070*$ C6 $0.2197(4)$ $0.4658(2)$ $0.4685(3)$ $0.0576(12)$ H6A 0.1724 0.4863 0.5239 $0.069*$ O3 $0.2834(2)$ $0.39923(13)$ $0.50214(17)$ $0.0406(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 $0.057*$ K8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 $0.053*$ 04 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 $0.052*$ C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 $0.049*$ H2 $0.625(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.044*$ H11B 0.7109 0.1333 0.3896 $0.048*$ C11 $0.6684(3)$ 0.2272 0.4239 $0.049*$ H12B 0.8004 0.2572 0.4239 $0.049*$ H12B $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0366(9)$ C11<	H1	0.329(3)	0.4852(19)	0.295(2)	0.052*
H5A 0.2661 0.5709 0.4185 0.070^* H5B 0.3706 0.5347 0.4954 0.070^* C6 $0.2197(4)$ $0.4658(2)$ $0.4685(3)$ $0.0576(12)$ H6A 0.1724 0.4863 0.5239 0.069^* H6B 0.1603 0.4538 0.4105 0.069^* O3 $0.2834(2)$ $0.39923(13)$ $0.50214(17)$ $0.0406(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 0.057^* K8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 0.053^* O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* L1 $0.6684(3)$ 0.2272 0.4239 $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C11 $0.6684(3)$ 0.2272 0.4239 0.049^* L12 $0.761(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 0.049^* L13 $0.3113(3)$ <td< td=""><td>C5</td><td>0.3108(4)</td><td>0.5236(2)</td><td>0.4372(3)</td><td>0.0581(12)</td></td<>	C5	0.3108(4)	0.5236(2)	0.4372(3)	0.0581(12)
H5B 0.3706 0.5347 0.4954 0.070^* C6 $0.2197(4)$ $0.4658(2)$ $0.4685(3)$ $0.0576(12)$ H6A 0.1724 0.4863 0.5239 0.069^* O3 $0.2834(2)$ $0.39923(13)$ $0.50214(17)$ $0.04466(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 0.057^* H7B 0.1572 0.3661 0.5954 0.057^* C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 0.053^* H8B 0.2225 0.2419 0.6106 $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10B 0.4336 0.1465 0.3843 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.0411(9)$ H11A 0.6215 0.1718 0.3026 0.048^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12B	H5A	0.2661	0.5709	0.4185	0.070*
C6 $0.2197(4)$ $0.4658(2)$ $0.4685(3)$ $0.0576(12)$ H6A 0.1724 0.4863 0.5239 $0.069*$ O3 $0.2834(2)$ $0.39923(13)$ $0.50214(17)$ $0.0406(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 $0.057*$ H7B 0.1572 0.3661 0.5954 $0.057*$ C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 $0.053*$ O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 $0.052*$ C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10B 0.4336 0.1465 0.3843 $0.049*$ H10B 0.4336 0.1465 0.3843 $0.049*$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.0412(10)$ H11A 0.6215 0.1718 0.3026 $0.048*$ C12 $0.7631(3)$ $0.2425(2)$ $0.3565(3)$ $0.0412(10)$ H12B 0.8301 0.2229 0.3159 $0.049*$ H12B 0.8301 0.2229 0.3159 $0.049*$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0366(9)$ C14 $0.3567(3)$ 0.27129 $0.1439(3)$ $0.0366(9)$ C15 $0.$	H5B	0.3706	0.5347	0.4954	0.070*
H6A 0.1724 0.4863 0.5239 0.069^* H6B 0.1603 0.4538 0.4105 0.069^* O3 $0.2834(2)$ $0.39923(13)$ $0.50214(17)$ $0.0406(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 0.057^* H7B 0.1572 0.3661 0.5954 0.057^* C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 0.053^* O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ 0.044^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C12 $0.7631(3)$ $0.29258(19)$ $0.1439(3)$ $0.0366(9)$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0364(9)$ C14 $0.3567(3)$ $0.2728(19)$ $0.1439(3)$ $0.0366(9)$ <td>C6</td> <td>0.2197(4)</td> <td>0.4658(2)</td> <td>0.4685(3)</td> <td>0.0576(12)</td>	C6	0.2197(4)	0.4658(2)	0.4685(3)	0.0576(12)
H6B 0.1603 0.4538 0.4105 0.069^* O3 $0.2834(2)$ $0.39923(13)$ $0.50214(17)$ $0.0406(6)$ C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 0.057^* H7B 0.1572 0.3661 0.5954 0.057^* C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 0.053^* O4 $0.3341(2)$ $0.224242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.042(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C12 $0.7631(3)$ $0.29258(19)$ $0.1439(3)$ $0.0366(9)$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0366(9)$ C14 $0.3567(3)$ $0.21497(19)$ $0.155(3)$ $0.0477(10)$ <td>H6A</td> <td>0.1724</td> <td>0.4863</td> <td>0.5239</td> <td>0.069*</td>	H6A	0.1724	0.4863	0.5239	0.069*
03 0.2834(2) 0.39923(13) 0.50214(17) 0.0406(6) C7 0.2026(3) 0.3442(2) 0.5399(2) 0.0475(10) H7A 0.1413 0.3280 0.4852 0.057* H7B 0.1572 0.3661 0.5954 0.057* C8 0.2770(3) 0.2783(2) 0.5783(3) 0.0445(10) H8A 0.3414 0.2953 0.6302 0.053* H8B 0.2225 0.2419 0.6106 0.0392(6) C9 0.3971(3) 0.1748(2) 0.5307(3) 0.0437(10) H9A 0.3359 0.1347 0.5423 0.052* C10 0.4814(3) 0.14978(19) 0.4509(2) 0.0411(9) H10A 0.5149 0.0991 0.4681 0.049* H10B 0.4336 0.1465 0.3843 0.049* N2 0.5828(3) 0.2010(18) 0.500(2) 0.044* C11 0.6684(3) 0.18081(19) 0.3684(2) 0.0402(10) H11A 0.62	H6B	0.1603	0.4538	0.4105	0.069*
C7 $0.2026(3)$ $0.3442(2)$ $0.5399(2)$ $0.0475(10)$ H7A 0.1413 0.3280 0.4852 $0.057*$ H7B 0.1572 0.3661 0.5954 $0.057*$ C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 $0.053*$ H8B 0.2225 0.2419 0.6106 $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 $0.052*$ H9B 0.4463 0.1843 0.5954 $0.052*$ C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 $0.049*$ H10B 0.4336 0.1465 0.3843 $0.049*$ N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.044*$ C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 $0.048*$ C12 $0.7631(3)$ $0.2249(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2272 0.4239 $0.049*$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.21497(19)$ $0.1515(3)$ $0.0477(10)$ C15 $0.2813(3)$ $0.21497(19)$ $0.1515(3)$ $0.0477(10)$ C14 <td< td=""><td>03</td><td>0.2834(2)</td><td>0.39923(13)</td><td>0.50214(17)</td><td>0.0406(6)</td></td<>	03	0.2834(2)	0.39923(13)	0.50214(17)	0.0406(6)
H7A 0.1413 0.3280 0.4852 $0.057*$ H7B 0.1572 0.3661 0.5954 $0.057*$ C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 $0.053*$ H8B 0.2225 0.2419 0.6106 $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 $0.052*$ C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 $0.049*$ H10B 0.4336 0.1465 0.3843 $0.049*$ H2 $0.625(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.0442*$ C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 $0.048*$ C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 $0.049*$ H12B 0.8301 0.2229 0.3159 $0.049*$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.31836(19)$ $0.196(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ 0.1963 $0.072*$ H18B 0.3612 0.1921 0.0855 $0.072*$ H18B 0.3612	C7	0.2026(3)	0.3442(2)	0.5399(2)	0.0475(10)
H7B 0.1572 0.3661 0.5954 $0.057*$ C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 $0.053*$ H8B 0.2225 0.2419 0.6106 $0.053*$ O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 $0.052*$ C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 $0.049*$ H10B 0.4336 0.1465 0.3843 $0.049*$ N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.044*$ C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 $0.048*$ C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 $0.049*$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0366(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ 0.1963 $0.072*$ H18B 0.3612 0.1921 0.0855 $0.072*$ H18B <td>H7A</td> <td>0.1413</td> <td>0.3280</td> <td>0.4852</td> <td>0.057*</td>	H7A	0.1413	0.3280	0.4852	0.057*
C8 $0.2770(3)$ $0.2783(2)$ $0.5783(3)$ $0.0445(10)$ H8A 0.3414 0.2953 0.6302 0.053^* H8B 0.2225 0.2419 0.6106 0.053^* O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* H9B 0.4463 0.1843 0.5954 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ 0.044^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 0.049^* C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0354(9)$ C16 $0.1884(3)$ $0.39450(19)$ $0.1681(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ 0.1963 0.072^* <td>H7B</td> <td>0.1572</td> <td>0.3661</td> <td>0.5954</td> <td>0.057*</td>	H7B	0.1572	0.3661	0.5954	0.057*
H8A 0.3414 0.2953 0.6302 0.053^* H8B 0.2225 0.2419 0.6106 0.053^* O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* H9B 0.4463 0.1843 0.5954 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ 0.044^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 0.049^* H12B 0.8301 0.2229 0.3159 0.049^* C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0354(9)$ C16 $0.1884(3)$ $0.39450(19)$ $0.1681(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ 0.1963 0.072^* <tr< td=""><td>C8</td><td>0.2770(3)</td><td>0.2783(2)</td><td>0.5783(3)</td><td>0.0445(10)</td></tr<>	C8	0.2770(3)	0.2783(2)	0.5783(3)	0.0445(10)
H8B 0.2225 0.2419 0.6106 0.053^* O4 $0.3341(2)$ $0.24242(13)$ $0.49762(16)$ $0.0392(6)$ C9 $0.3971(3)$ $0.1748(2)$ $0.5307(3)$ $0.0437(10)$ H9A 0.3359 0.1347 0.5423 0.052^* H9B 0.4463 0.1843 0.5954 0.052^* C10 $0.4814(3)$ $0.14978(19)$ $0.4509(2)$ $0.0411(9)$ H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ 0.044^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 0.049^* H12B 0.8301 0.2229 0.3159 0.049^* C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0354(9)$ C16 $0.1884(3)$ $0.39450(19)$ $0.1681(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ 0.1963 0.072^* H18B 0.3612 0.1921 0.0855 0.072^* <t< td=""><td>H8A</td><td>0.3414</td><td>0.2953</td><td>0.6302</td><td>0.053*</td></t<>	H8A	0.3414	0.2953	0.6302	0.053*
04 0.3341(2) 0.24242(13) 0.49762(16) 0.0392(6) C9 0.3971(3) 0.1748(2) 0.5307(3) 0.0437(10) H9A 0.3359 0.1347 0.5423 0.052* H9B 0.4463 0.1843 0.5954 0.052* C10 0.4814(3) 0.14978(19) 0.4509(2) 0.0411(9) H10A 0.5149 0.0991 0.4681 0.049* H10B 0.4336 0.1465 0.3843 0.049* N2 0.5828(3) 0.20283(17) 0.4444(2) 0.0366(8) H2 0.625(3) 0.2010(18) 0.500(2) 0.044* C11 0.6684(3) 0.18081(19) 0.3684(2) 0.0402(10) H11A 0.6215 0.1718 0.3026 0.044* C12 0.7631(3) 0.2419(2) 0.3565(3) 0.0412(10) H12A 0.8004 0.2572 0.4239 0.049* C12 0.7631(3) 0.2419(2) 0.3565(3) 0.049* C13	H8B	0.2225	0.2419	0.6106	0.053*
C9 0.3971(3) 0.1748(2) 0.5307(3) 0.0437(10) H9A 0.3359 0.1347 0.5423 0.052* H9B 0.4463 0.1843 0.5954 0.052* C10 0.4814(3) 0.14978(19) 0.4509(2) 0.0411(9) H10A 0.5149 0.0991 0.4681 0.049* H10B 0.4336 0.1465 0.3843 0.049* N2 0.5828(3) 0.20283(17) 0.4444(2) 0.0366(8) H2 0.625(3) 0.2010(18) 0.500(2) 0.0402(10) H11A 0.6684(3) 0.18081(19) 0.3684(2) 0.0402(10) H11B 0.7109 0.1333 0.3896 0.044* C12 0.7631(3) 0.2419(2) 0.3565(3) 0.0412(10) H12A 0.8004 0.2572 0.4239 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0366(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15	04	0.3341(2)	0.24242(13)	0.49762(16)	0.0392(6)
H9A0.33590.13470.54230.052*H9B0.44630.18430.59540.052*C100.4814(3)0.14978(19)0.4509(2)0.0411(9)H10A0.51490.09910.46810.049*H10B0.43360.14650.38430.049*N20.5828(3)0.20283(17)0.4444(2)0.0366(8)H20.625(3)0.2010(18)0.500(2)0.044*C110.6684(3)0.18081(19)0.3684(2)0.0402(10)H11A0.62150.17180.30260.048*C120.7631(3)0.2419(2)0.3565(3)0.0412(10)H12B0.80040.25720.42390.049*C130.3113(3)0.29258(19)0.1439(3)0.0360(9)C140.3567(3)0.3535(2)0.0906(2)0.0366(9)C150.2813(3)0.4169(2)0.1046(3)0.0364(9)C160.1884(3)0.39450(19)0.1681(3)0.0353(9)C170.2064(3)0.31836(19)0.1926(2)0.0350(9)C180.3655(3)0.21497(19)0.1515(3)0.0477(10)H18A0.31950.18500.19630.072*H18B0.36120.19210.08550.072*H18C0.45040.21800.17750.072*C190.4695(3)0.3515(2)0.0262(3)0.0492(10)	C9	0.3971(3)	0.1748(2)	0.5307(3)	0.0437(10)
H9B0.44630.18430.59540.052*C100.4814(3)0.14978(19)0.4509(2)0.0411(9)H10A0.51490.09910.46810.049*H10B0.43360.14650.38430.049*N20.5828(3)0.20283(17)0.4444(2)0.0366(8)H20.625(3)0.2010(18)0.500(2)0.044*C110.6684(3)0.18081(19)0.3684(2)0.0402(10)H11A0.62150.17180.30260.048*H11B0.71090.13330.38960.048*C120.7631(3)0.2419(2)0.3565(3)0.0412(10)H12A0.80040.25720.42390.049*C130.3113(3)0.29258(19)0.1439(3)0.0360(9)C140.3567(3)0.3535(2)0.0906(2)0.0366(9)C150.2813(3)0.4169(2)0.1046(3)0.0364(9)C160.1884(3)0.39450(19)0.1681(3)0.0353(9)C170.2064(3)0.31836(19)0.1926(2)0.0350(9)C180.3655(3)0.21497(19)0.1515(3)0.0477(10)H18A0.31950.18500.19630.072*H18B0.36120.19210.08550.072*H18C0.45040.21800.17750.072*C190.4695(3)0.3515(2)0.0262(3)0.0492(10)	H9A	0.3359	0.1347	0.5423	0.052*
C100.4814(3)0.14978(19)0.4509(2)0.0411(9)H10A0.51490.09910.46810.049*H10B0.43360.14650.38430.049*N20.5828(3)0.20283(17)0.4444(2)0.0366(8)H20.625(3)0.2010(18)0.500(2)0.044*C110.6684(3)0.18081(19)0.3684(2)0.0402(10)H11A0.62150.17180.30260.048*C120.7631(3)0.2419(2)0.3565(3)0.0412(10)H12A0.80040.25720.42390.049*C130.3113(3)0.29258(19)0.1439(3)0.0360(9)C140.3567(3)0.3535(2)0.0906(2)0.0366(9)C150.2813(3)0.4169(2)0.1046(3)0.0364(9)C160.1884(3)0.39450(19)0.1681(3)0.0353(9)C170.2064(3)0.31836(19)0.1926(2)0.0350(9)C180.3655(3)0.21497(19)0.1515(3)0.0477(10)H18A0.31950.18500.19630.072*H18B0.36120.19210.08550.072*H18C0.45040.21800.17750.072*C190.4695(3)0.3515(2)0.0262(3)0.0499(10)	H9B	0.4463	0.1843	0.5954	0.052*
H10A 0.5149 0.0991 0.4681 0.049^* H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.044*$ C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 $0.048*$ C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 $0.049*$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0354(9)$ C16 $0.1884(3)$ $0.39450(19)$ $0.1681(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ $0.1926(2)$ $0.0350(9)$ C18 0.3612 0.1921 0.0855 $0.072*$ H18B 0.3612 0.1921 0.0855 $0.072*$ H18C $0.4695(3)$ $0.3515(2)$ $0.0262(3)$ $0.0499(10)$	C10	0.4814(3)	0.14978(19)	0.4509(2)	0.0411(9)
H10B 0.4336 0.1465 0.3843 0.049^* N2 $0.5828(3)$ $0.20283(17)$ $0.4444(2)$ $0.0366(8)$ H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ $0.044*$ C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 $0.048*$ H11B 0.7109 0.1333 0.3896 $0.048*$ C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 $0.049*$ C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0364(9)$ C16 $0.1884(3)$ $0.39450(19)$ $0.1681(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ $0.1926(2)$ $0.0350(9)$ C18 $0.3655(3)$ $0.21497(19)$ $0.1515(3)$ $0.0477(10)$ H18A 0.3195 0.1850 0.1963 $0.072*$ H18B 0.3612 0.1921 0.0855 $0.072*$ H18C $0.4695(3)$ $0.3515(2)$ $0.0262(3)$ $0.0499(10)$	H10A	0.5149	0.0991	0.4681	0.049*
N2 0.5828(3) 0.20283(17) 0.4444(2) 0.0366(8) H2 0.625(3) 0.2010(18) 0.500(2) 0.044* C11 0.6684(3) 0.18081(19) 0.3684(2) 0.0402(10) H11A 0.6215 0.1718 0.3026 0.048* H11B 0.7109 0.1333 0.3896 0.048* C12 0.7631(3) 0.2419(2) 0.3565(3) 0.0412(10) H12A 0.8004 0.2572 0.4239 0.049* H12B 0.8301 0.2229 0.3159 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0366(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) <tr< td=""><td>H10B</td><td>0.4336</td><td>0.1465</td><td>0.3843</td><td>0.049*</td></tr<>	H10B	0.4336	0.1465	0.3843	0.049*
H2 $0.625(3)$ $0.2010(18)$ $0.500(2)$ 0.044^* C11 $0.6684(3)$ $0.18081(19)$ $0.3684(2)$ $0.0402(10)$ H11A 0.6215 0.1718 0.3026 0.048^* H11B 0.7109 0.1333 0.3896 0.048^* C12 $0.7631(3)$ $0.2419(2)$ $0.3565(3)$ $0.0412(10)$ H12A 0.8004 0.2572 0.4239 0.049^* H12B 0.8301 0.2229 0.3159 0.049^* C13 $0.3113(3)$ $0.29258(19)$ $0.1439(3)$ $0.0360(9)$ C14 $0.3567(3)$ $0.3535(2)$ $0.0906(2)$ $0.0366(9)$ C15 $0.2813(3)$ $0.4169(2)$ $0.1046(3)$ $0.0364(9)$ C16 $0.1884(3)$ $0.39450(19)$ $0.1681(3)$ $0.0353(9)$ C17 $0.2064(3)$ $0.31836(19)$ $0.1926(2)$ $0.0350(9)$ C18 $0.3655(3)$ $0.21497(19)$ $0.1515(3)$ $0.0477(10)$ H18A 0.3195 0.1850 0.1963 0.072^* H18B 0.3612 0.1921 0.0855 0.072^* H18C $0.4695(3)$ $0.3515(2)$ $0.0262(3)$ $0.0499(10)$	N2	0.5828(3)	0.20283(17)	0.4444(2)	0.0366(8)
C110.6684(3)0.18081(19)0.3684(2)0.0402(10)H11A0.62150.17180.30260.048*H11B0.71090.13330.38960.048*C120.7631(3)0.2419(2)0.3565(3)0.0412(10)H12A0.80040.25720.42390.049*H12B0.83010.22290.31590.049*C130.3113(3)0.29258(19)0.1439(3)0.0360(9)C140.3567(3)0.3535(2)0.0906(2)0.0366(9)C150.2813(3)0.4169(2)0.1046(3)0.0364(9)C160.1884(3)0.39450(19)0.1681(3)0.0353(9)C170.2064(3)0.31836(19)0.1926(2)0.0350(9)C180.3655(3)0.21497(19)0.1515(3)0.0477(10)H18A0.31950.18500.19630.072*H18B0.36120.19210.08550.072*H18C0.45040.21800.17750.072*C190.4695(3)0.3515(2)0.0262(3)0.0499(10)	H2	0.625(3)	0.2010(18)	0.500(2)	0.044*
H11A 0.6215 0.1718 0.3026 0.048* H11B 0.7109 0.1333 0.3896 0.048* C12 0.7631(3) 0.2419(2) 0.3565(3) 0.0412(10) H12A 0.8004 0.2572 0.4239 0.049* H12B 0.8301 0.2229 0.3159 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0360(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	C11	0.6684(3)	0.18081(19)	0.3684(2)	0.0402(10)
H11B 0.7109 0.1333 0.3896 0.048* C12 0.7631(3) 0.2419(2) 0.3565(3) 0.0412(10) H12A 0.8004 0.2572 0.4239 0.049* H12B 0.8301 0.2229 0.3159 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0360(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	H11A	0.6215	0.1718	0.3026	0.048*
C12 0.7631(3) 0.2419(2) 0.3565(3) 0.0412(10) H12A 0.8004 0.2572 0.4239 0.049* H12B 0.8301 0.2229 0.3159 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0360(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072* H18C 0.4504 0.2180 0.1775 0.072*	H11B	0.7109	0.1333	0.3896	0.048*
H12A 0.8004 0.2572 0.4239 0.049* H12B 0.8301 0.2229 0.3159 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0360(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	C12	0.7631(3)	0.2419(2)	0.3565(3)	0.0412(10)
H12B 0.8301 0.2229 0.3159 0.049* C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0360(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	H12A	0.8004	0.2572	0.4239	0.049*
C13 0.3113(3) 0.29258(19) 0.1439(3) 0.0360(9) C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	H12B	0.8301	0.2229	0.3159	0.049*
C14 0.3567(3) 0.3535(2) 0.0906(2) 0.0366(9) C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	C13	0.3113(3)	0.29258(19)	0.1439(3)	0.0360(9)
C15 0.2813(3) 0.4169(2) 0.1046(3) 0.0364(9) C16 0.1884(3) 0.39450(19) 0.1681(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072*	C14	0.3567(3)	0.3535(2)	0.0906(2)	0.0366(9)
C16 0.1884(3) 0.39450(19) 0.1881(3) 0.0353(9) C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072* (19 0.4695(3) 0.3515(2) 0.0262(3) 0.0499(10)	C15	0.2813(3)	0.4169(2)	0.1046(3)	0.0364(9)
C17 0.2064(3) 0.31836(19) 0.1926(2) 0.0350(9) C18 0.3655(3) 0.21497(19) 0.1515(3) 0.0477(10) H18A 0.3195 0.1850 0.1963 0.072* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072* (19) 0.4695(3) 0.3515(2) 0.0262(3) 0.0499(10)	C16	0.1884(3)	0.39450(19)	0.1681(3)	0.0353(9)
C_{18} $0.3655(3)$ $0.21497(19)$ $0.1515(3)$ $0.0477(10)$ H18A 0.3195 0.1850 0.1963 $0.072*$ H18B 0.3612 0.1921 0.0855 $0.072*$ H18C 0.4504 0.2180 0.1775 $0.072*$ (19) $0.4695(3)$ $0.3515(2)$ $0.0262(3)$ $0.0499(10)$	C10	0.2064(3)	0.31836(19)	0.1926(2)	0.0350(9)
H18A 0.3195 0.1850 0.1963 0.0/2* H18B 0.3612 0.1921 0.0855 0.072* H18C 0.4504 0.2180 0.1775 0.072* (19) 0.4695(3) 0.3515(2) 0.0262(3) 0.0499(10)		0.3655(3)	0.2149/(19)	0.1515(3)	0.04//(10)
$\Pi 18D$ 0.3612 0.1921 0.0855 0.072^* H18C 0.4504 0.2180 0.1775 0.072^* (19) $0.4695(3)$ $0.3515(2)$ $0.0262(3)$ $0.0499(10)$		0.3195	0.1850	0.1963	0.072*
ΠΙΟC U.4504 U.2180 U.1//5 U.0/2^* (19 0.4695(3) 0.3515(2) 0.0262(3) 0.0400(10)		0.3612	0.1921	0.0855	0.072*
	(10	0.4504	0.2100	0.1775	0.072*

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Table 2	(continued)	
IUDIC 2	(continucu)	

Atom	x	у	Z	U _{iso} */U _{eq}
H19A	0.5000	0.2996	0.0224	0.075*
H19B	0.5351	0.3838	0.0574	0.075*
H19C	0.4454	0.3699	-0.0423	0.075*
C20	0.2902(3)	0.4927(2)	0.0539(3)	0.0535(11)
H20A	0.2911	0.5326	0.1053	0.080*
H20B	0.2186	0.4997	0.0053	0.080*
H20C	0.3666	0.4950	0.0183	0.080*
C21	0.0851(3)	0.44569(19)	0.1991(3)	0.0496(11)
H21A	0.1198	0.4947	0.2206	0.074*
H21B	0.0444	0.4226	0.2555	0.074*
H21C	0.0244	0.4529	0.1414	0.074*
C22	0.1287(3)	0.27075(19)	0.2596(3)	0.0434(10)
H22A	0.0792	0.3038	0.3004	0.065*
H22B	0.1833	0.2395	0.3046	0.065*
H22C	0.0734	0.2382	0.2171	0.065*

of ZnCp*₂. The title compound has been obtained as a crystallized product of a partial metathesis reaction, while the remaining ingredients, Zn^{2+} cations as well as $[Si_4]^{4-}$ and $[Si_9]^{4-}$ cluster anions, were not found as parts of crystalline phases after this experiment.

[Rb(diaza-18-crown-6)]Cp* crystallizes in space group $P2_1/c$ with all atoms at general positions. The Rb⁺ cation is coordinated by one diaza-18-crown-6 molecule and one Cp* anion. While pure RbCp* is found to crystallize in polymeric "multidecker" strands [10], here the presence of the crown ether causes the formation of molecular units, similar to the effect of 18-crown-6 on RbCp* in THF [11]. The Rb⁺ cation is situated near the centre of the diaza-18-crown-6 molecule but apart from the ring plane shifted in direction of the Cp* anion as previously found for [Rb(diaza-18-crown-6)] complexes in Fulleride salts [12]. Rb is bound to the Cp* ligand via two short Rb-C bonds of 3.075(3) Å and 3.210(3) Å which are in the same range as those observed for the η^5 coordination in [Rb(18-crown-6)]Cp* [11]. All atoms of the Cp* ligand are in plane and the cyclopentadienyl ring is a nearly perfect pentagon (C–C bond lengths between 1.398(4) Å and 1.418(4) Å, C-C-C angles between 107.3(3)° and 108.8(3)°) which differs clearly from the shape of the neutral Cp*–H molecule [13], suggesting that the negative charge is located at Cp*. Confirming the neutral nature of the diaza-18-crown-6 molecule, one H atom close to each N atom could have been located from the Fourier map. In contrast to the structure of the free diaza-18-crown-6 molecule [14], where the N-H bonds are parallel, both the N–H bonds of the [Rb(diaza-18-crown-6)] complex are directed almost perpendicular to the ring plane. Probably the orthogonal N-H bond hampers the formation of the symmetric η^5 coordination, possibly by forming N-H···C hydrogen bonds instead.

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References

- Rigaku Oxford Diffraction: *CrysAlis CCD, CrysAlis RED* Version 1.171.33.34d. Oxford Diffraction Ltd., Yarnton, Oxfordshire, UK (2009).
- Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. A64 (2008) 112–122.
- Sheldrick, G. M.: Crystal structure refinement with SHELXL. Acta Crystallogr. C71 (2015) 3–8.
- Brandenburg, K.: DIAMOND. Visual Crystal Structure Information System. Version 3.2i. Crystal Impact, Bonn, Germany (2012).
- Quéneau, V.; Todorov, E.; Sevov, S. C.: Synthesis and structure of isolated silicon clusters of nine atoms. J. Am. Chem. Soc. 120 (1998) 3263–3264.
- Blom, R.; Boersma, J.; Budzelaar, P. H. M.; Fischer, B.; Haaland, A.; Volden, H. V.; Weidlein, J.: The preparation of bis(pentamethylcyclopentadienyl)zinc and bis(trimethylsilylcyclopentadienyl)zinc, and their molecular structures determined by gas electron diffraction. Acta Chem. Scand. A 40 (1986) 113–120.
- Bentlohner, M. M.; Jantke, L.-A.; Henneberger, T.; Fischer, C.; Mayer, K.; Klein, W.; Fässler, T. F.: On the nature of cridging

metal atoms in intermetalloid clusters: synthesis and structure of the metal-atom-bridged zintl clusters $[Sn(Ge_9)_2]^{4-}$ and $[Zn(Ge_9)_2]^{6-}$. Chem. Eur. J. **22** (2016) 13946–13952.

- Benda, C. B.; Henneberger, T.; Klein, W.; Fässler, T. F.: [Si₄]⁴⁻ and [Si₉]⁴⁻ clusters crystallized from liquid ammonia solution – synthesis and characterization of K₈[Si₄][Si₉](NH₃)_{14.6}.
 Z. Anorg. Allg. Chem. 643 (2017) 146–148.
- Henneberger, T.; Klein, W.; Fässler, T. F.: Silicon containing nine atom clusters from liquid ammonia solution: crystal structures of the first protonated clusters [HSi₉]³⁻ and [H₂{Si/Ge}₉]².
 Z. Anorg. Allg. Chem. 644 (2018) 1018–1027.
- Behrens, U.; Dinnebier, R. E.; Neander, S.; Olbrich, F.: Solid-state structures of base-free rubidium and cesium pentamethylcyclopentadienides. Determination by high-resolution powder diffraction. Organometallics 27 (2008) 5398–5400.
- Neander, S.; Behrens, U.; Olbrich, F.: Novel 18-crown-6 organometallic rubidium and cesium complexes containing cyclopentadienyl, indenyl, pentamethylcyclopentadienyl, and fluorenyl as carbanions. J. Organomet. Chem. 604 (2000) 59–67.
- Boeddinghaus, M. B.; Wahl, B.; Fässler, T. F.; Jakes, P.; Eichel, R.-A.: Three salts containing the fullerene tetra-anion C₆₀⁴⁻⁻ – synthesis, X-ray single-crystal structure determination and EPR investigation. Z. Anorg. Allg. Chem. **638** (2012) 2205–2212.
- Benda, C. B.; Klein, W.; Fässler, T. F.: Crystal structure of 1,2,3,4,5-pentamethyl-1,3-cyclopentadiene, C₁₀H₁₆.
 Z. Kristallogr. NCS 232 (2017) 511–512.
- Dokurno, P.; Trokowski, R.; Kościuszko-Panek, B.; Ossowski, T.; Konitz, A.; Blażejowski, J.: Crystal structure of three diaza-crowns-18. Z. Kristallogr. 212 (1997) 362–366.