

Fe ₂ P	<i>hP</i> 9	(189) <i>P</i> -62 <i>m</i> – gfd
-------------------	-------------	-----------------------------------

Fe₂P [2], barringerite, Strukturbericht notation C22; Ni₂P (see remark); Mg₂In [8]; US₂ γ [6]
 Structural features: Infinite columns of base-linked PFe₆Fe₃ tricapped trigonal prisms share atoms to form a 3D-framework (a framework of base- and edge-linked PFe₆ trigonal prisms with single prism columns shifted by *c*/2 in channels). See Fig. IV.2.

Carlsson B. et al. (1973) [1]

Fe₂P

a = 0.58675, *c* = 0.34581 nm, *c/a* = 0.589, *V* = 0.1031 nm³, *Z* = 3

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.25683	0	1/2		cuboctahedron P ₄ Fe ₈
Fe2	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.59461	0	0		pseudo Frank-Kasper P ₆ Fe ₁₂
P3	2 <i>d</i>	-6..	1/3	2/3	1/2		tricapped trigonal prism Fe ₉
P4	1 <i>a</i>	-62 <i>m</i>	0	0	0		tricapped trigonal prism Fe ₉

Transformation from published data: origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.032

Remarks: Strukturbericht notation C22 was originally defined on the superseded structure proposal. Structure proposals in space group (150) *P*321 for Fe₂P [4] and Ni₂P [5] are superseded (see [2]). Refinements on neutron diffraction data are reported in [3] and [7], where the magnetic structure is studied. Mg₂In with *c/a* = 0.4 is sometimes considered as a structure type branch.

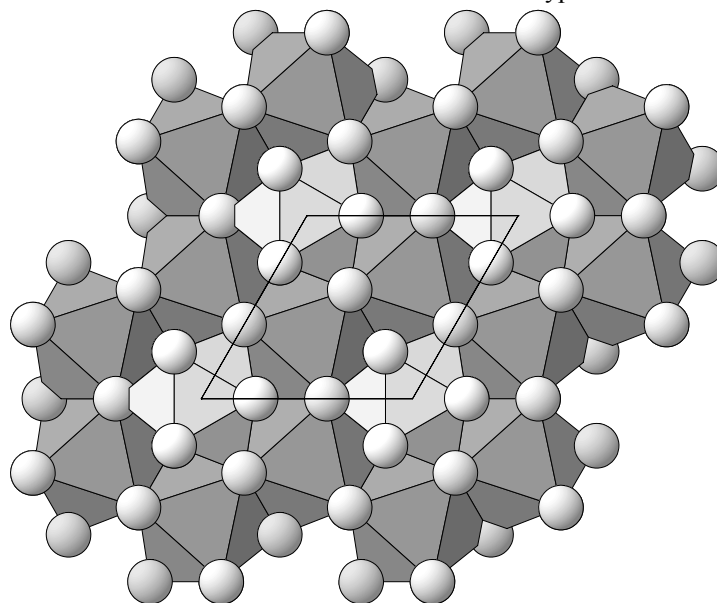


Fig. IV.2. **Fe₂P**

Arrangement of PFe₆Fe₃ tricapped trigonal prisms viewed along [001]. Light and dark prisms are shifted by *c*/2.

References: [1] Carlsson B., Gölin M., Rundqvist S. (1973), J. Solid State Chem. 8, 57-67. [2] Rundqvist S., Jellinek F. (1959), Acta Chem. Scand. 13, 425-432. [3] Fujii H., Komura S., Takeda T., Okamoto T., Ito Y., Akimitsu J. (1979), J. Phys. Soc. Jpn. 46, 1616-1621. [4] Hendricks S.B., Kesting P.R. (1930), Z. Kristallogr. 74, 511-533. [5] Nowotny H., Henglein E. (1938), Z. Phys. Chem., Abt. B 40, 281-284. [6]

Daoudi A., Levet J.C., Potel M., Noel H. (1996), Mater. Res. Bull. 31, 1213-1218. [7] Koumina A., Bacmann M., Fruchart D., Soubeyroux J.L., Wolfers P., Tobola J., Kaprzyk S., Niziol S., Mesnaoui M., Zach R. (1998), Ann. Chim. (Paris) 23, 177-180. [8] Schubert K., Gauzzi F., Frank K. (1963), Z. Metallkd. 54, 422-429.