Electronic Supplementary Material (ESI) for RSC Advances.

Electronic structure and transport properties of antiferromagnetic double perovskite Y_2AlCrO_6

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Supporting information

Table ESI1 Structural parameters for YAC as obtained from Rietveld analysis of XRD pattern.

Space group = $P2_1/n$

Lattice parameter: a = 5.215(3) Å, b = 5.429(3) Å, c = 7.455(4) Å, β = 90.01º

Refinement parameters: R_p = 2.15, R_{wp} = 2.74, R_{exp} = 2.66, χ^2 = 1.05

Atom	Wyckoff site	x	y	z	B (Å)	Occupancy	Bond length (Å)
Y	4e	0.513(5)	0.559(2)	0.247(6)	0.63	2	Cr-O_1(x2) = 2.00
Cr	2a	0.0	0.5	0.0	0.87	1	Cr-O_2(x2) = 2.04
Al	2c	0.5	0.0	0.0	0.91	1	Cr-O_3(x2) = 2.12
O_1	4e	0.402(1)	0.973(1)	0.240(3)	0.90	2	Al-O_1 (x2) = 1.87
O_2	4e	0.311(3)	0.271(3)	0.017(3)	0.84	2	Al-O_2 (x2) = 1.78
O_3	4e	0.216(3)	0.817(2)	0.068(2)	0.43	2	Al-O_3 (x2) = 1.85

<Cr-O_1-Al> =148.11

<Cr-O_2-Al> = 159.80

<Cr-O_3-Al> = 142.62

Table ESI2 Symmetry and frequencies of calculated Raman modes of YAC.

Band no	Position (Cm^{-1})	FWHM	Assignment
1	154.4	5.5	T
2	165.0	8.0	T
3	185.8	6.2	T
4	192.1	4.5	T
5	219.6	4.5	T
6	258.1	8.0	L
7	270.1	19.1	L
8	281.9	11.6	L
9	303.6	11.4	L
10	310.0	12.0	L
11	334.0	20.0	L
12	345.2	8.6	υ_5
13	374.2	33.7	υ_5
14	398.0	16.4	υ_5
15	424.1	29.6	υ_5
16	480.4	36.3	υ_5
17	459.6	27.1	υ_5
18	505.5	29.6	υ_5
19	524.3	29.1	υ_2
20	565.1	42.5	υ_2
21	595.1	42.6	υ_2
22	625.0	25.0	υ_2
23	702.3	34.8	υ_1
24	720.4	28.8	υ_1