New Tables S1-C and S2-C

Table S1-C. 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	8*f*	1	0.3435(3)	0.5789(4)	0.3195(6)	0.8(1)
Sr2	8*f*	1	0.1109(4)	0.3184(4)	0.0882(6)	0.9(1)
Al1	8*f*	1	0.921(1)	0.097(1)	0.232(2)	1.2(2)

[a] R_{wp} = 7.22%, R_p = 5.35%, R_I = 1.95%, S = 2.83.

Table S2-C. 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	8*f*	1	0.3435	0.5789	0.3195	0.4(1)
Sr2	8*f*	1	0.1109	0.3184	0.0882	0.7(1)
Al1	8*f*	1	0.921	0.097	0.232	0.1(2)
D1	8*f*	1	0.9994(7)	0.1094(7)	0.077(1)	1.9(2)
D2	8*f*	1	0.8514(7)	0.9606(7)	0.117(1)	2.8(3)
D3	8*f*	1	0.0158(6)	0.9878(8)	0.341(1)	1.5(2)
D4	8*f*	1	0.8385(6)	0.0798(8)	0.379(1)	1.6(2)
D5	8*f*	1	0.9895(6)	0.2419(7)	0.3291(9)	0.9(2)
D6	8*f*	1	0.8248(6)	0.2058(7)	0.1157(8)	0.8(2)
D7	8*f*	1	0.6875(6)	0.8537(7)	0.3189(9)	2.3(2)

[a] Space group *I*2/*a* (No. 15); 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 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.