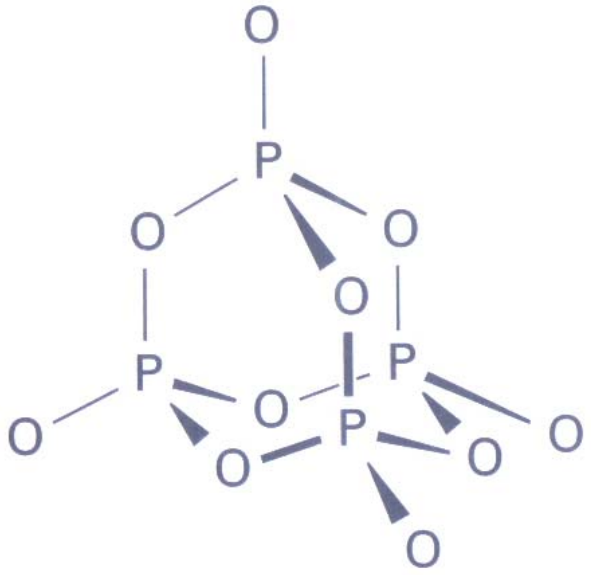
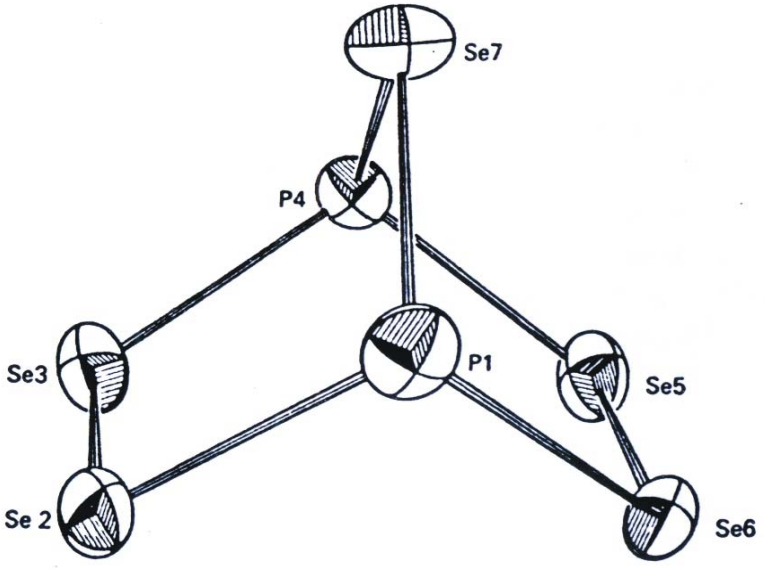
Molecular structures of „P_2O_5“ and P_2Se_5





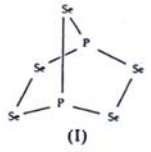
P_4O_{10} dimers of „P_2O_5“ (T_d – 43m)

The norbornane like structure of P_2Se_5 (~C_{2v} – mm2)

Crystal and Molecular structure of P_2Se_5

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-

P_2Se_5 has
40 ve's → 20 ep's
8 bonds + 12 E's

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P_2Se_5

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Abstract

The structure of 2,3,5,6,7-pentaselena-1,4-diphospha-bicyclo[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.

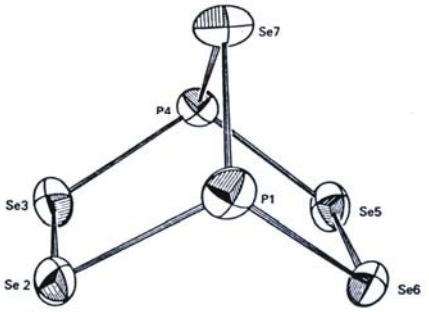

Fig. 1. Structure of the P_2Se_5 molecule.

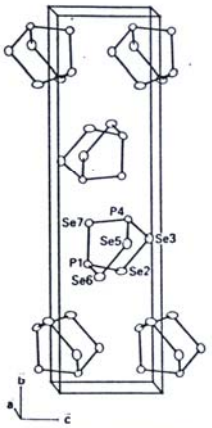

Fig. 2. Structure of P_2Se_5 viewed along [100].

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

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Professor H. J. Seifert zum 65. Geburtstag gewidmet

P_4S_6 has
56 ve's → 28 ep's
12 bonds + 16 E's

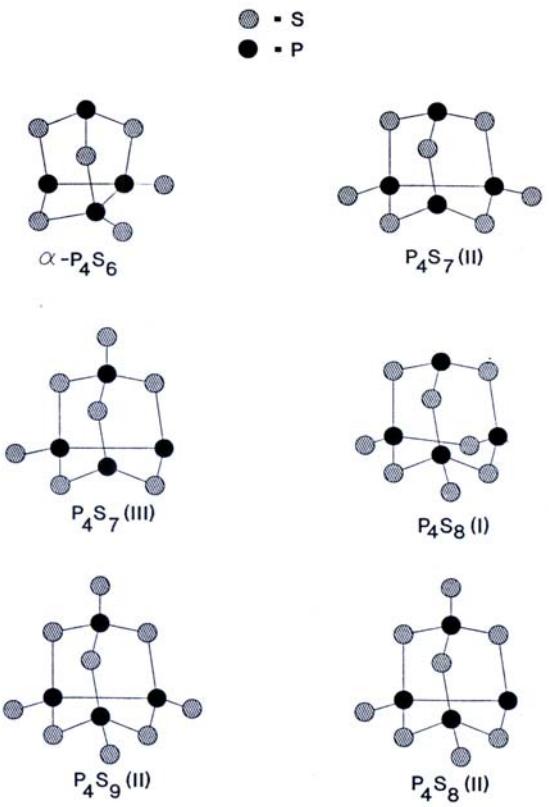


Abb. 3 Vermutete Strukturen neuer P_4S_n-Isomere (P_4S_8(I)) nach [18], α-P_4S_6 nach [21]

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

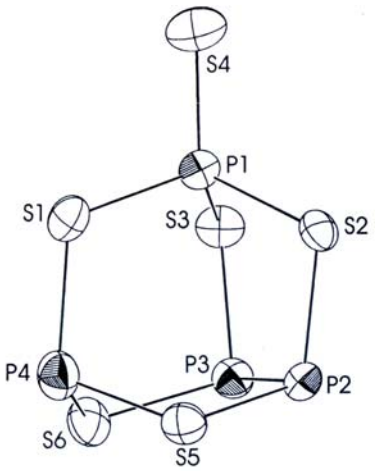


Abb. 4 Struktur des P_4S_6 Moleküls mit Schwingungsellipsoiden

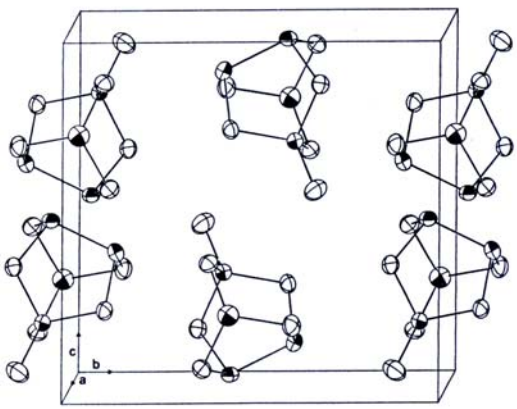
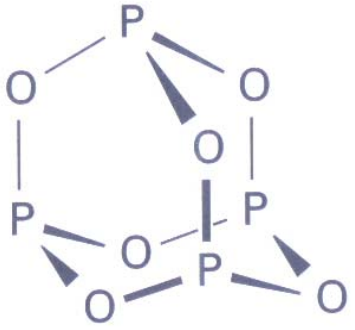


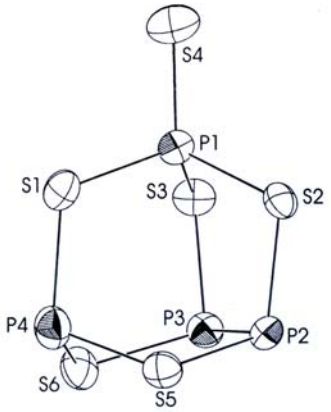
Abb. 5 Kristallstruktur von β-P_4S_6 in Richtung [100]

Molecular structures of „P_2O_3“ and β-P_4Se_6

56 ve's → 28 ep's, 12/13 bonds + 16/15 E's



P_4O_6 dimers of „P_2O_3“
(T_d – 43m)

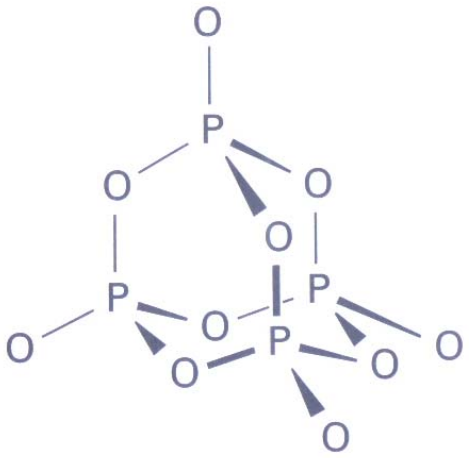


The structure of β-P_4Se_6
(C_s = m)

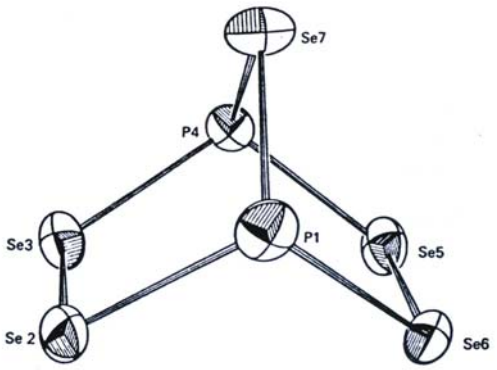
Molecular structures of „P_2O_5“ and P_2Se_5

P_4O_{10}: 80 ve's → 40 ep's, 20 bonds + 20 E's

P_2Se_5: 40 ve's → 20 ep's, 8 bonds + 12 E's



P_4O_{10} dimers of „P_2O_5“
(T_d – 43m)



The norbornane like structure of P_2Se_5 (~C_{2v} – mm2)