$H_9Ce_6Nd_7[SO_4]_{27}[H_2O]_{72.33}$	*hP*474	(176) $P6_3/m$ – $i^{34}h^{10}ec$

$H_9Ce_6Nd_7(SO_4)_{27}\cdot 72.33H_2O$ [1]
Structural features: CeO_6O_3 and $Nd(OH_2)_6O_3$ tricapped trigonal prisms are interconnected via SO_4 and $S(O_3[OH])$ tetrahedra to form infinite slabs perpendicular to [001]; additional H_2O in channels (partial disorder).

Barnes J.C. et al. (1993) [1]
$Ce_6H_{147.64}Nd_7O_{180.32}S_{27}$
a = 1.9165, c = 2.506 nm, c/a = 1.308, V = 7.9713 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ce1	12*i*	1	0.01604	0.345	0.14449		tricapped trigonal prism O_9
$(OH_2)2$	12*i*	1	0.021	0.1443	0.1994	0.5	single atom (OH_2)
O3	12*i*	1	0.0393	0.4484	0.0818		single atom S
$(OH_2)4$	12*i*	1	0.0692	0.1512	0.0814		non-colinear $(OH_2)_2$
O5	12*i*	1	0.0731	0.2961	0.2024		single atom S
O6	12*i*	1	0.0733	0.4505	0.2028		single atom S
$(OH_2)7$	12*i*	1	0.0743	0.0485	0.0287	0.16	non-colinear $(OH_2)_2$
O8	12*i*	1	0.0807	0.3141	0.0756		single atom S
$(OH_2)9$	12*i*	1	0.1474	0.065	0.1961	0.5	single atom (OH_2)
O10	12*i*	1	0.1629	0.4273	0.1272		single atom S
S11	12*i*	1	0.16703	0.37605	0.08402		tetrahedron O_4
$(OH_2)12$	12*i*	1	0.1825	0.6035	0.0891		single atom (OH_2)
O13	12*i*	1	0.2019	0.422	0.0353		single atom S
O14	12*i*	1	0.2108	0.3367	0.1017		single atom S
$(OH_2)15$	12*i*	1	0.2368	0.2266	0.1739		single atom Nd
$(OH_2)16$	12*i*	1	0.2373	0.2295	0.0396		single atom Nd
O17	12*i*	1	0.2448	0.0473	0.1289		single atom S
O18	12*i*	1	0.2523	0.097	0.0393		single atom S
S19	12*i*	1	0.29656	0.10842	0.08864		tetrahedron O_4
$(OH_2)20$	12*i*	1	0.3011	0.5642	0.1793		single atom Nd
$(OH_2)21$	12*i*	1	0.3282	0.4091	0.1795		single atom Nd
O22	12*i*	1	0.3285	0.1898	0.1086		single atom S
Nd23	12*i*	1	0.33318	0.32349	0.10674		tricapped trigonal prism $O_3(OH_2)_6$
$(OH_2)24$	12*i*	1	0.3418	0.4168	0.033		single atom Nd
O25	12*i*	1	0.3628	0.0901	0.0808		single atom S
O26	12*i*	1	0.3711	0.0874	0.2035		single atom S
$(OH_2)27$	12*i*	1	0.428	0.3191	0.1731		single atom Nd
$(OH_2)28$	12*i*	1	0.4344	0.3235	0.044		single atom Nd
O29	12*i*	1	0.4755	0.0725	0.138		single atom S
S30	12*i*	1	0.4911	0.03074	0.09367		tetrahedron O_4
$(OH_2)31$	12*i*	1	0.5182	0.2401	0.1066	0.82	non-colinear O_2
O32	12*i*	1	0.5234	0.0812	0.0463		single atom S
O33	12*i*	1	0.5438	0.0021	0.1115		single atom S
$(OH_2)34$	12*i*	1	0.6124	0.2489	0.0001	0.24	non-coplanar triangle $(OH_2)_3$
O35	6*h*	*m*..	0.0599	0.5501	$^1/_4$		single atom S
S36	6*h*	*m*..	0.0997	0.5027	$^1/_4$		tetrahedron O_4
S37	6*h*	*m*..	0.1224	0.3037	$^1/_4$		tetrahedron O_4
O38	6*h*	*m*..	0.1353	0.2353	$^1/_4$		single atom S
O39	6*h*	*m*..	0.1864	0.5532	$^1/_4$		single atom S
O40	6*h*	*m*..	0.1969	0.3791	$^1/_4$		single atom S
(OH)41	6*h*	*m*..	0.2825	0.1225	$^1/_4$		single atom S

S42	6*h*	*m*..	0.3702	0.131	$^1/_4$	tetrahedron $O_3(OH)$
O43	6*h*	*m*..	0.4187	0.2104	$^1/_4$	single atom S
(OH_2)44	6*h*	*m*..	0.5738	0.1053	$^1/_4$	non-coplanar triangle $O(OH_2)_2$
(OH_2)45	4*e*	3..	0	0	0.1568	non-coplanar triangle $(OH_2)_3$
Nd46	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$	tricapped trigonal prism $(OH_2)_6O_3$

Experimental: single crystal, diffractometer, X-rays, R = 0.038, T = 293 K

Remarks: H positions were refined but not published. 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] Barnes J.C., Paton J.D., Seaward K.F. (1993), Acta Crystallogr. C 49, 2057-2060.