$Ca_4Pb_6[Si_2O_7]_3Cl_2$	*hP*78	(176) $P6_3/m$ – $i^5hfdcba$

$Ca_4Pb_6(Si_2O_7)_3Cl_2$ [1], nasonite
Structural features: Infinite columns of face-linked CaO_6 trigonal prisms, units of two vertex-linked SiO_4 tetrahedra and $:PbO_3$ ψ-tetrahedra share atoms to form a 3D-framework; Cl in channels parallel to [001] (infinite columns of face-linked $ClPb_6$ octahedra and trigonal prisms).

Giuseppetti G. et al. (1971) [1]
$Ca_4Cl_2O_{21}Pb_6Si_6$
a = 1.008, c = 1.327 nm, c/a = 1.316, V = 1.1677 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.1455	0.5203	0.1275		single atom Si
Pb2	12*i*	1	0.26493	0.25801	0.10862		non-coplanar triangle O_3
O3	12*i*	1	0.3291	0.071	0.0556		single atom Si
Si4	12*i*	1	0.4198	0.0259	0.1356		tetrahedron O_4
O5	12*i*	1	0.6051	0.1412	0.1208		single atom Si
O6	6*h*	*m*..	0.383	0.0714	$^1/_4$		non-colinear Si_2
Ca7	4*f*	3..	$^1/_3$	$^2/_3$	0.0064		trigonal prism O_6
Ca8	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		tricapped trigonal prism O_9
Ca9	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		trigonal prism O_6
Cl10	2*b*	-3..	0	0	0		octahedron Pb_6
Cl11	2*a*	-6..	0	0	$^1/_4$		trigonal prism Pb_6

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.054

Remarks: Natural specimen from Franklin, New Jersey. The structure was refined on X-ray diffraction data in space group (176) $P6_3/m$ in [2] (coordinates not published), however, electron microscopy studies indicated deviations from hexagonal symmetry.

References: [1] Giuseppetti G., Rossi G., Tadini C. (1971), Am. Mineral. 56, 1174-1179. [2] Brès F.F., Waddington W.G., Hutchison J.L., Cohen S., Mayer I., Voegel J.C. (1987), Acta Crystallogr. B 43, 171-174.