| $H_9Ce_6Tb_7[SO_4]_{27}[H_2O]_{72.2}$ | *hP*466 | (176) $P6_3/m$ – $i^{33}h^{10}fec$ |
|---|---|---|

**$H_9Ce_6Tb_7(SO_4)_{27}\cdot 72.2H_2O$** [1]
Structural features: $CeO_6O_3$ and $Tb(OH_2)_6O_3$ 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). Variant of $H_9Ce_6Nd_7(SO_4)_{27}\cdot 72.33H_2O$.

Barnes J.C. (1995) [1]
$Ce_6H_{148.40}O_{180.70}S_{27}Tb_7$
$a = 1.9341$, $c = 2.5688$ nm, $c/a = 1.328$, $V = 8.3218$ nm$^3$, $Z = 2$

| site | Wyck. | sym. | *x* | *y* | *z* | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| Ce1 | 12*i* | 1 | 0.0156 | 0.34501 | 0.14474 | | tricapped trigonal prism $O_9$ |
| O2 | 12*i* | 1 | 0.0392 | 0.4479 | 0.0817 | | single atom S |
| $(OH_2)3$ | 12*i* | 1 | 0.066 | 0.1497 | 0.0797 | | non-colinear $(OH_2)_2$ |
| O4 | 12*i* | 1 | 0.0722 | 0.4511 | 0.2027 | | single atom S |
| O5 | 12*i* | 1 | 0.0727 | 0.2957 | 0.2024 | | single atom S |
| $(OH_2)6$ | 12*i* | 1 | 0.073 | 0.047 | 0.0298 | 0.17 | non-coplanar square $(OH_2)_4$ |
| O7 | 12*i* | 1 | 0.0802 | 0.3143 | 0.0757 | | single atom S |
| $(OH_2)8$ | 12*i* | 1 | 0.1205 | 0.0064 | 0.1994 | 0.5 | single atom $(OH_2)$ |
| $(OH_2)9$ | 12*i* | 1 | 0.1478 | 0.0653 | 0.1952 | 0.5 | single atom $(OH_2)$ |
| O10 | 12*i* | 1 | 0.1628 | 0.4276 | 0.1271 | | single atom S |
| S11 | 12*i* | 1 | 0.1663 | 0.3765 | 0.08415 | | tetrahedron $O_4$ |
| $(OH_2)12$ | 12*i* | 1 | 0.1833 | 0.6026 | 0.0898 | | non-colinear $(OH_2)O$ |
| O13 | 12*i* | 1 | 0.2015 | 0.4232 | 0.0356 | | single atom S |
| O14 | 12*i* | 1 | 0.2101 | 0.3365 | 0.1011 | | single atom S |
| $(OH_2)15$ | 12*i* | 1 | 0.2346 | 0.2268 | 0.1741 | | single atom Tb |
| $(OH_2)16$ | 12*i* | 1 | 0.2364 | 0.2284 | 0.04 | | single atom Tb |
| O17 | 12*i* | 1 | 0.2454 | 0.0462 | 0.1296 | | single atom S |
| O18 | 12*i* | 1 | 0.2519 | 0.0959 | 0.0394 | | single atom S |
| S19 | 12*i* | 1 | 0.2966 | 0.1081 | 0.08881 | | tetrahedron $O_4$ |
| $(OH_2)20$ | 12*i* | 1 | 0.3001 | 0.5638 | 0.1783 | | single atom Tb |
| $(OH_2)21$ | 12*i* | 1 | 0.3274 | 0.4089 | 0.1799 | | single atom Tb |
| O22 | 12*i* | 1 | 0.3282 | 0.1889 | 0.1087 | | single atom S |
| Tb23 | 12*i* | 1 | 0.33255 | 0.32358 | 0.10689 | | tricapped trigonal prism $O_3(OH_2)_6$ |
| $(OH_2)24$ | 12*i* | 1 | 0.3421 | 0.4168 | 0.0329 | | single atom Tb |
| O25 | 12*i* | 1 | 0.3637 | 0.0903 | 0.0807 | | single atom S |
| O26 | 12*i* | 1 | 0.3717 | 0.0871 | 0.2032 | | single atom S |
| $(OH_2)27$ | 12*i* | 1 | 0.4277 | 0.3184 | 0.1731 | | single atom Tb |
| $(OH_2)28$ | 12*i* | 1 | 0.4343 | 0.3234 | 0.0437 | | single atom Tb |
| O29 | 12*i* | 1 | 0.4751 | 0.0722 | 0.1379 | | single atom S |
| S30 | 12*i* | 1 | 0.4908 | 0.0305 | 0.09356 | | tetrahedron $O_4$ |
| $(OH_2)31$ | 12*i* | 1 | 0.5161 | 0.2386 | 0.1029 | 0.78 | non-colinear $O_2$ |
| O32 | 12*i* | 1 | 0.5235 | 0.0817 | 0.0466 | | single atom S |
| O33 | 12*i* | 1 | 0.5433 | 0.0008 | 0.1113 | | single atom S |
| O34 | 6*h* | *m*.. | 0.0597 | 0.5502 | $^1/_4$ | | single atom S |
| S35 | 6*h* | *m*.. | 0.099 | 0.5022 | $^1/_4$ | | tetrahedron $O_4$ |
| S36 | 6*h* | *m*.. | 0.1218 | 0.304 | $^1/_4$ | | tetrahedron $O_4$ |
| O37 | 6*h* | *m*.. | 0.135 | 0.2349 | $^1/_4$ | | single atom S |
| O38 | 6*h* | *m*.. | 0.1861 | 0.5508 | $^1/_4$ | | single atom S |
| O39 | 6*h* | *m*.. | 0.1962 | 0.3776 | $^1/_4$ | | single atom S |
| (OH)40 | 6*h* | *m*.. | 0.287 | 0.1248 | $^1/_4$ | | single atom S |
| S41 | 6*h* | *m*.. | 0.3716 | 0.1313 | $^1/_4$ | | tetrahedron $O_3(OH)$ |

| | | | | | | |
|---|---|---|---|---|---|---|
| O42 | 6*h* | *m*.. | 0.4116 | 0.2052 | $^1/_4$ | single atom S |
| $(OH_2)$43 | 6*h* | *m*.. | 0.5765 | 0.1056 | $^1/_4$ | non-coplanar triangle $O(OH_2)_2$ |
| $(OH_2)$44 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.019 | non-coplanar triangle $(OH_2)_3$ |
| $(OH_2)$45 | 4*e* | 3.. | 0 | 0 | 0.1568 | non-coplanar triangle $(OH_2)_3$ |
| Tb46 | 2*c* | -6.. | $^1/_3$ | $^2/_3$ | $^1/_4$ | tricapped trigonal prism $(OH_2)_6O_3$ |

Experimental: single crystal, diffractometer, X-rays, R = 0.069, T = 120 K

Remarks: Part of H required for charge balance was not located; the author states that most of these protons are probably associated with water molecules. We set the occupancy of site $(OH_2)$44 equal to unity (refined value 1.51(17)). 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. (1995), Acta Crystallogr. C 51, 2466-2469.