

# Lithium dicyanoargentate(I) acetonitrile disolvate

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**Key indicators**

Single-crystal X-ray study  
 T = 200 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
 R factor = 0.031  
 wR factor = 0.079  
 Data-to-parameter ratio = 20.4

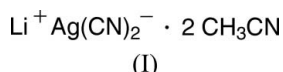
For details of how these key indicators were  
 automatically derived from the article, see  
<http://journals.iucr.org/e>.

The structure of the title compound, poly[diacetonitriledi- $\mu$ -cyano-lithium(I)silver(I)],  $[\text{AgLi}(\text{CN})_2(\text{CH}_3\text{CN})_2]_n$ , shows infinite chains of the anionic silver dicyanide unit connected by an Li atom, which is itself coordinated by two further acetonitrile groups.

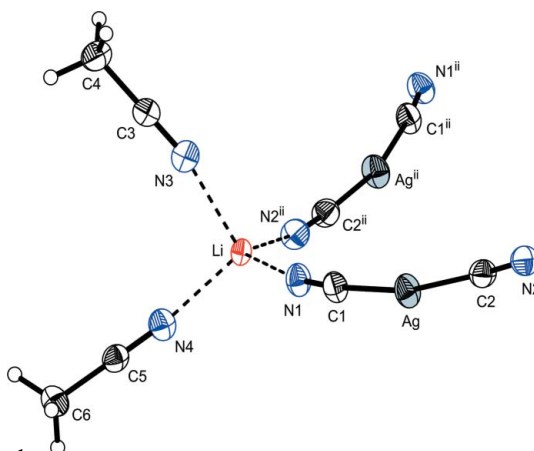
**Comment**

Dicyanoargentates(I) have been known for many years; lithium dicyanoargentate was prepared as early as 1921 (Meyer, 1921; Perret & Perrot, 1932; Jones, 1963; Rossmannith, 1965). Complexes of rubidium and caesium dicyanoargentates with 18-crown-6 were synthesized and structural details were reported a few years ago (Manskaya *et al.*, 1998). In some of our earlier work, we also characterized dicyanoargentate salts by X-ray diffraction, *viz.*  $[(\text{CH}_3)_3\text{Te}][\text{Ag}(\text{CN})_2]$  and  $[(\text{C}_6\text{H}_5)_3\text{Te}][\text{Ag}(\text{CN})_2]$  (Klapötke *et al.*, 2002). In this contribution, we present the structure of the lithium salt of dicyanoargentate(I), which was obtained as a side-product with the intended preparation of a tellurium-containing material.

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The structure of the title compound, (I), exists as infinite chains with the  $\text{Ag}(\text{CN})_2^-$  anions connected by  $\text{Li}^+$  cations. The  $\text{Li} \cdots \text{N1}/\text{Li} \cdots \text{N2}^{\text{ii}}$  (for symmetry code, see caption of Fig. 1) distances [1.995 (4)/2.009 (4) Å] are significantly shorter than the van der Waals radii (Li + N = 3.10 Å; Bondi, 1964). Compared to known structures of [Cs(18-crown-



**Figure 1** Part of the polymeric structure of (I), with displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (ii)  $-1 + x, \frac{1}{2} - y, -\frac{1}{2} + z$ .]

6)]Ag(CN)<sub>2</sub>] and [(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>Te][Ag(CN)<sub>2</sub>], the distances within the Ag(CN)<sub>2</sub> units are nearly the same [Ag—C1 = 2.062 (3) Å, C1—N1 = 1.138 (4) Å, Ag—C2 = 2.052 (3) Å and C2—N2 = 1.142 (4) Å compared to Ag—C = 2.05–2.07 Å and C—N = 1.13 Å for the Cs salt, or Ag—C = 2.06–2.07 Å and C—N = 1.14 Å for the telluronium salt]. The C1—Ag—C2 angle [168.78 (11)°] is smaller than the angles in the latter dicyanoargentates [171.8 (4)° for the Cs salt and 175–180° for the telluronium salt] and therefore further away from the expected linearity. The Li<sup>+</sup> cation is further coordinated by two molecules of acetonitrile with slightly longer Li···N distances compared to the cyano group [Li···N3 = 2.096 (5) Å and Li···N4 = 2.064 (5) Å], which leads to a distorted tetrahedral coordination of Li.

## Experimental

Tellurium (2.0 mmol) and LiBHEt<sub>3</sub> [3.9 mmol, 1 M solution in tetrahydrofuran (THF)] were stirred for 15 min with gentle heating. The solution was cooled to 273 K and TeBr<sub>4</sub> (2.0 mmol) in THF (12.5 ml) was added dropwise. The green reaction mixture was separated from elemental tellurium and all volatile materials were removed *in vacuo* to give an orange oil. To a solution of the oil in CH<sub>3</sub>CN (5 ml) was added AgCN (3.2 mmol) at 273 K and the yellow suspension was stirred for an hour in the dark. After an extended storage period at 253 K, colourless crystals were obtained.

### Crystal data

[AgLi(CN) <sub>2</sub> (C <sub>2</sub> H <sub>3</sub> N) <sub>2</sub> ]	Z = 4
<i>M<sub>r</sub></i> = 248.95	<i>D<sub>x</sub></i> = 1.636 (1) Mg m <sup>-3</sup>
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 7.7799 (2) Å	<i>μ</i> = 1.95 mm <sup>-1</sup>
<i>b</i> = 17.6741 (4) Å	<i>T</i> = 200 (2) K
<i>c</i> = 7.3680 (2) Å	Block, colourless
<i>β</i> = 94.0056 (11)°	0.19 × 0.14 × 0.07 mm
<i>V</i> = 1010.65 (4) Å <sup>3</sup>	

### Data collection

Nonius KappaCCD diffractometer	<i>X-RED</i> (Stoe & Cie, 1997)
<i>φ</i> scans	<i>T</i> <sub>min</sub> = 0.618, <i>T</i> <sub>max</sub> = 0.708
Absorption correction: numerical	16742 measured reflections
Crystal faces optimized with	2264 independent reflections
<i>X-SHAPE</i> (Stoe & Cie, 1997)	1806 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction with	<i>R</i> <sub>int</sub> = 0.048
	<i>θ</i> <sub>max</sub> = 27.3°

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.2798P]$
$R[F^2 > 2\sigma(F^2)] = 0.031$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.079$	( $\Delta/\sigma$ ) <sub>max</sub> < 0.001
<i>S</i> = 1.08	$\Delta\rho_{max} = 0.49 \text{ e } \text{Å}^{-3}$
2264 reflections	$\Delta\rho_{min} = -0.68 \text{ e } \text{Å}^{-3}$
111 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically (C—H = 0.98 Å) and refined as riding, with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C).

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1996); software used to prepare material for publication: *SHELXL97*.

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