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Supplementary Material for

Synthesis and Crystal Structure of Sr_2AlH_7: a New Structural Type of Alkaline Earth Aluminum Hydride

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Structural refinement of Sr_2AlD_7

The Rietveld refinement for the X-ray diffraction data of the deuteride sample was first carried out with a Rietveld refinement program RIETAN-2000. The refined position coordinates and isotropic thermal displacement parameters for Sr_2AlD_7 are listed in Table S1. Then the neutron powder diffraction data of the deuteride sample were analyzed by a Rietveld refinement program RIETAN-2001T. During the refinement, the Sr and Al atom coordinates of the deuteride Sr_2AlD_7 were fixed as those refined from the X-ray data of the deuteride sample. The deuterium positions were initially located by placing the atoms in the octahedral and tetrahedral holes formed by Sr and Al atoms. The occupation factors of the deuterium positions were fixed at unity because they were close to 1 (the differences were smaller than 3σ) during the refinement. The finally refined position coordinates and isotropic thermal displacement parameters of Sr_2AlD_7 are summarized in Table S2.

Table S1. Atomic coordinates and isotropic thermal parameters for Sr_2AlD_7 refined from X-ray diffraction data[a]

Atom	Site	*g*	*x*	*y*	*z*	*B* (Å^2)
Sr1	4*c*	1	0.0935(3)	0.3289(4)	0.3195(6)	0.8(1)
Sr1'	4*c*	1	0.9065(3)	0.6711(4)	0.1805(6)	0.8(1)
Sr2	4*c*	1	0.8609(4)	0.0684(4)	0.0882(6)	0.9(1)
Sr2'	4*c*	1	0.1391(4)	0.9316(4)	0.4118(6)	0.9(1)
Al1	4*c*	1	0.671(1)	0.847(1)	0.232(2)	1.2(2)
Al1'	4*c*	1	0.329(1)	0.153(1)	0.268(2)	1.2(2)

[a] R_{wp} = 7.22%, R_p = 5.35%, R_I = 1.95%, S = 2.83. The coordinates and isotropic thermal displacement parameters of atoms A and A' were constrained by $x' = 1-x$, $y' = 1-y$, $z' = 0.5-z$ and $B' = B$.

Table S2. Atomic coordinates and isotropic thermal parameters for Sr_2AlD_7 finally refined from neutron powder diffraction data[a]

Atom	Site	*g*	*x*	*y*	*z*	*B* (Å^2)
Sr1	4*c*	1	0.0935	0.3289	0.3195	0.4(1)
Sr1'	4*c*	1	0.9065	0.6711	0.1805	0.4(1)
Sr2	4*c*	1	0.8609	0.0684	0.0882	0.7(1)
Sr2'	4*c*	1	0.1391	0.9316	0.4118	0.7(1)
Al1	4*c*	1	0.671	0.847	0.232	0.1(2)
Al1'	4*c*	1	0.329	0.153	0.268	0.1(2)
D1	4*c*	1	0.7494(7)	0.8594(7)	0.077(1)	1.9(2)
D1'	4*c*	1	0.2506(7)	0.1406(7)	0.423(1)	1.9(2)
D2	4*c*	1	0.6014(7)	0.7106(7)	0.117(1)	2.8(3)
D2'	4*c*	1	0.3986(7)	0.2894(7)	0.383(1)	2.8(3)
D3	4*c*	1	0.7658(6)	0.7378(8)	0.341(1)	1.5(2)
D3'	4*c*	1	0.2342(6)	0.2622(8)	0.159(1)	1.5(2)
D4	4*c*	1	0.5885(6)	0.8298(8)	0.379(1)	1.6(2)
D4'	4*c*	1	0.4115(6)	0.1702(8)	0.121(1)	1.6(2)
D5	4*c*	1	0.7395(6)	0.9919(7)	0.3291(9)	0.9(2)
D5'	4*c*	1	0.2605(6)	0.0081(7)	0.1709(9)	0.9(2)
D6	4*c*	1	0.5748(6)	0.9558(7)	0.1157(8)	0.8(2)
D6'	4*c*	1	0.4252(6)	0.0442(7)	0.3843(8)	0.8(2)
D7	4*c*	1	0.4375(6)	0.6037(7)	0.3189(9)	2.3(2)
D7'	4*c*	1	0.5625(6)	0.3963(7)	0.1811(9)	2.3(2)

[a] Space group *I*2 (No. 5-3); cell parameters: a = 12.552(1) Å, b = 9.7826(8) Å, c = 7.9816(7) Å, β = 100.286(4)°, V = 964.3(1) Å^3, Z = 8; R_{wp} = 2.72%, R_p = 2.15%, R_I = 5.33%, S = 2.28. The coordinates and isotropic thermal displacement parameters of atoms A and A' were constrained by $x' = 1-x$, $y' = 1-y$, $z' = 0.5 - z$ and $B' = B$. The Sr and Al atom coordinates were fixed as those refined from the X-ray data. The occupation factors were fixed at unity because they were close to 1 (the differences were smaller than 3σ) during the refinement.