Crystal structure of bis[bis(diethylether)lithium (trimethylsilyl)methyl-cyanocuprate], $[(C_4H_{10}O)_2Li(C_3H_9)SiCH_2CuCN]_2$

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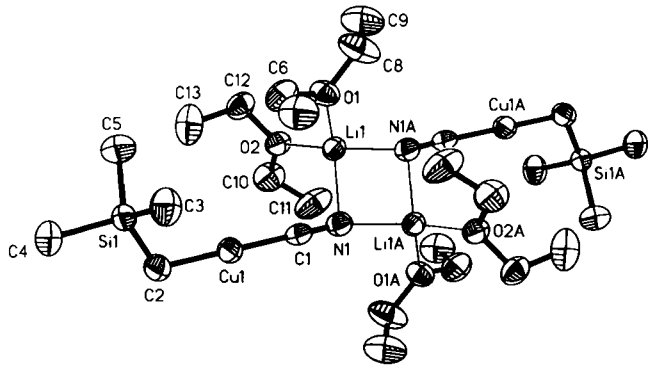

Abstract

$C_{26}H_{62}Cu_2Li_2N_2O_4Si_2$, monoclinic, $P12_1/c1$ (No. 14), a = 10.0080(8) Å, b = 11.1636(6) Å, c = 18.029(2) Å, β = 106.091(9)°, V = 1935.4 Å^3, Z = 2, $R_{gt}(F)$ = 0.031, $wR_{ref}(F^2)$ = 0.074, T = 193 K.

Source of material

The synthesis was done according to [1].

Discussion

The first X-ray crystal structure of a lower order cyano cuprate [1], $[tBuCuC(CN)Li(OEt_2)_2]_\infty$, has been published only recently [2]. The most significant different between this structure and the structure published here is the absence of a $Cu^I(d^{10})$–$Cu^I(d^{10})$ bonding interaction in the latter one (see also [3]).

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.4 × 0.4 × 1.0 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.87 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, Δφ = 1°
$2\theta_{max}$:	51.78°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	14200, 3585
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2601
$N(param)_{refined}$:	179
Programs:	SHELXS-97 [4], SHELXL-97 [5], DIFABS [6]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	4e	0.8314	1.0246	0.3728	0.057
H(2B)	4e	0.9372	0.9255	0.3593	0.057
H(3A)	4e	1.0942	1.0719	0.2375	0.092
H(3B)	4e	1.2001	1.0094	0.3103	0.092
H(3C)	4e	1.2134	1.1495	0.2949	0.092
H(4A)	4e	1.0807	1.1445	0.4884	0.093
H(4B)	4e	1.2031	1.1995	0.4577	0.093
H(4C)	4e	1.1939	1.0579	0.4690	0.093
H(5A)	4e	0.8999	1.2685	0.2684	0.094
H(5B)	4e	1.0252	1.3284	0.3328	0.094
H(5C)	4e	0.8866	1.2884	0.3540	0.094
H(6A)	4e	0.7583	1.2215	0.1302	0.078
H(6B)	4e	0.8021	1.3310	0.0849	0.078
H(7A)	4e	0.9793	1.1928	0.1196	0.112
H(7B)	4e	0.9238	1.2012	0.0275	0.112
H(7C)	4e	0.8788	1.0909	0.0720	0.112
H(8A)	4e	0.7425	1.3342	–0.0427	0.101
H(8B)	4e	0.6599	1.2237	–0.0908	0.101
H(9A)	4e	0.5369	1.3850	–0.1334	0.138
H(9B)	4e	0.5471	1.4300	–0.0477	0.138
H(9C)	4e	0.4553	1.3149	–0.0819	0.138
H(10A)	4e	0.2460	1.2087	0.1350	0.081
H(10B)	4e	0.3594	1.1182	0.1857	0.081
H(11A)	4e	0.1789	1.0111	0.1064	0.125
H(11B)	4e	0.3178	0.9874	0.0810	0.125
H(11C)	4e	0.2018	1.0771	0.0320	0.125
H(12A)	4e	0.3743	1.3664	0.1244	0.067
H(12B)	4e	0.5189	1.3541	0.1035	0.067
H(13A)	4e	0.5710	1.3983	0.2322	0.127
H(13B)	4e	0.6132	1.2610	0.2267	0.127
H(13C)	4e	0.4717	1.2940	0.2470	0.127

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	4*e*	0.77836(3)	0.97960(3)	0.23662(2)	0.0427(2)	0.0424(2)	0.0404(2)	–0.0061(1)	0.0080(1)	0.0001(1)
Si(1)	4*e*	1.02747(6)	1.11692(6)	0.35167(3)	0.0400(3)	0.0413(4)	0.0355(3)	–0.0004(3)	0.0110(2)	–0.0010(3)
C(1)	4*e*	0.6668(2)	0.9570(2)	0.1356(1)	0.041(1)	0.029(2)	0.049(1)	–0.0030(9)	0.012(1)	0.002(1)
O(1)	4*e*	0.6555(2)	1.2268(2)	0.01875(9)	0.0445(9)	0.056(1)	0.0511(9)	–0.0084(8)	0.0168(7)	0.0100(8)
N(1)	4*e*	0.5990(2)	0.9449(2)	0.0736(1)	0.042(1)	0.038(1)	0.047(1)	–0.0024(8)	0.0091(9)	0.0015(8)
Li(1)	4*e*	0.5097(4)	1.1194(3)	0.0313(2)	0.042(2)	0.036(2)	0.041(2)	–0.003(2)	0.015(2)	–0.003(2)
O(2)	4*e*	0.4200(2)	1.1994(2)	0.10204(9)	0.0508(9)	0.039(1)	0.0540(9)	–0.0011(7)	0.0280(8)	–0.0025(7)
C(2)	4*e*	0.8922(2)	1.0027(2)	0.3400(1)	0.052(1)	0.049(2)	0.043(1)	–0.007(1)	0.012(1)	0.003(1)
C(3)	4*e*	1.1482(3)	1.0829(3)	0.2914(2)	0.054(2)	0.077(2)	0.057(2)	–0.004(1)	0.023(1)	–0.011(1)
C(4)	4*e*	1.1398(3)	1.1314(3)	0.4539(1)	0.067(2)	0.066(2)	0.048(1)	–0.007(1)	0.005(1)	–0.009(1)
C(5)	4*e*	0.9507(3)	1.2686(3)	0.3233(2)	0.064(2)	0.049(2)	0.076(2)	0.003(1)	0.019(1)	0.007(1)
C(6)	4*e*	0.7787(3)	1.2446(3)	0.0815(2)	0.058(2)	0.056(2)	0.079(2)	–0.016(1)	0.016(1)	–0.011(2)
C(7)	4*e*	0.9002(3)	1.1767(3)	0.0746(2)	0.049(2)	0.079(3)	0.092(2)	–0.006(2)	0.010(2)	0.011(2)
C(8)	4*e*	0.6571(4)	1.2852(3)	–0.0517(2)	0.092(2)	0.089(3)	0.087(2)	0.015(2)	0.048(2)	0.042(2)
C(9)	4*e*	0.5402(4)	1.3594(4)	–0.0809(2)	0.087(2)	0.077(3)	0.110(3)	0.012(2)	0.022(2)	0.036(2)
C(10)	4*e*	0.3160(3)	1.1473(3)	0.1326(2)	0.069(2)	0.067(2)	0.084(2)	–0.010(2)	0.049(2)	–0.003(2)
C(11)	4*e*	0.2480(3)	1.0475(3)	0.0840(2)	0.085(2)	0.055(2)	0.135(3)	–0.019(2)	0.074(2)	–0.020(2)
C(12)	4*e*	0.4592(3)	1.3167(2)	0.1326(2)	0.062(2)	0.044(2)	0.068(2)	0.003(1)	0.029(1)	–0.010(1)
C(13)	4*e*	0.5354(3)	1.3176(4)	0.2169(2)	0.074(2)	0.110(3)	0.071(2)	–0.006(2)	0.021(2)	–0.030(2)

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