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New ambient pressure organic superconductors κ_H- and κ_L-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF)

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Hydrogen bonds in κ_H-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF)

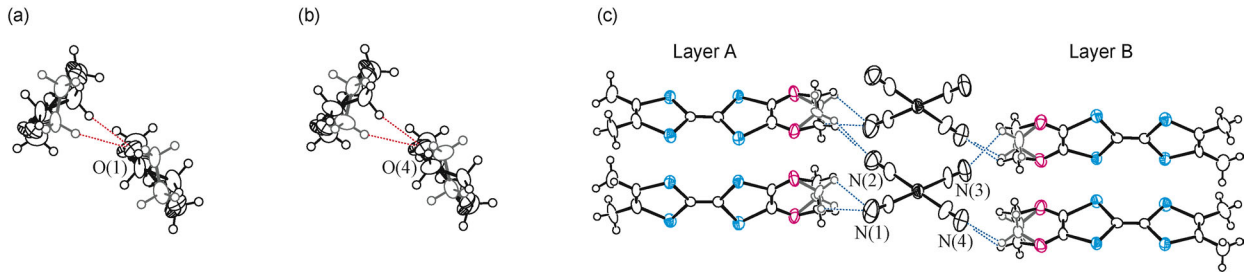

Fig. 1 Hydrogen bonds in κ_H-phase. Red dotted lines indicate CH···O hydrogen bonds; (a) in the layer A and (b) the layer B. (c) Blue dotted lines indicate CH···N hydrogen bonds between the donor and the anion. Gray atoms and bonds indicate minor orientation of the disordered ethylene bridge.

Table 1 Hydrogen bond distances[a] for κ_H-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF) less than 3.0 Å

Atom	Atom	Distance / Å	ADC[b]	Atom	Atom	Distance / Å	ADC[b]
In layer A				In layer B			
			HCH···O				
			For the major orientation of the ethylene group				
O(1)	**H(7A1)**	**2.497**	**4**	**O(4)**	**H(18B)**	**2.517**	**55404**
			For the minor orientation of the ethylene group				
O(1)	**H(8B2)**	**2.675**	**4**	**O(4)**	**H(17D)**	**2.696**	**55404**
			H_2CH···O				
O(1)	H(9C)	2.959	2	O(3)	H(20C)	2.883	65703
O(2)	H(9A)	2.989	3				
Molecule A-Anion				Molecule B-Anion			
			HCH···N				
			For the major orientation of the ethylene group				
N(1)	H(7A2)	2.810	4	N(3)	H(17A)	2.773	4
N(1)	H(8A1)	2.990	4	N(3)	H(17A)	2.789	1
N(2)	**H(8A2)**	**2.548**	**1**	**N(3)**	**H(18A)**	**2.698**	**1**
				N(4)	**H(18A)**	**2.671**	**4**
				N(3)	H(18B)	2.808	1
			For the minor orientation of the ethylene group				
N(1)	**H(7B1)**	**2.590**	**4**	**N(3)**	**H(17C)**	**2.671**	**1**
N(1)	**H(7B2)**	**2.592**	**4**	N(3)	H(17C)	2.934	4
N(2)	**H(8B1)**	**2.746**	**1**	N(3)	H(17D)	2.886	1
N(2)	H(8B1)	2.965	4	**N(4)**	**H(18C)**	**2.535**	**4**
				N(3)	H(18C)	2.905	1
				N(4)	H(18D)	2.844	4
			H_2CH···N				
N(1)	**H(10A)**	**2.495**	**55602**	N(4)	H(19A)	2.960	66703
				N(4)	**H(19C)**	**2.589**	**65602**

[a] The hydrogen bonds shorter than sum of the van der Waals radii are represented by the pink characters; sum of the van der van der Waals radii; O···H = 2.72 Å; N···H = 2.75 Å; A. Bondi, *J. Phys. Chem*., 1964, **68**, 411–451. [b] Symmetry operators: (1) +X, +Y, +Z; (2) –X, 1/2+Y, 1/2–Z; (3) –X, –Y, –Z; (4) +X, 1/2–Y, 1/2+Z.

Hydrogen bonds in κ_L-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF)

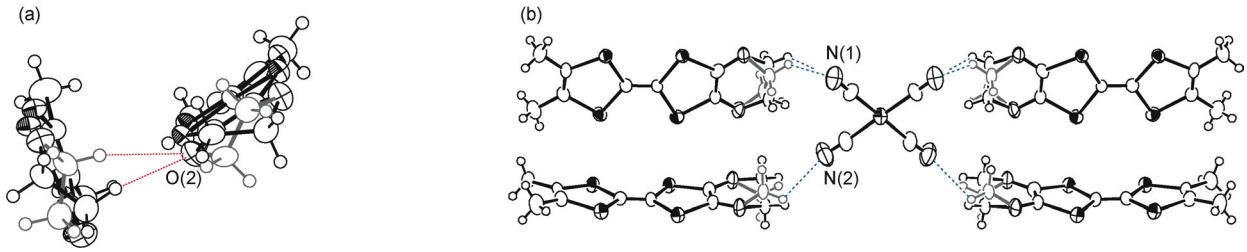

Fig. 2 Hydrogen bonds in κ_L-phase. (a) Red dotted lines indicate CH···O hydrogen bonds in the donor layer. (b) Blue dotted lines indicate CH···N hydrogen bonds between the donor and the anion. Gray atoms and bonds indicate minor orientation of the disordered ethylene bridge.

Table 2 Hydrogen bond distances[a] for κ_L-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF) less than 3.0 Å

Atom	Atom	Distance / Å	ADC[b]	Atom	Atom	Distance / Å	ADC[b]
HCH···O (For the major orientation)				HCH···O (For the minor orientation)			
O(2)	**H(7A2)**	**2.582**	**55608**	O(2)	H(8B1)	2.791	55608
			H_2CH···O				
O(2)	H(9C)	2.853	56504				
HCH···N (For the major orientation)				HCH···N (For the minor orientation)			
N(1)	**H(7A1)**	**2.599**	**1**	**N(1)**	**H(7B1)**	**2.381**	**1**
N(2)	H(7A1)	2.820	55608	N(1)	H(7B2)	2.823	1
N(2)	H(7A2)	2.792	55608	N(2)	H(7B1)	2.963	55608
N(2)	H(8A1)	2.793	1	N(2)	H(8B1)	2.843	55608
N(2)	H(8A1)	2.826	55608	N(2)	H(8B2)	2.949	1
				N(2)	**H(8B2)**	**2.716**	**55608**
			H_2CH···N				
N(1)	**H(10A)**	**2.447**	**66605**	N(1)	H(10C)	2.927	56404

[a] The hydrogen bonds shorter than sum of the van der Waals radii are represented by the pink characters; sum of the van der van der Waals radii; O···H = 2.72 Å; N···H = 2.75 Å. [b] Symmetry operators: (1) +X, +Y, +Z; (2) 1/2+X, 1/2−Y, 1/2−Z; (3) −X, 1/2+Y, −Z; (4) 1/2−X, −Y, 1/2+Z; (5) −X, −Y, −Z; (6) 1/2−X, 1/2+Y, 1/2+Z; (7) +X, 1/2−Y, +Z; (8) 1/2+X, +Y, 1/2−Z.

Molecular packing of κ_L-(DMEDO-TSeF)$_2$[Au(CN)$_4$](THF)

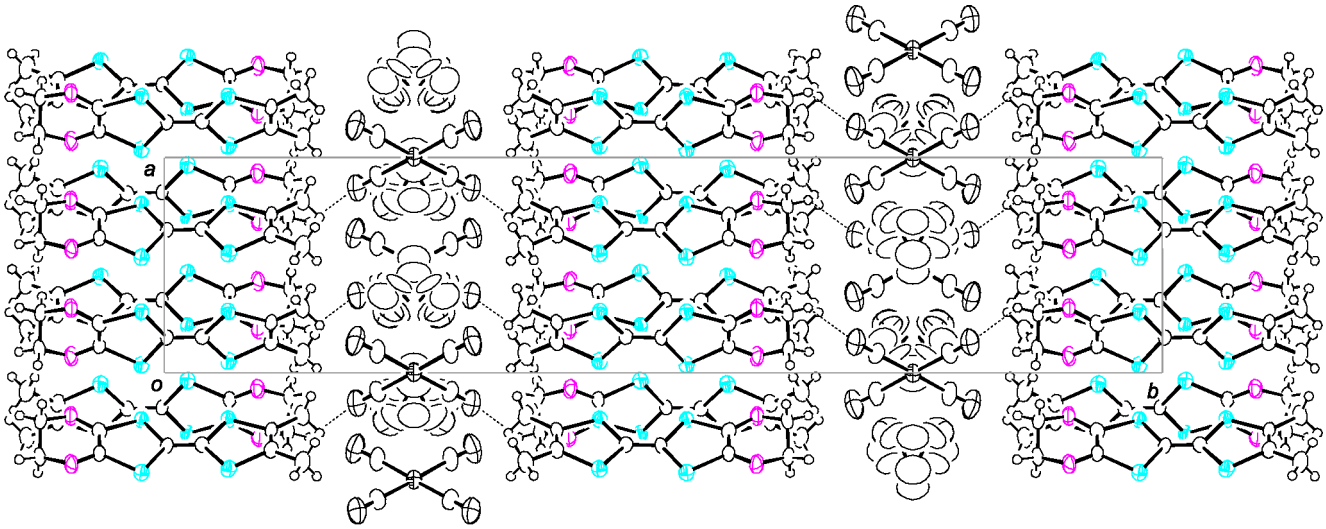

Fig. 3 Molecular packing of the κ_L-phase viewed along the crystallographic *c*-axis. Dotted lines indicate CH···N hydrogen bonds less than 2.75 Å. The minor orientations of the disordered ethylene bridge of the donor molecule are omitted for clarity.

Crystal structures for the insulating layer of the κ_H- and κ_L-phase

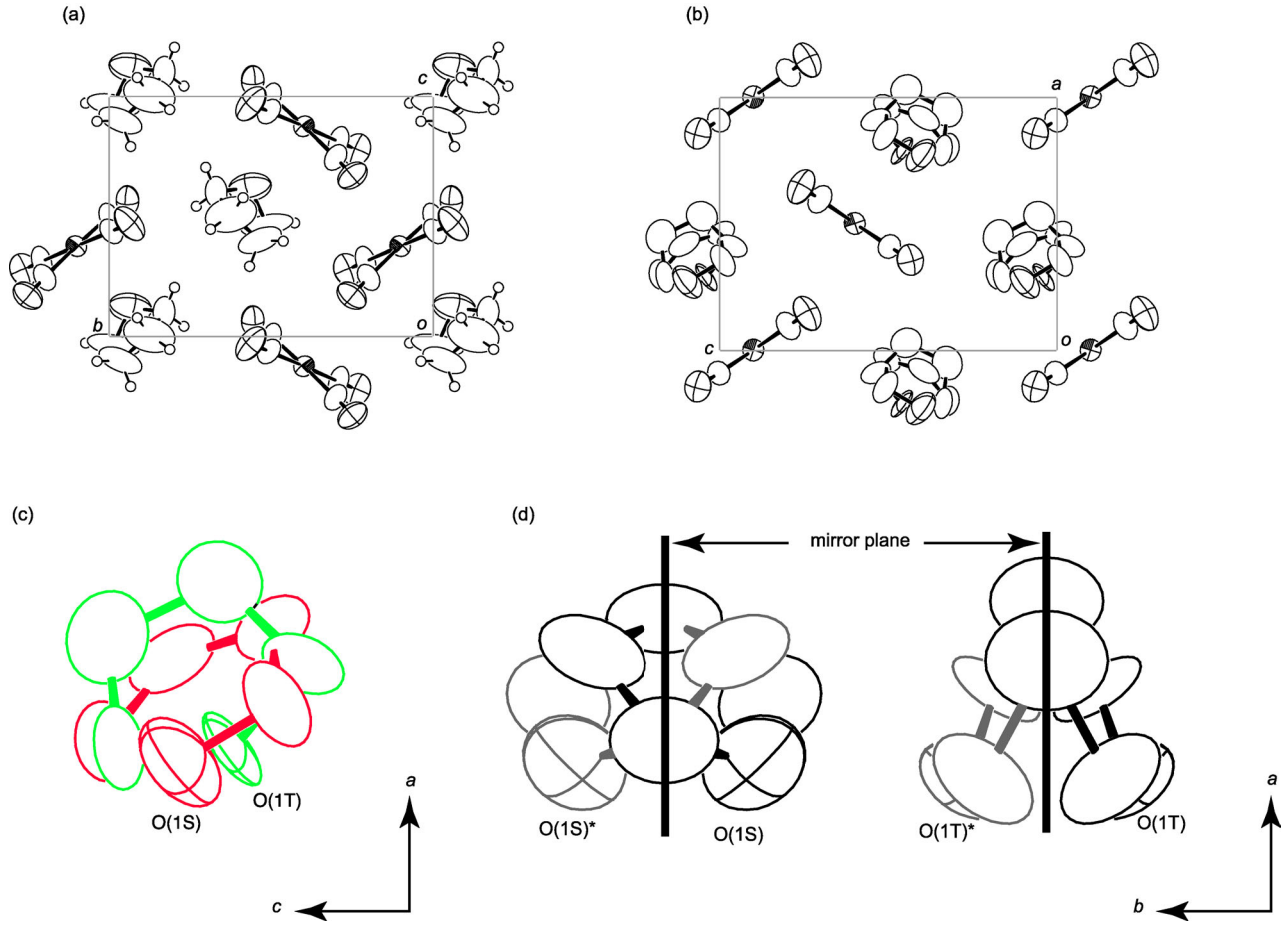

Fig. 4 Crystal structure for the insulating layer; (a) κ_H-phase projection onto the *bc*-plane; (b) κ_L-phase projection onto the *ac*-plane. (c) Red and green lines indicate each orientation of the disordered THF molecule in the κ_L-phase viewed along the crystallographic *b*-axis. Only the asymmetric units are indicated. (d) Structures for each orientation of THF molecule viewed along the crystallographic *c*-axis. Gray lines indicate the atoms and bonds generated by the mirror symmetry.