The Space Group of (TTM-TTF)$^{2+}$(AuCl$_4^-$)$_2$ [TTM-TTF = Tetra(methylthio)tetrathiofulvalene]

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Tetra(methylthio)tetrathiofulvalene

The space group of the title compound is probably C2/*m* rather than the previously reported C2.

During the preparation of a review article on the crystal structures of gold compounds, it was noticed that the structure of (TTM-TTF)$^{2+}$(AuCl$_4^-$)$_2$, presented in space group C2 with cell constants a = 14.799, b = 11.513, c = 8.034 Å, β = 97.05° [1], displayed several unusual features. The atoms Au, Cl(2), Cl(4) and C(1) lay in or near the planes y = 0 or 1/2; other atoms occurred in pairs with similar x and z coordinates, and y coordinates summing to 0 or 1; and some chemically equivalent bond lengths differed appreciably (Au–Cl 2.247–2.309 Å, S–C(1) 1.573, 1.787 Å). All these features could be explained if the true space group were C2/*m*, *i.e.* if a crystallographic centre of symmetry had been overlooked [2].

The deposited structure factors were obtained from the Fachinformationszentrum Energie, Physik, Mathematik, 7514 Eggenstein-Leopoldshafen 2 (deposition number CSD 52689). Anisotropic refinement in C2/*m* proceeded smoothly to an R value of 0.032 for 1511 reflections, 70 parameters (*cf.* 0.028 for 1581 reflections, 140 parameters in C2; only 1512 reflections were present in the deposited material and one was clearly in error). Atoms Au, Cl(2) and Cl(3) (in the new numbering scheme, see Tables I and II) were fixed in the mirror planes. The weighting scheme was $w = \sigma^{-2}(F)$, with σ values calculated by the method of Cruickshank [3] (no σ values had been deposited). H atoms were not included. The program system was SHELX-76, locally modified by its author Prof. G. M. Sheldrick.

The new refinement leads to more regular geometry, with Au–Cl 2.255–2.275 Å, C(1)–S(1) 1.684 Å, and to much lower e.s.d.'s [2]. The descrip-

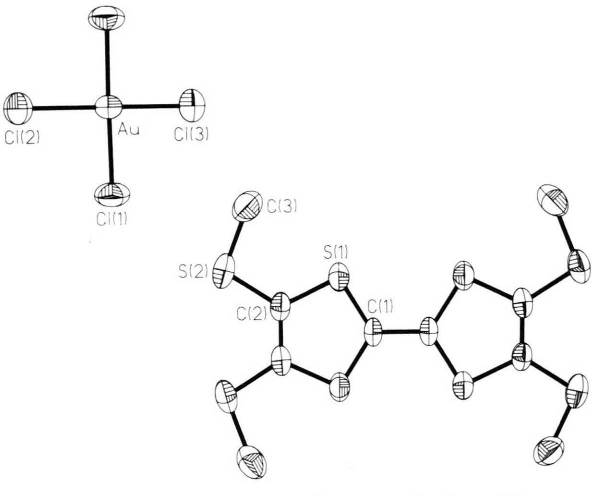

Fig. 1. Thermal ellipsoid plot (50% level) of the title compound, showing the numbering of the asymmetric unit in C2/*m*.

Table I. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2×10^3).

	x	y	z	U(eq)*
Au	1448.9(2)	0	1147.5(4)	44(1)
Cl(1)	1498(2)	1974(2)	1252(3)	72(1)
Cl(2)	2495(2)	0	– 689(4)	67(1)
Cl(3)	350(3)	0	2860(5)	83(1)
S(1)	470(1)	3756(2)	8307(2)	50(1)
S(2)	1376(1)	3584(2)	5204(2)	60(1)
C(1)	211(6)	5000	9244(9)	40(2)
C(2)	959(4)	4390(6)	6722(7)	42(2)
C(3)	1360(6)	2137(9)	6067(10)	72(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U$_{ij}$ tensor.

Table II. Bond lengths (Å) and angles (°).

Au–Cl(1)	2.275(2)	Au–Cl(2)	2.266(3)
Au–Cl(3)	2.255(4)	S(1)–C(1)	1.684(5)
S(1)–C(2)	1.704(6)	S(2)–C(2)	1.707(7)
S(2)–C(3)	1.806(10)	C(1)–C(1a)	1.433(16)
Cl(1)–Au–Cl(2)	90.2(1)	Cl(1)–Au–Cl(3)	90.0(1)
Cl(2)–Au–Cl(3)	177.0(1)	Cl(1)–Au–Cl(1b)	174.8(1)
C(1)–S(1)–C(2)	96.4(3)	C(2)–S(2)–C(3)	101.8(4)
S(1)–C(1)–S(1c)	116.5(5)	S(1)–C(1)–C(1a)	121.7(2)
S(1)–C(2)–S(2)	121.7(4)	S(1)–C(2)–C(2c)	115.4(2)
S(2)–C(2)–C(2c)	122.9(2)		

Symmetry operators: (a) $-x,y,2-z$; (b) $x,-y,z$; (c) $x,1-y,z$

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tion in C2/*m* thus seems preferable. The anion possesses exact *m* symmetry and the cation exact 2/*m* symmetry.

Observed and calculated structure factors in C2/*m* and anisotropic thermal parameters have been deposited as above. Any request for this material should quote the new reference number CSD 53456 and a full literature citation.

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