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Die molekulare Zusammensetzung von erstarrten Phosphor-Schwefel-Schmelzen und die Kristallstruktur von β-P_4S_6

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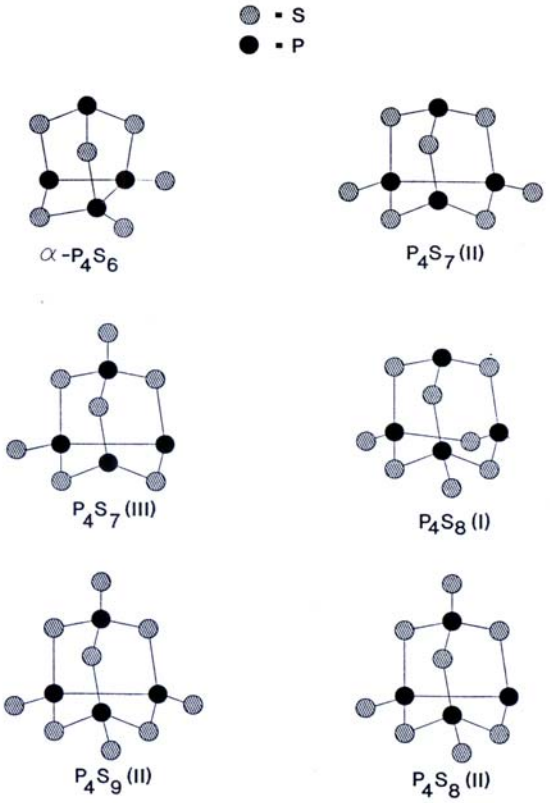

Abb. 3 Vermutete Strukturen neuer P_4S_n-Isomere (P_4S_8(I)) nach [18], α-P_4S_6 nach [21]

mensetzung sind darauf zurückzuführen, daß die Schmelzen aus P_4S_{10} und Schwefel nach dem Tempern nicht abgeschreckt, sondern langsam abgekühlt wurden.

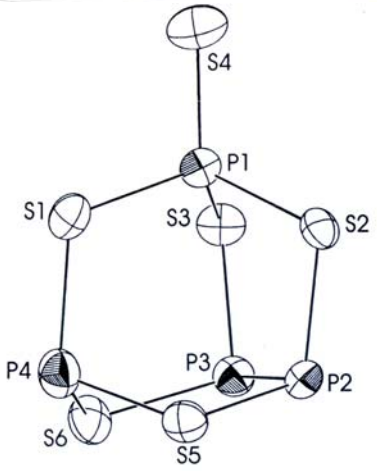

Abb. 4 Struktur des P_4S_6 Moleküls mit Schwingungsellipsoiden

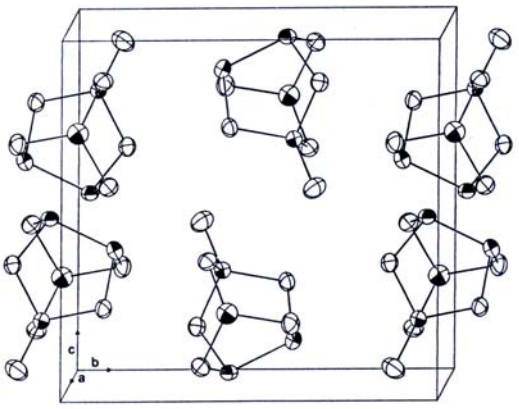

Abb. 5 Kristallstruktur von β-P_4S_6 in Richtung [100]

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Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71748 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SH1073]

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P_2Se_5

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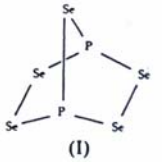
Abstract

The structure of 2,3,5,6,7-pentaselena-1,4-diphosphabicyclo[2.2.1]heptane is built from separate norbornane-like molecules with Se atoms in the bridging position. The P—Se bond lengths fall in the range 2.234 (2)–2.254 (2) Å and the Se—Se bond lengths are 2.387 (1) and 2.390 (1) Å.

Comment

A view of the molecule (I) is shown in Fig. 1. The X-ray structure analysis confirms the constitution of the molecule deduced from ^{31}P and ^{77}Se NMR data (Blachnik, Lönnecke & Tattershall, 1991) as 2,3,5,6,7-pentaselena-1,4-diphospabicyclo[2.2.1]heptane, a P—Se norbornane which consists of two



(I)

nearly regular five-membered rings. A view of the structure along [100] is shown in Fig. 2. The P_2Se_5 molecules form approximately hexagonal close-packed layers parallel to (010). These layers are shifted successively by $\vec{a}/2$ or $\vec{b}/2$, leading to a coordination number of ten for each P_2Se_5 molecule. The corresponding interlayer distances are 5.02 and 5.10 Å, respectively.

The P—Se bond distances are found in the range 2.234 (2)–2.254 (2) Å and correspond to the single-

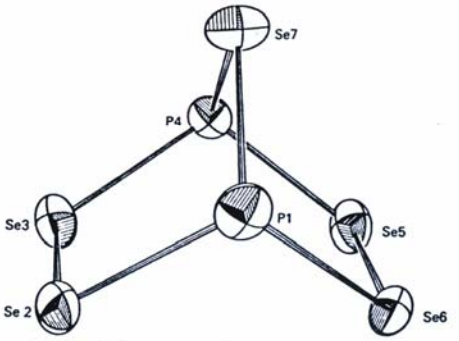


Fig. 1. Structure of the P_2Se_5 molecule.

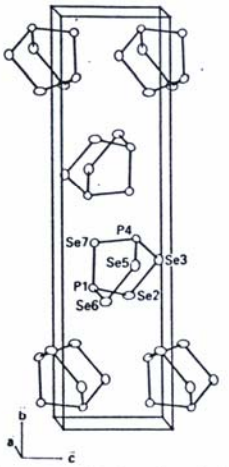


Fig. 2. Structure of P_2Se_5 viewed along [100].