Structure of $[\mu-S_2[\text{Ru(PCy}_3)('S_4')]_2] \cdot 2.5 \text{ THF} \cdot 0.5 \text{ Et}_2\text{O}$

Containing Homochiral Metal Complex Fragments

$['S_4^{2-} = 1,2\text{-Bis(mercaptophenylthio)-ethane (2–)}]$  

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Crystal Structure, Ruthenium-Sulfur Complexes  

A crystal of the title compound $[\mu-S_2\{\text{Ru(PCy}_3)('S_4')\}_2] \cdot 2.5 \text{ THF} \cdot 0.5 \text{ Et}_2\text{O}$ (1 $\cdot$ 2.5 THF $\cdot$ 0.5 Et$_2$O), grown from a THF/Et$_2$O solution, was investigated by single-crystal X-ray analysis. 1 $\cdot$ 2.5 THF $\cdot$ 0.5 Et$_2$O crystallizes in the triclinic space group $P\overline{1}$ with $a = 14.209(4)$, $b = 15.390(4)$, $c = 19.526(6)$ Å, $\alpha = 111.29(2)$, $\beta = 100.43(2)$, $\gamma = 95.65(2)$°, and $Z = 2$. The crystal structure was solved by direct methods ($wR_2 = 0.1520$ for 12565 reflections; $R_1 = 0.0507$ for 9205 observed reflections). The molecular structure of 1 $\cdot$ 2.5 THF $\cdot$ 0.5 Et$_2$O is characterized by a trans $\eta^1$-$\eta^1$-$S_2$ bridge connecting two homochiral [Ru(PCy$_3$)('S$_4'$)] fragments. The S-S bond length of 1.982(2) Å and a mean Ru-S(bridge) distance of 2.234(2) Å indicate partial double bond character of these bonds. The RuSSRu unit in 1 $\cdot$ 2.5 THF $\cdot$ 0.5 Et$_2$O is a chromophore as indicated by its UV spectrum and can be described by a delocalized 4c-6e $\pi$ system.