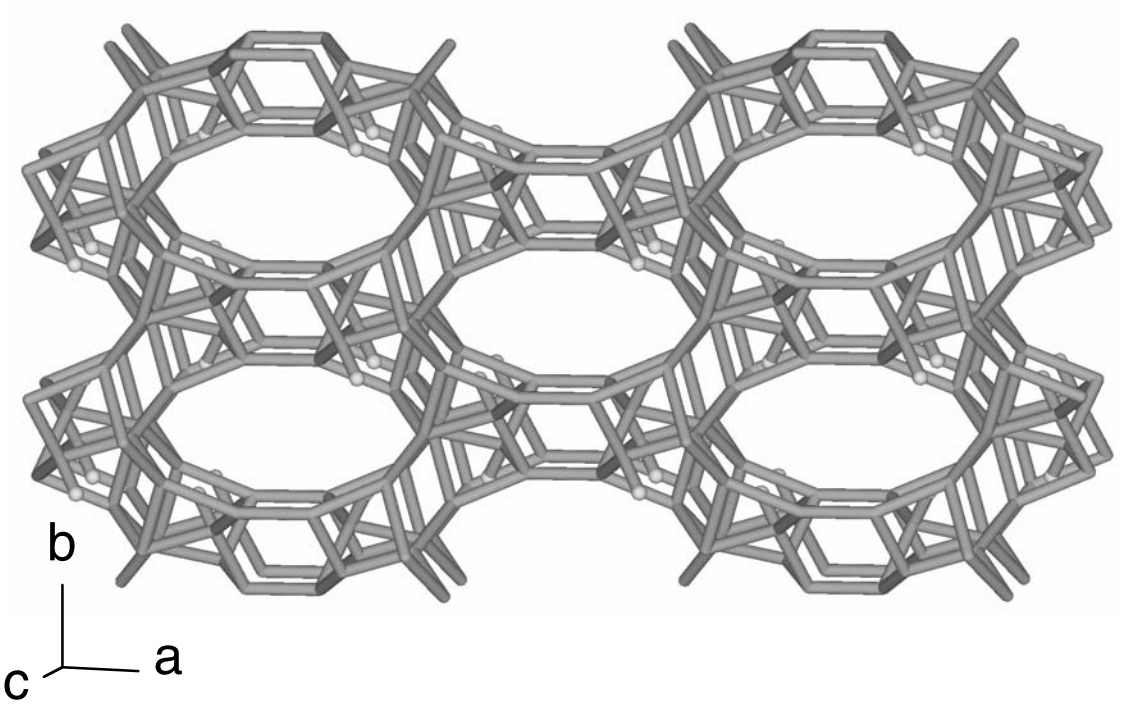
PAR

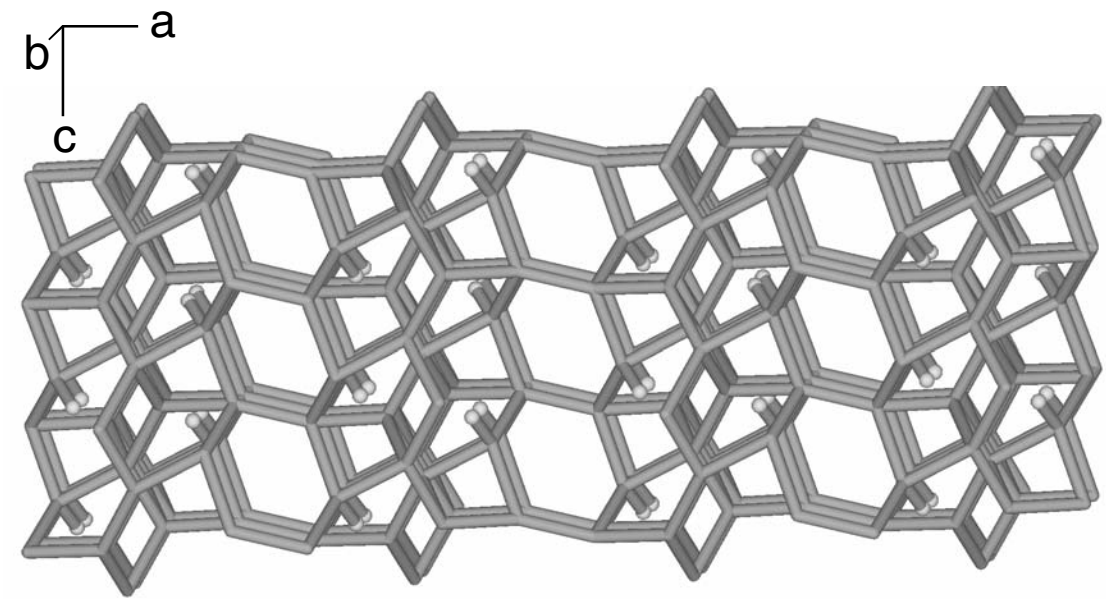
PAR.1 Zeolite framework type and topology

The framework type code is named after the mineral **PAR**théite, $Ca_2Al_4Si_4O_{15}(OH)_2 \cdot 4H_2O$, first found in the Taurus Mountains (Southwest Turkey) and described by Sarp et al. [79Sar1, cited after 84Eng1]. A first description of its aluminosilicate framework structure was given by Engel and Yvon [84Eng1] in space group *C* 1 2/c 1 representing the highest possible topological symmetry. The interrupted framework structure (Fig. PAR.1.1) consists of one-dimensional 10-ring channels parallel **c** crosslinked by a complex network of Si and Al atoms which cannot be described in terms of simple polyhedral building units. Every second Al atom (Al 1) has a terminal OH group interrupting the framework. The linkage around the 10-ring opening is shown in Fig. PAR.1.2 and the building scheme is shown in Fig. PAR.1.3.



a View parallel **c** rotated by 4° about **b** and **b**×**c**.

Fig. PAR.1.1. The framework structure of PAR-type compounds in the highest possible topological symmetry *C* 1 2/c 1. Terminal OH groups are indicated by small circles with bonds to Al 1 atoms.



b View parallel **b** rotated by 2° about **c** and **b**×**c**.

Fig. PAR.1.1. (continued). The framework structure of PAR-type compounds in the highest possible topological symmetry *C*1 2/c 1. Terminal OH groups are indicated by small circles with bonds to Al 1 atoms.

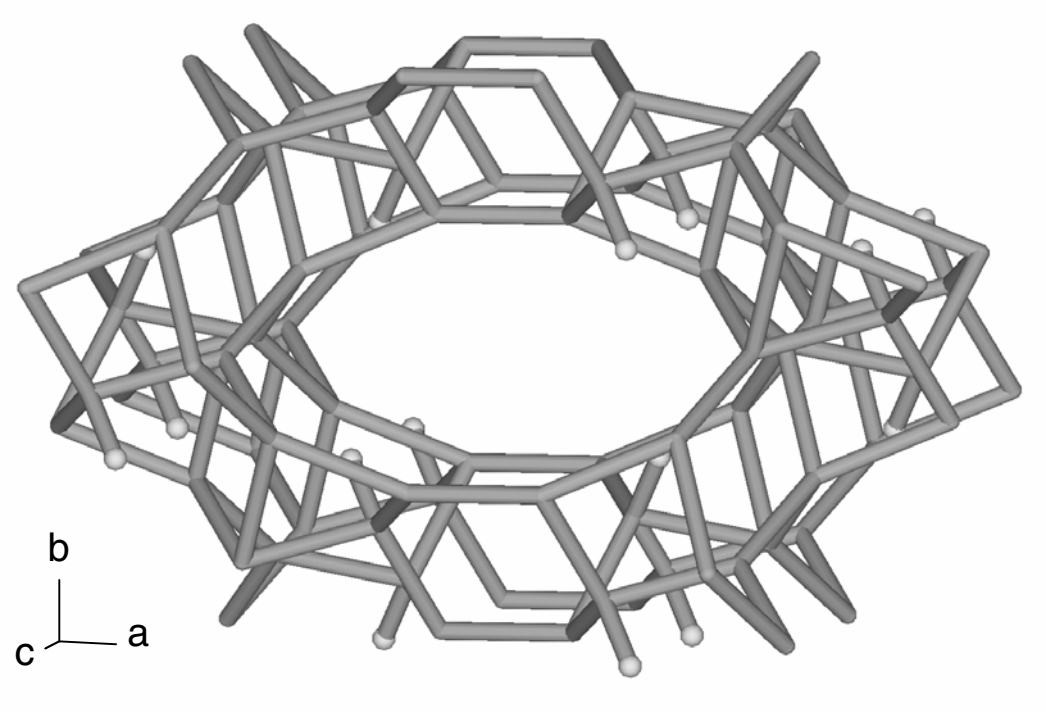


Fig. PAR.1.2. The linkage of T-atoms around the 10-ring opening. Terminal OH groups are indicated by small circles with bonds to Al 1 atoms. View parallel **c** rotated by 8° about **b** and 4° about **b**×**c**.

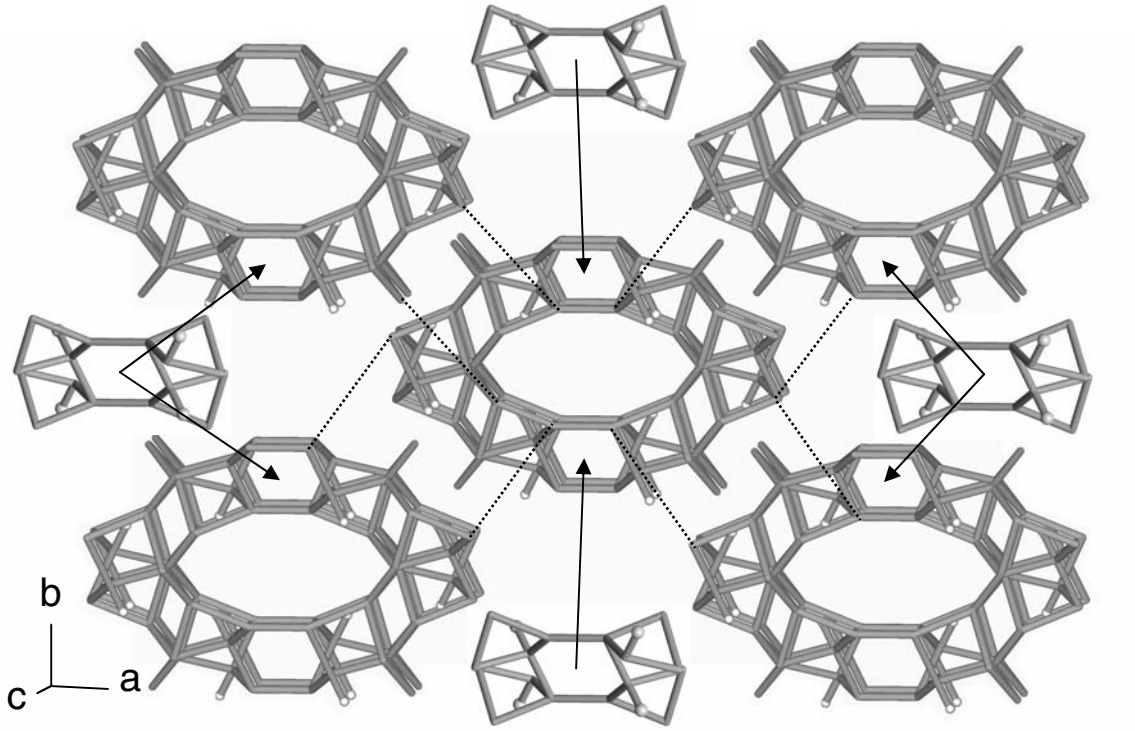


Fig. PAR.1.3. The building scheme of PAR-type compounds. The 10-ring channels are linked according to the C-centering of the unit cell with T16 units [2006van1] in the 6-ring nodes between adjacent channels as indicated by the arrows. View parallel **c** rotated by 2° about **b** and **b**×**c**.

PAR.2 Compounds and crystal data

Table PAR.2.1 Chemical data.

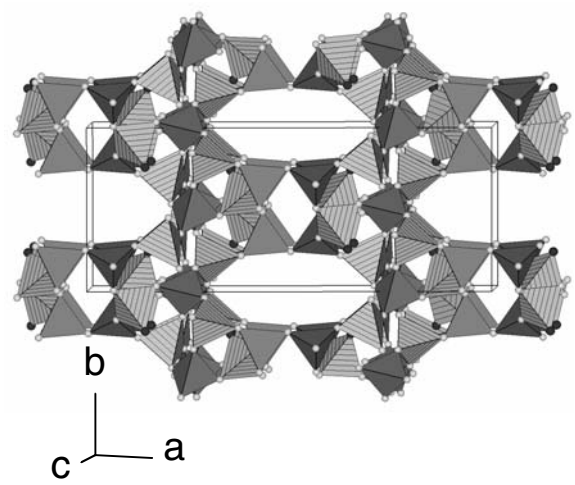
FD = framework density CE = cation exchange TT = thermal treatment REF = reference
SM = source of material SR = sorbate T = temperature of thermal treatment [K]

code	chemical composition	FD	SM	CE	SR	TT	T	REF
PAR-I *C* 1 2/c 1								
PAR1984a01	$Ca_8 \cdot Al_{16}Si_{16}O_{60}(OH)_8 \cdot 16H_2O$	18.2	M	-	H_2O	-	-	84Eng1

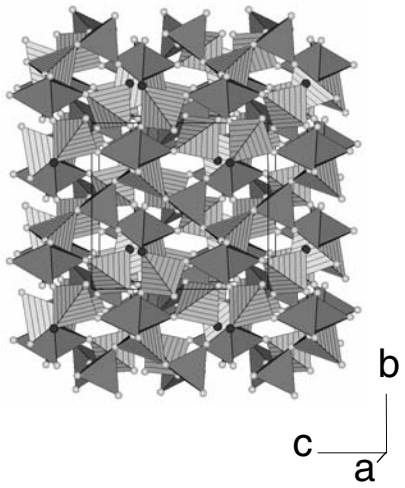
Table PAR.2.2 Structural parameters of PAR-type compound.

code	*a* [Å]	*b* [Å]	*c* [Å]	β [°]	*V* [Å^3]	*T* [K]	reference
PAR-I *C* 1 2/c 1							
PAR1984a01	21.555(3)	8.761(1)	9.304(2)	91.55(2)	1756	n.s.	84Eng1

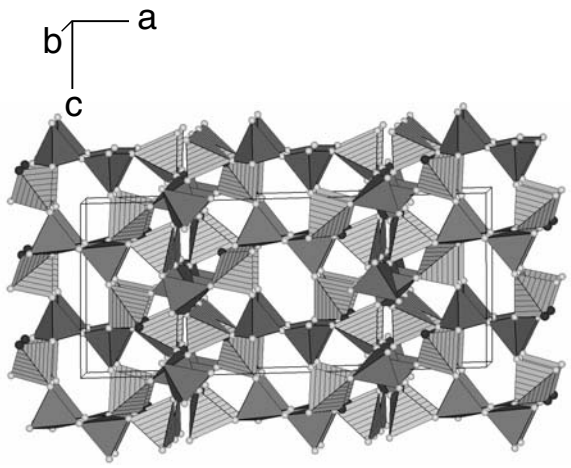
PAR.3 Framework structure of PAR-I compound (*C* 1 2/c 1, IT #15)



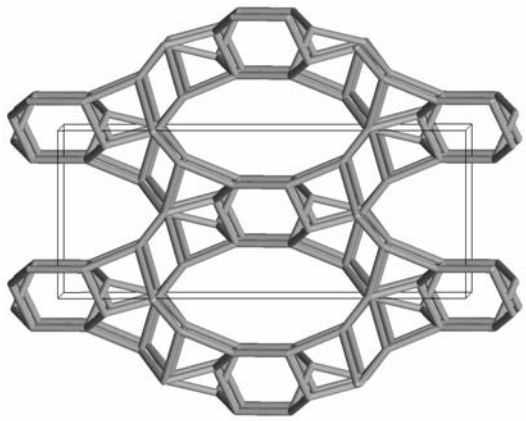
a View parallel **c**] rotated by 2° about **b** and **b**×**c**.



b View parallel **a** rotated by 1° about **b** and **a**×**b**.



c View parallel **b** rotated by 2° about **a** and **a**×**b**.



b Ball and stick model corresponding to a) slightly extended parallel **c**.

Fig. PAR.3.1 Projections of the PAR-I crystal structure of parthéite $Ca_8 \cdot Al_{16}Si_{16}O_{68}H_8 \cdot 16H_2O$ (PAR1984a01, 84Eng1).

Table PAR.3.1 Atomic coordinates and site definitions for PAR-I, parthéite, $Ca_8 \cdot Al_{16}Si_{16}O_{68}H_8 \cdot 16H_2O$ 84Eng1).

atom	*x*	*y*	*z*	B_{eq} [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Si1	0.06729(9)	0.1832(3)	0.2896(2)	0.53	1	8(f)	8
Si2	0.23983(9)	0.0077(3)	0.4621(2)	0.46	1	8(f)	8
Al 1	0.1161(1)	0.0844(3)	0.6006(3)	0.56	1	8(f)	8
Al2	0.1999(1)	0.3162(3)	0.2858(2)	0.51	1	8(f)	8
O1	0.0695(2)	0.0181(7)	0.2162(6)	0.73	1	8(f)	8
O2	0.0725(2)	0.1719(7)	0.4626(6)	0.84	1	8(f)	8
O3	0.1222(2)	0.2883(7)	0.2295(6)	0.90	1	8(f)	8
O4	0.1722(2)	0.0363(6)	0.0250(6)	0.86	1	8(f)	8
O5	0.2081(2)	0.4669(6)	0.4096(6)	0.71	1	8(f)	8
O6	0.2345(3)	0.1550(6)	0.3605(6)	0.84	1	8(f)	8
O7	0.2340(2)	0.3599(6)	0.1221(6)	0.76	1	8(f)	8
O8	0	0.2632(9)	¼	0.63	2	4(e)	4
OH9	0.3523(3)	0.2673(7)	0.2918(6)	1.11	1	8(f)	8
Ca1	0.35586(7)	0.1991(2)	0.0444(2)	0.93	1	8(f)	8
OW1	0.0712(3)	0.5050(8)	0.0159(9)	2.63	1	8(f)	8
OW2	0.4541(3)	0.3070(8)	0.0800(7)	1.72	1	8(f)	8

Table PAR.3.1.2 Selected interatomic distances and angles for PAR-I, parthéite, $Ca_8 \cdot Al_{16}Si_{16}O_{68}H_8 \cdot 16H_2O$ 84Eng1).

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Si1 - O1	1.601(7)	138.9(3)	Si2 - O6	1.602(6)	156.4(4)
Si1 - O3	1.612(6)	132.7(4)	Si2 - O7	1.623(6)	138.9(4)
Si1 - O2	1.614(6)	141.4(4)	Si2 - O5	1.631(5)	129.6(3)
Si1 - O8	1.644(4)	129.5(5)	Si2 - O4	1.632(5)	129.0(3)
mean	1.617	135.6	mean	1.622	138.5
Al 1 - O1	1.741(6)	138.9(3)	Al2 - O6	1.734(6)	156.4(4)
Al 1 - O2	1.748(6)	141.4(4)	Al2 - O7	1.751(6)	138.9(4)
Al 1 - OH9	1.766(7)	-	Al2 - O5	1.758(6)	129.6(3)
Al 1 - O4	1.767(5)	129.0(3)	Al2 - O3	1.758(5)	132.7(4)
mean	1.755	136.4	mean	1.750	139.4

PAR.4 Chemical composition

	D																
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	L	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

Fig. PAR.4.1 Chemical elements (highlighted) occurring in PAR-type compounds. Framework cations are in grey fields.

PAR.5 Flexibility and apertures

There is insufficient information available about the PAR-type to judge its flexibility.

The 10-ring openings in the PAR-type framework are compressed into ellipses, with diameters approximately 3.5 Å by 7 Å, as compared with the more regular dimensions of the MFI-type where they are about 5 Å by 5.5 Å.

PAR.6 Other information

No useful properties have been reported for PAR-type compounds.

PAR.7 References

79Sar1 Sarp, H., Deferne, J., Bizouard, H., Liebich, B.W.: Bull. Suisse Min. Petrogr. **59** (1979) 5.

84Eng1 Engel, N., Yvon, K.: Z. Kristallogr. **169** (1984) 165.

2006van1 van Koningsveld, H.: http://topaz.ethz.ch/IZA-SC/ModelBuilding.htm

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