

Synthesis and Crystal Structure of $(\text{dmaaH})_2(\text{dmaH})_2[\text{P}_{12}\text{S}_{12}\text{N}_{12}(\text{NH})_2] \cdot 4 \text{ dmaa}$, $\text{dmaa} = \text{N,N-Dimethylacetamide}$, $\text{dma} = \text{Dimethylamine}$, an Anhydrous Example of the $\text{P}_{12}\text{N}_{14}$ Cage

Stephan Roth and Wolfgang Schnick

Department of Chemistry, University of Munich (LMU),
Butenandtstraße 5-13 (block D), D-81377 Munich (Germany)

Reprint requests to Prof. Dr. W. Schnick, Fax: +49-(0)89-2180-7440.

E-mail: wsc@cup.uni-muenchen.de

Z. Naturforsch. **56 b**, 1020–1024 (2001); received July 18, 2001

Phosphorus, Cage Compounds

The title compound $(\text{dmaaH})_2(\text{dmaH})_2[\text{P}_{12}\text{S}_{12}\text{N}_{12}(\text{NH})_2] \cdot 4 \text{ dmaa}$ (**1**) was obtained by crystallization from a saturated solution of anhydrous $\text{P}_{12}\text{S}_{12}\text{N}_8(\text{NH})_6$ in N,N-dimethylacetamide (dmaa) as large single crystals. According to the X-ray structure determination ($P2_1/n$, $a = 1421.8(1)$, $b = 1556.5(2)$, $c = 1645.8(1)$ pm, $\beta = 112.207(6)^\circ$, $Z = 2$, 6388 observed reflections, $R1 = 0.046$, $wR2 = 0.111$) the anionic cage is built up from twelve P_3N_3 rings in boat conformation. N,N-dimethylammonium ions (dmaH^+) are directly connected to the cage, and pairs of N,N-dimethylacetamidonium ions (dmaaH^+) and N,N-dimethylacetamide molecules (dmaa) are interconnected by hydrogen-bonds.