$Fe_{21}Al_4[PO_4]_{17}O_6[OH]_{12}[H_2O]_{24}$	*hP*310	(176) $P6_3/m$ – $i^{16}h^{18}f^2c$

$Al(Al,Fe)_3Fe_{21}O_6(OH)_{12}(PO_4)_{17}(H_2O)_{24}$·~51$H_2O$ [1], cacoxenite
Structural features: Infinite chains of edge- and vertex-linked $Fe(O,OH,OH_2)_6$ octahedra and units of twelve edge- and vertex-linked $Fe(O,OH,OH_2)_6$ octahedra are interconnected via $Al(O_3[OH][OH_2]_2)$ octahedra, $Al(O_2[OH_2]_3)$ trigonal bipyramids and PO_4 tetrahedra to form a 3D-framework with large channels parallel to [001].

Moore P.B., Shen J. (1983) [1]
$Al_4Fe_{21}H_{60}O_{110}P_{17}$
a = 2.7559, c = 1.055 nm, c/a = 0.383, V = 6.9392 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Fe1	12*i*	1	0.0525	0.5125	0.1025		octahedron $O_5(OH)$
O2	12*i*	1	0.1022	0.4819	0.128		non-colinear PFe
O3	12*i*	1	0.2062	0.5907	0.015		non-colinear PFe
(OH_2)4	12*i*	1	0.241	0.51	0.047		single atom Fe
O5	12*i*	1	0.3533	0.5239	0.122		non-colinear PFe
O6	12*i*	1	0.3606	0.4256	0.122		non-colinear PFe
O7	12*i*	1	0.3839	0.0171	0.077		non-colinear PAl
P8	12*i*	1	0.3954	0.4061	0.049		tetrahedron O_4
O9	12*i*	1	0.3989	0.3591	0.119		non-colinear PFe
(OH)10	12*i*	1	0.4816	0.332	0.115		non-colinear Fe_2
O11	12*i*	1	0.5284	0.1817	0.113		non-colinear PFe
O12	12*i*	1	0.5403	0.1053	0.021		non-colinear PFe
O13	12*i*	1	0.5428	0.0001	0.031		single atom P
Fe14	12*i*	1	0.5471	0.3242	0.1066		octahedron $O_3(OH)_2(OH_2)$
P15	12*i*	1	0.5522	0.1657	0.0		tetrahedron O_4
O16	12*i*	1	0.606	0.2979	0.114		single atom P
(OH)17	6*h*	*m*..	0.0025	0.4505	$^1/_4$		non-coplanar triangle $AlFe_2$
O18	6*h*	*m*..	0.0672	0.3941	$^1/_4$		non-colinear PAl
O19	6*h*	*m*..	0.074	0.5596	$^1/_4$		non-coplanar triangle Fe_3
P20	6*h*	*m*..	0.1129	0.4574	$^1/_4$		tetrahedron O_4
O21	6*h*	*m*..	0.1709	0.4646	$^1/_4$		single atom P
(OH_2)22	6*h*	*m*..	0.256	0.636	$^1/_4$	0.5	
(OH_2)23	6*h*	*m*..	0.259	0.603	$^1/_4$	0.5	
(OH_2)24	6*h*	*m*..	0.271	0.427	$^1/_4$		single atom Fe
(OH_2)25	6*h*	*m*..	0.325	0.034	$^1/_4$		single atom Al
Fe26	6*h*	*m*..	0.3619	0.4759	$^1/_4$		octahedron $O_5(OH_2)$
(OH_2)27	6*h*	*m*..	0.376	0.262	$^1/_4$		single atom Fe
Al28	6*h*	*m*..	0.3831	0.0107	$^1/_4$		octahedron $O_3(OH)(OH_2)_2$
Fe29	6*h*	*m*..	0.4398	0.3458	$^1/_4$		octahedron $O_2(OH)_2(OH_2)_2$
(OH_2)30	6*h*	*m*..	0.443	0.094	$^1/_4$		single atom Al
(OH)31	6*h*	*m*..	0.5172	0.2646	$^1/_4$		non-coplanar triangle Fe_3
(OH_2)32	6*h*	*m*..	0.57	0.079	$^1/_4$		single atom Fe
Fe33	6*h*	*m*..	0.5717	0.233	$^1/_4$		octahedron $O_5(OH)$
O34	6*h*	*m*..	0.6294	0.215	$^1/_4$		non-coplanar triangle Fe_3
O35	4*f*	3..	$^1/_3$	$^2/_3$	0.078		colinear PAl
P36	4*f*	3..	$^1/_3$	$^2/_3$	0.562		tetrahedron O_4
Al37	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		

Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.118

Remarks: Natural specimen from Shady, Arkansas. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Moore P.B., Shen J. (1983), Nature (London) 306, 356-358.