PON

PON.1 Zeolite framework type and topology

The framework type code (FTC) is named after the origin of the type material IST-1 (**I**nstituto **S**uperior **T**écnico, Lisboa) first synthesized by [2001Bor1] in **P**ortugal assigning sequence number **ON**e. The framework structure (Fig. PON.1.1) was solved by Jordá et al. [2003Jor1]. It can be described as being built from *bb39* ($4^2 4^2 6^2$) units forming one-dimensional channels outlined by 10-rings parallel **a** as shown in Fig. PON.1.2.

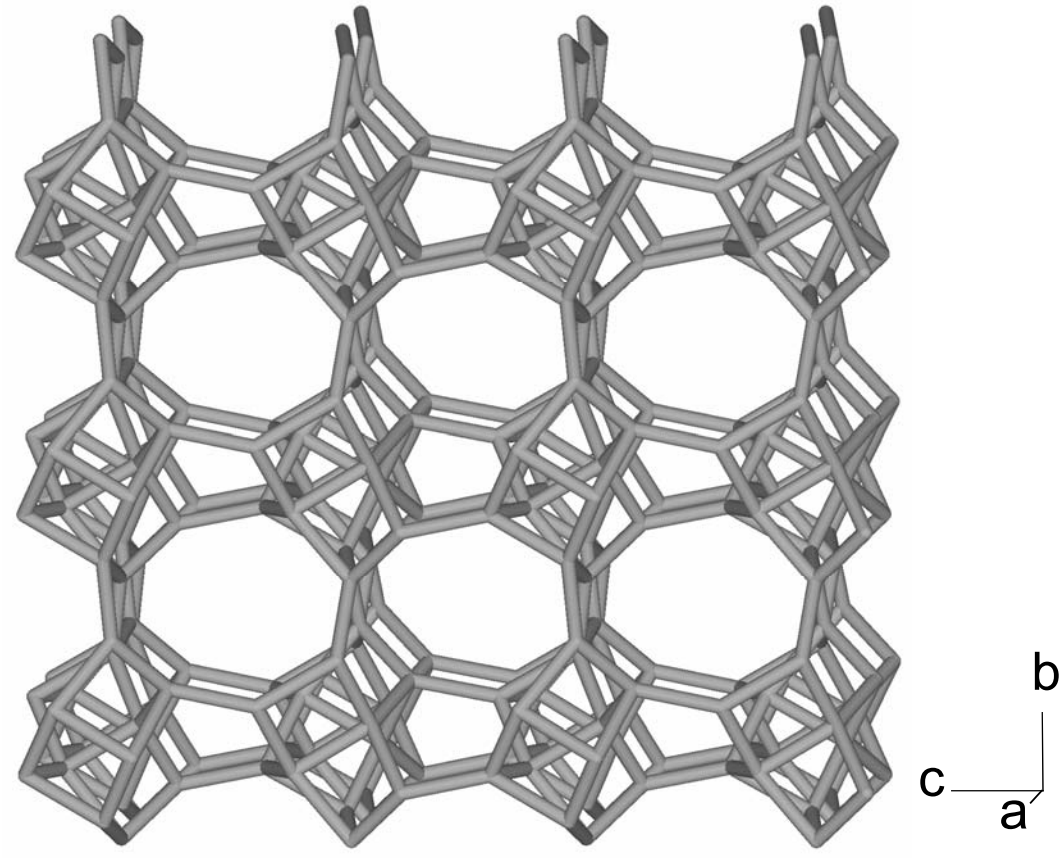
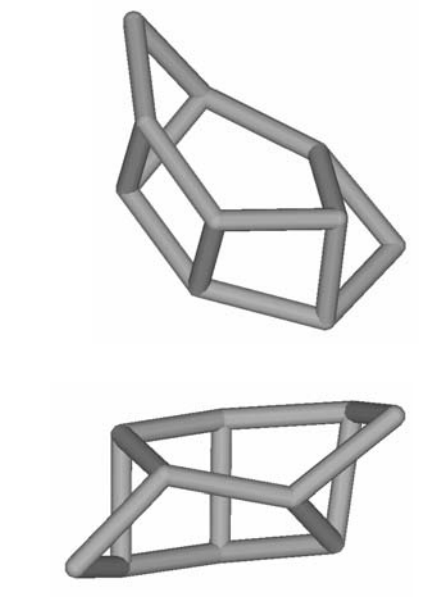
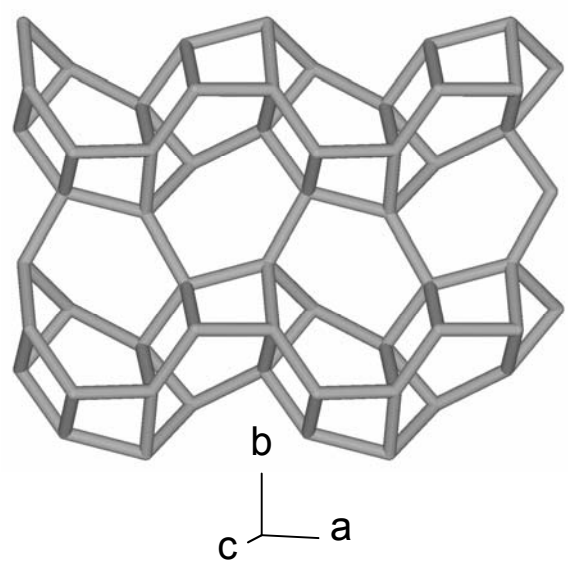


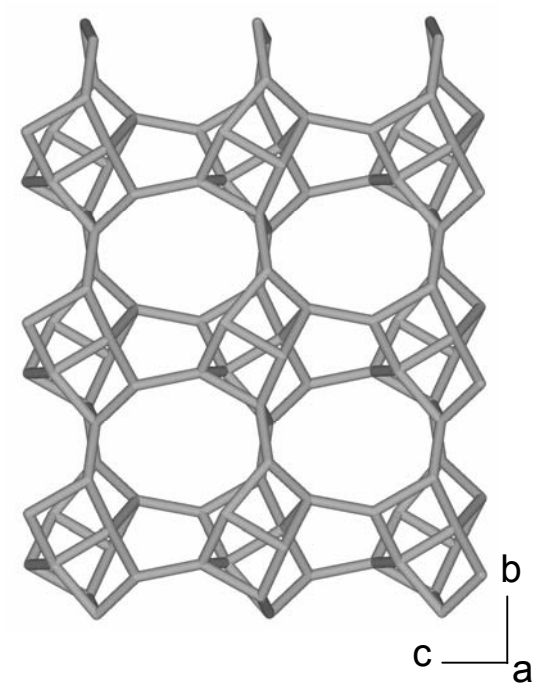
Fig. PON.1.1. The framework structure of PON-type compounds in the highest possible topological symmetry *P c a* 2_1. View parallel **a** rotated by 4° about **b** and **c**.



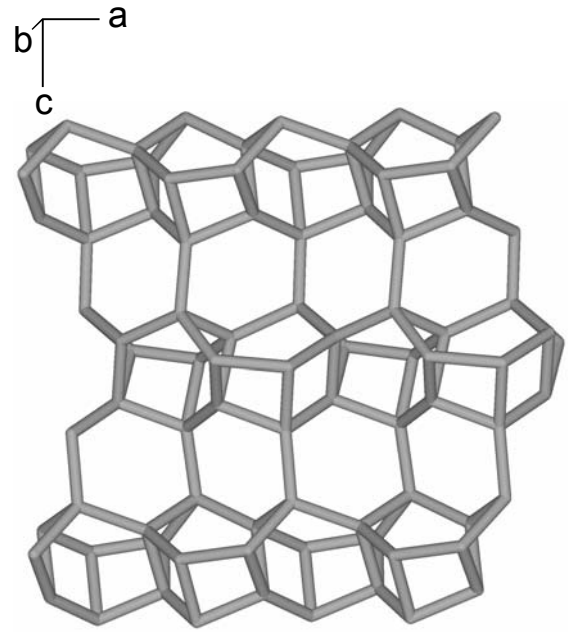
a The *bb39* unit in two different orientations.



b View parallel **c** rotated by 2° about **a** and **b**. The *bb39* units are directly linked parallel **a** and crosslinked by additional bonds parallel **b**.



c View parallel **a**. The *bb39* units are crosslinked parallel **b** and **c** forming the one-dimensional channels.



d View parallel **b** rotated by 4° about **a** and 8° about **c**. The *bb39* units are directly linked parallel **a** and crosslinked by additional bonds parallel **c**.

Fig. PON.1.2 Two-dimensional linkage of the *bb39* units in the main planes of the unit cell.

PON.2 Compounds and crystal data

Table PON.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
PON-I ***Pca*2$_1$**								
PON2003a0 1	$Al_{12}P_{12}O_{48} \cdot 4CH_3NH_2$ $4CH_3NH_3$ 4OH	13.4	S	-	MMA, OH HMMA	-	-	2003Jor1

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

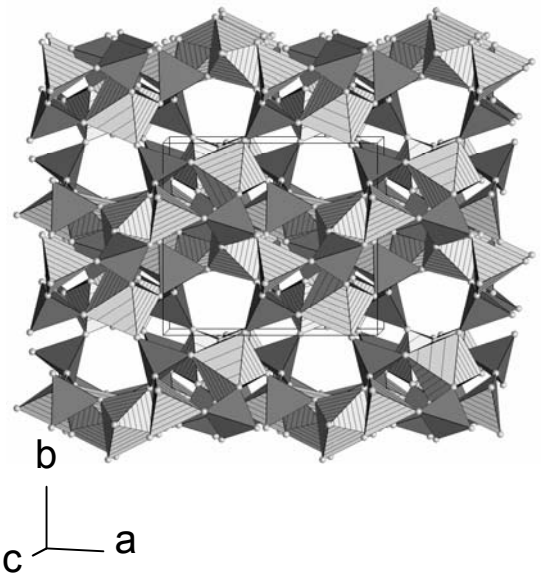
code	*a* [Å]	*b* [Å]	*c* [Å]	*V* [Å^3]	*T* [K]	reference
PON-I ***Pca*2$_1$**						
PON2003a01	9.61523(1)	8.67024(1)	16.21957(2)	1352	n.s.	2003Jor1

PON.3 Framework structure of PON-I (*Pca*2$_1$, IT #29)

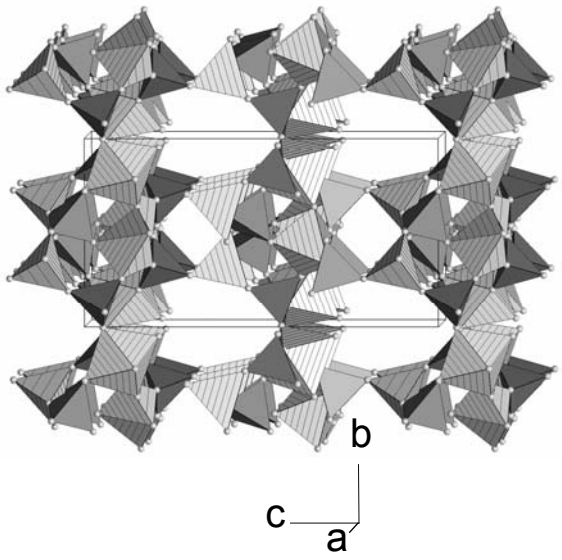
Table PON.3.1 Atomic coordinates and site definitions for PON-I, IST-1, $Al_{12}P_{12}O_{48} \cdot 4CH_3NH_2$ $4CH_3NH_3$ 4OH, PON2003a01, 2003Jor1).

atom	*x*	*y*	*z*	*B* [Å^2]	site symmetry	Wyckoff position	no. of atoms in unit cell
Al 1	0.1950(3)	0.8346(3)	0.3921(2)	0.43(2)	1	4(a)	4
Al2	0.0171(3)	0.6502(3)	0.1040(2)	0.43(2)	1	4(a)	4
Al3	0.1780(3)	0.4521(3)	0.3614(2)	0.43(2)	1	4(a)	4
P4	0.0380(3)	0.3284(3)	0.7909	0.43(2)	1	4(a)	4
P5	0.1877(3)	0.5844(3)	0.5345(2)	0.43(2)	1	4(a)	4
P6	0.0259(2)	0.1513(3)	0.4455(2)	0.43(2)	1	4(a)	4
O1	0.3738(5)	0.8960(6)	0.4306(4)	0.59(3)	1	4(a)	4
O2	0.1470(6)	0.7320(6)	0.4927(3)	0.59(3)	1	4(a)	4
O3	0.0188(5)	0.7988(5)	0.3478(4)	0.59(3)	1	4(a)	4
O4	0.1226(5)	0.0127(6)	0.4409(5)	0.59(3)	1	4(a)	4
O5	0.2011(5)	0.3396(6)	0.8031(3)	0.59(3)	1	4(a)	4
O6	0.9740(5)	0.4831(5)	0.8070(4)	0.59(3)	1	4(a)	4
O7	0.0198(6)	0.2780(5)	0.7014(4)	0.59(3)	1	4(a)	4
O8	-0.0371(5)	0.7890(6)	0.0367(4)	0.59(3)	1	4(a)	4
O9	0.1931(5)	0.6098(6)	0.0977(4)	0.59(3)	1	4(a)	4
O10	0.9400(6)	0.4761(6)	0.0856(4)	0.59(3)	1	4(a)	4
O11	0.0676(5)	0.2760(6)	0.3868(4)	0.59(3)	1	4(a)	4
O12	0.2282(5)	0.4627(6)	0.4698(3)	0.59(3)	1	4(a)	4
OH13	0.7393(4)	0.3535(5)	0.8459(3)	0.59(3)	1	4(a)	4
C1	0.1528(6)	0.9036(8)	0.7281(4)	3.95	1	4(a)	6.00
N1	0.2603(7)	0.9621(7)	0.7855(4)	3.95	1	4(a)	5.16
C2	0.1442(7)	0.1472(8)	0.1047(4)	3.95	1	4(a)	6.00
N2	0.1317(6)	0.1829(7)	0.0146(3)	3.95	1	4(a)	5.72

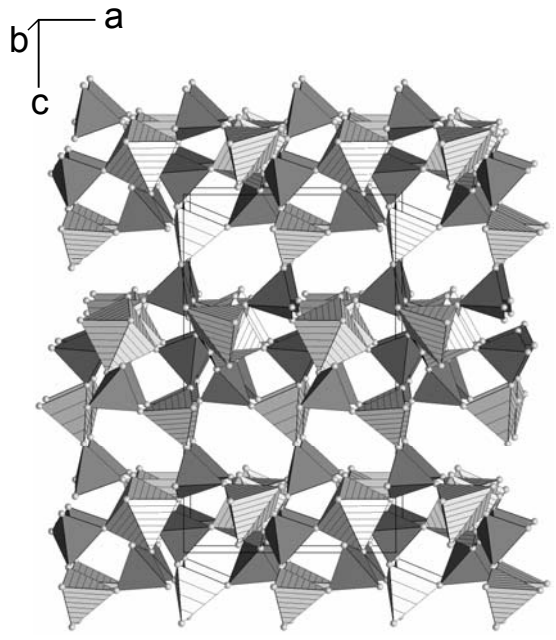
The only observed crystal structure of this type (IST-1) has 6-coordinated Al 1 and 5-coordinated Al3 atoms. However, the crystal structure can be described as a 4-connected framework if the additional N1-atom and the OH13 group are omitted.



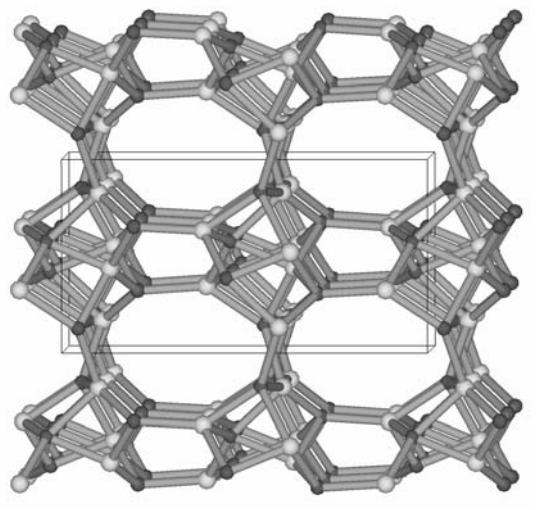
a View parallel **c** rotated by 1° about **a** and **b**.



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



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



d Ball and stick model corresponding to b).

Fig. PON.3.1 Projections of the PON-I crystal structure of IST-1, $Al_{12}P_{12}O_{48}$ · $4CH_3NH_2$ $4CH_3NH_3$ 4OH, PON2003a01, 2003Jor1). AlO_4NOH groups and AlO_4 tetrahedra are light grey and hatched. PO_4 tetrahedra are dark grey.

Table PON.3.2 Selected interatomic distances and angles for PON-I, IST-1, $Al_{12}P_{12}O_{48}$ · $4CH_3NH_2$ $4CH_3NH_3$ 4OH, PON2003a01, 2003Jor1). Atoms OH13 and N1 are not part of the four-connected framework.

	T - O [Å]	T - O - T [°]		T - O [Å]	T - O - T [°]
Al 1 - O3	1.866(6)	132.3(3)	Al3 - O5	1.788(6)	138.0(4)
Al 1 - O4	1.870(6)	154.3(5)	Al3 - O6	1.797(6)	134.4(4)
Al 1 - O1	1.905(6)	146.6(4)	Al3 - O12	1.826(6)	128.7(3)
Al 1 - O2	1.915(6)	135.9(4)	Al3 - O11	1.905(6)	150.1(4)
Al 1 - OH13	1.903(5)	125.1(3)	Al3 - OH13	1.881(5)	125.1(3)
Al 1 - N1	2.097(7)	-	mean of first four	1.829	137.8
mean of first four	1.889	142.8	mean of all five	1.839	135.3
mean of first five	1.892	139.3			
mean of all six	1.926	-			
Al2 - O8	1.706(6)	144.5(4)	P4 - O6	1.499(5)	134.4(4)
Al2 - O10	1.708(6)	136.6(4)	P4 - O7	1.526(6)	141.9(3)
Al2 - O9	1.731(6)	142.1(4)	P4 - O3	1.538(6)	132.3(3)
Al2 - O7	1.735(7)	141.9(3)	P4 - O5	1.584(6)	138.0(4)
Mean	1.720	141.3	mean	1.537	136.7
P5 - O2	1.500(6)	135.9(4)	P6 - O11	1.495(6)	150.1(4)
P5 - O12	1.538(6)	128.7(3)	P6 - O4	1.521(6)	154.3(5)
P5 - O9	1.553(6)	142.1(4)	P6 - O1	1.538(6)	146.6(4)
P5 - O10	1.572(7)	136.6(4)	P6 - O8	1.571(7)	144.5(4)
mean	1.541	135.8	mean	1.531	148.9

PON.4 Chemical composition

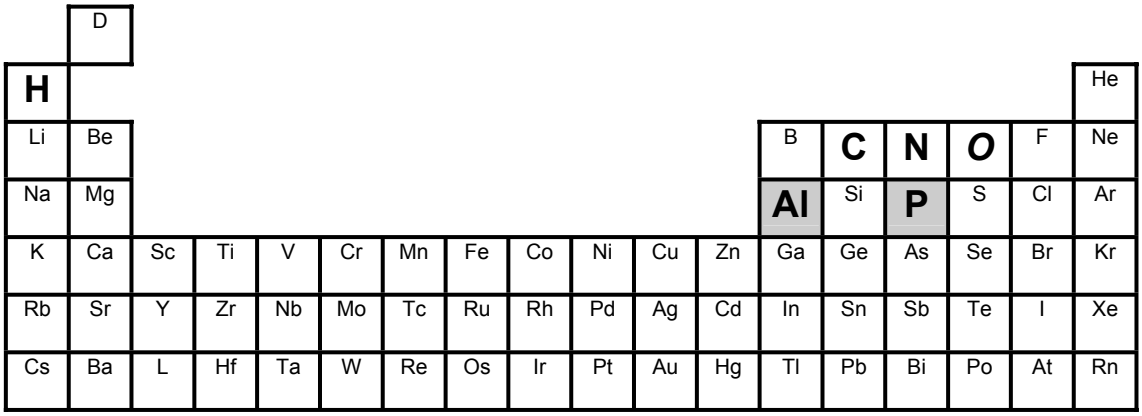


Fig. PON.4.1 Chemical elements (highlighted) occurring in PON-type compounds. Framework cations are in grey fields.

PON.5 Flexibility and apertures

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

The 10-rings in the framework of PON-type are deformed and buckled with openings around 4.5 Å and therefore clearly narrower than in the MFI-type, where they measure about 5 Å to 5.5 Å.

PON.6 Other information

Useful properties have not been reported for PON-type compounds.

PON.7 References

2001Bor1 Borges, C., Ribeiro, M.F., Henriques, C., Duarte, M.T., Laurenço, J.P., Gabelica, Z.: Stud. Surf. Sci. Catal. (2001) 194 (CD-ROM ref. 02-P-33).

2003Jor1 Jordá, J.L., McCusker, L.B., Baerlocher, C., Morais, C.M., Rocha, J., Fernandez, C., Borges, C., Laurenço, J.P., Ribeiro, M.F., Gabelica, Z.: Microporous Mesoporous Mater. (2003) 43.

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