$Ca_{17}[NO_3]_{34}[H_2O]_{21}$	*hP*364	(176) $P6_3/m$ – $i^{26}h^5f^4ed$

$Ca(NO_3)_2 \cdot 1.24H_2O$ [1]
Structural features: CaO_{12} icosahedra, $Ca(O_9[OH_2])$, $Ca(O_8[OH_2]_2)$ and $Ca(O_{10}[OH_2])$ polyhedra share atoms with NO_3 trigonal units (in part orientational disorder); additional NO_3 (partial orientational disorder) coordinated by H_2O.

Leclaire A. (1976) [1]
$Ca_{17}H_{42}N_{34}O_{123}$
$a = 1.3226$, $c = 3.237$ nm, $c/a = 2.447$, $V = 4.9038$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	12*i*	1	0.00614	0.22466	0.04765		single atom N
O2	12*i*	1	0.01576	0.10129	0.19146		single atom N
O3	12*i*	1	0.03251	0.40915	0.17477		single atom N
Ca4	12*i*	1	0.11313	0.42801	0.01431		bicapped square prism $(OH_2)O_9$
$(OH_2)5$	12*i*	1	0.13109	0.13408	0.11054		single atom Ca
$(OH_2)6$	12*i*	1	0.14649	0.4436	0.08695		single atom Ca
O7	12*i*	1	0.19355	0.33393	0.21617		single atom N
O8	12*i*	1	0.23586	0.63108	0.1706	0.333	
Ca9	12*i*	1	0.24204	0.19792	0.17426		bicapped square prism $(OH_2)_2O_8$
O10	12*i*	1	0.26977	0.17671	0.0391		single atom N
O11	12*i*	1	0.2799	0.036	0.1422		single atom N
N12	12*i*	1	0.28031	0.09055	0.0313		coplanar triangle O_3
$(OH_2)13$	12*i*	1	0.28967	0.37449	0.13398		single atom Ca
O14	12*i*	1	0.30888	0.57813	0.17889	0.333	
N15	12*i*	1	0.3334	0.03096	0.17311		coplanar triangle O_3
O16	12*i*	1	0.34378	0.09502	0.20418		single atom N
O17	12*i*	1	0.34549	0.57896	0.02595		single atom N
O18	12*i*	1	0.35756	0.10269	0.00551		single atom N
O19	12*i*	1	0.43485	0.36855	0.19891		single atom N
O20	12*i*	1	0.45137	0.288	0.14261		single atom N
N21	12*i*	1	0.49718	0.35842	0.17173		coplanar triangle O_3
O22	12*i*	1	0.50409	0.12067	0.09025		single atom N
O23	12*i*	1	0.52501	0.02727	0.03844		single atom N
O24	12*i*	1	0.53769	0.33736	0.05464		single atom N
N25	12*i*	1	0.56175	0.11548	0.06183		coplanar triangle O_3
O26	12*i*	1	0.58314	0.18872	0.17444		single atom N
$(OH_2)27$	6*h*	*m*..	0.12621	0.54689	$^1/_4$		single atom Ca
N28	6*h*	*m*..	0.20263	0.29552	$^1/_4$		coplanar triangle O_3
O29	6*h*	*m*..	0.22529	0.21252	$^1/_4$		single atom N
Ca30	6*h*	*m*..	0.48544	0.07433	$^1/_4$		octahedron $(OH_2)O_5$
O31	6*h*	*m*..	0.55834	0.29134	$^1/_4$		single atom N
N32	4*f*	3..	$^1/_3$	$^2/_3$	0.02607		coplanar triangle O_3
O33	4*f*	3..	$^1/_3$	$^2/_3$	0.11873		single atom N
N34	4*f*	3..	$^1/_3$	$^2/_3$	0.15701		7-vertex polyhedron O_7
Ca35	4*f*	3..	$^1/_3$	$^2/_3$	0.61431		icosahedron O_{12}
N36	4*e*	3..	0	0	0.19206		coplanar triangle O_3
N37	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		coplanar triangle O_3

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$
Experimental: single crystal, diffractometer, X-rays, R = 0.039

Remarks: 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] Leclaire A. (1976), Acta Crystallogr. B 32, 1950-1953.