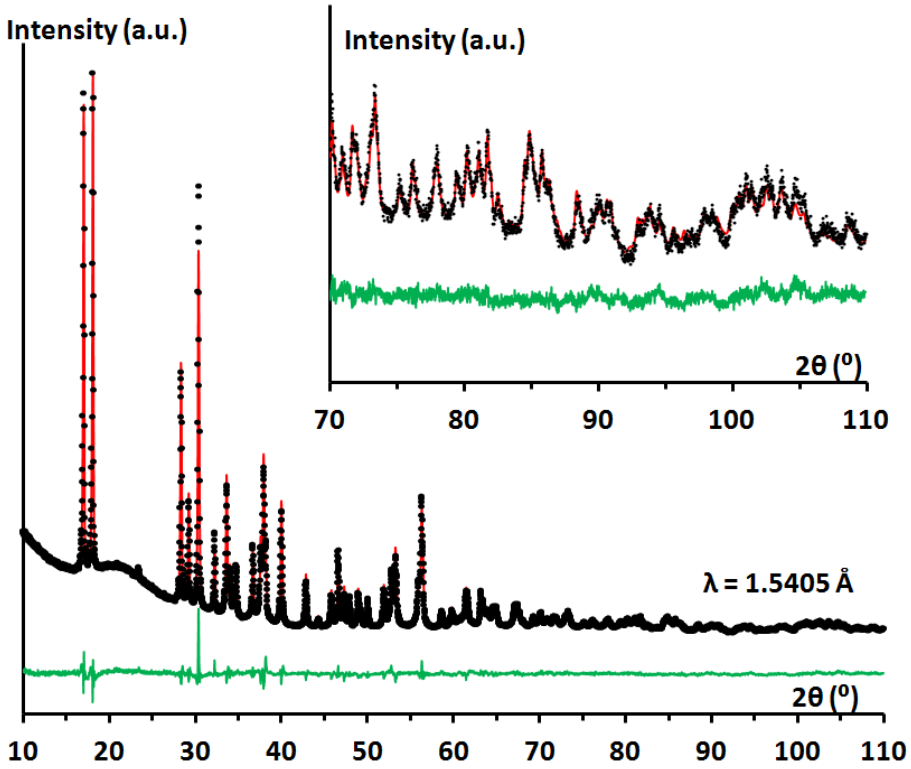
Electronic Supplementary Material (ESI) for Dalton Transactions

Supplementary Information

Na_2AgF_4: 1D antiferromagnet with unusually short Ag(II)···Ag(II) separation

Dominik Kurzydłowski[1#], Zoran Mazej[2] and Wojciech Grochala[1,3#]

1. Powder x-ray diffraction pattern of Na_2AgF_4

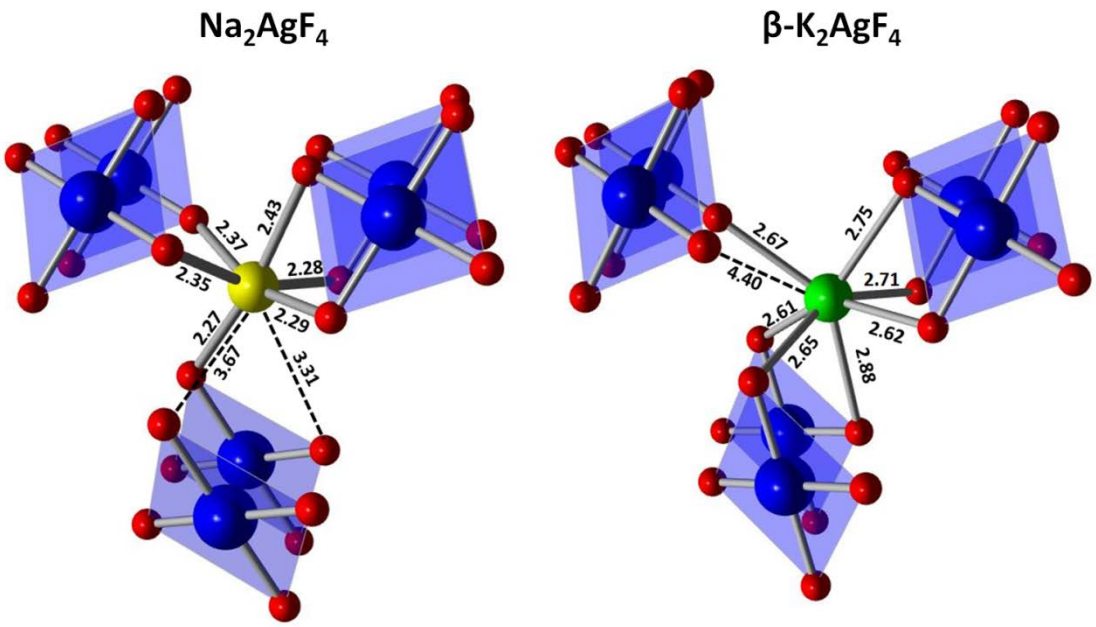


The Rietveld fit in the Na_2CuF_4-type structure is depicted by a red line. Green lines depict the difference between the fit and experimental points.

2. Selected crystallographic data for Na_2AgF_4

	Na_2AgF_4 **$P2_1/c$ (no. 14) Z = 2**
a, b, c (Å)	3.34160(5), 10.4012(1), 6.07607(9)
β (°)	65.971(1)
V (Å^3)	192.883(5)
Ag (x,y,z)	2a (0, 0, 0)
U^{equiv}(Ag)	0.047
Na (x,y,z)	4e (0.2487(8) 0.8472(2) 0.4672(5))
U^{iso}(Na)	0.0201(8)
F1 (x,y,z)	(0.4356(12) 0.4397(3) 0.7886(7))
U^{iso}(F1)	0.0465(14)
F2 (x,y,z)	(0.0436(14) 0.1681(4) 0.8121(7))
U^{iso}(F2)	0.0512(14)
GOF, R_p, R_{wp}	2.29, 3.18 %, 4.11 %

3. Comparison of the first coordination sphere of Na^+ and K^+ in Na_2AgF_4 and β-K_2AgF_4



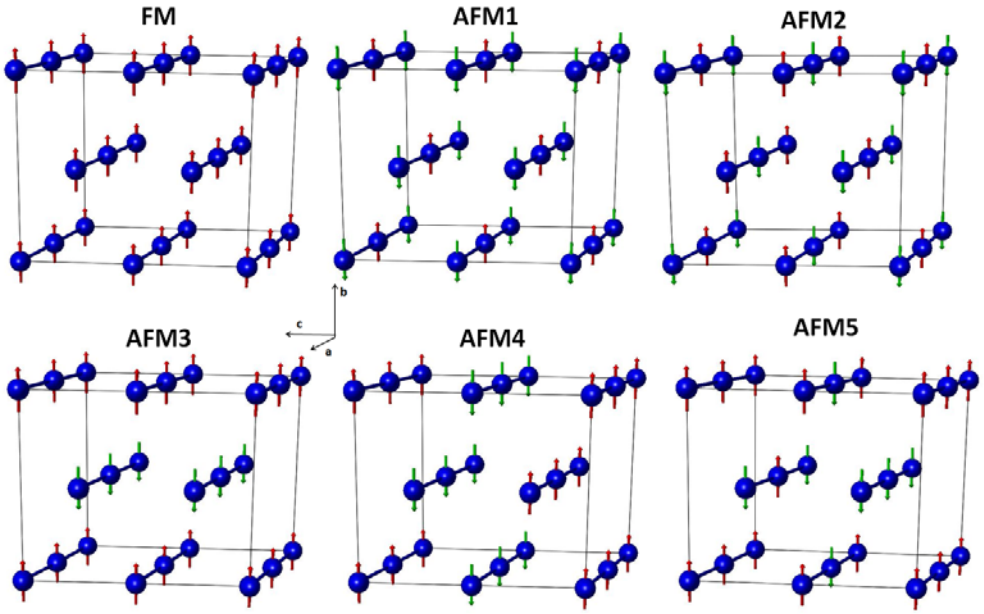
Blue/red/yellow/green balls depict Ag/F/Na/K atoms. Distances are given in Å.

4. Comparison of experimental and theoretical geometry of Na_2AgF_4 and β-K_2AgF_4.

	Na_2AgF_4			β-K_2AgF_4		
	exp.[#]	DFT+U[#]	diff. (%)	exp.*	DFT+U[#]	diff. (%)
R_{Ag-F1}	2.081	2.118	1.8	2.103	2.140	1.8
$R_{Ag\cdots F1}$	2.769	2.830	2.2	2.710	2.803	3.4
R_{Ag-F2}	2.061	2.115	2.6	2.059	2.119	2.9
$r_{intra-chain}$	3.342	3.406	1.9	3.717	3.815	2.6
$r_{inter-chain}$	5.617	5.695	1.4	7.290	7.404	1.5
	6.023	6.125	1.7	6.048	6.156	1.8
	6.076	6.194	1.9	6.386	6.506	1.9
	6.259	6.353	1.5	7.048	7.170	1.7
	7.464	7.608	1.9	7.150	7.313	2.3
	8.039	8.216	2.2	7.486	7.678	2.6

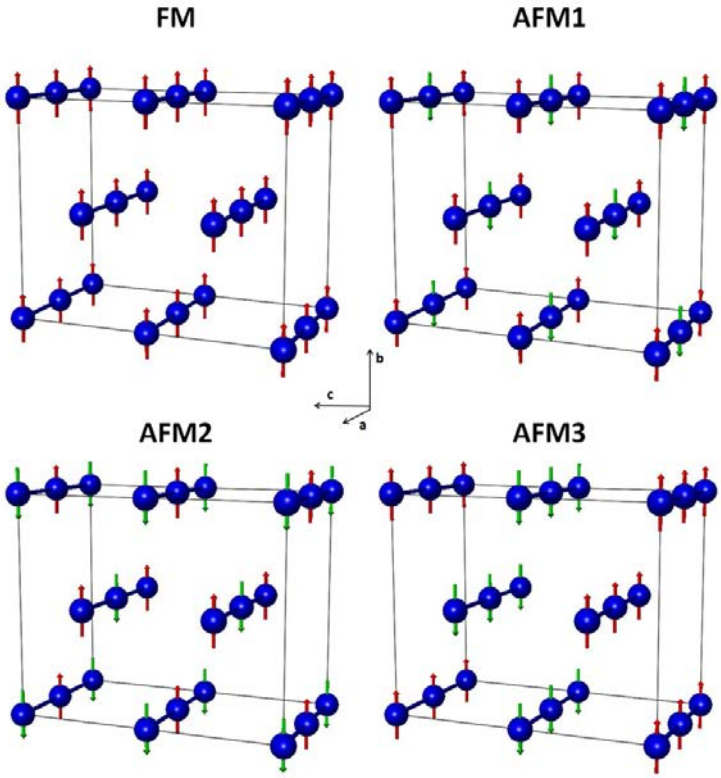
Distances are given in Å; * ref. [1]; [#] this work

5. Spin-ordered states of Na_2AgF_4 depicted in the 1x2x2 supercell



Red/green arrows depict up/down spin sites.

6. Spin-ordered states of β-K_2AgF_4 depicted in the 1x2x2 supercell



Red/green arrows depict up/down spin sites.

7. Comparison of super-exchange paths in Na_2AgF_4 at 0 GPa and 10 GPa as obtained from DFT+U calculations

Pressure	**0 GPa**		**10 GPa**	
	Coupling constant	**Ag(II)···Ag(II) distance**	**Coupling constant**	**Ag(II)···Ag(II) distance**
J_1	–0.31	3.406	–0.75	3.176 (–7 %)
J_2	0.46	5.695	0.42	5.499 (–3 %)
J_3	0.17	6.125	0.27	5.755 (–6 %)
J_4	0.09	6.194	–0.31	5.805 (–6 %)
J_5	0.23	6.353	0.40	6.036 (–5 %)

Values of coupling constants are given in meV, distances in Å.

8. References

[1] D. Kurzydłowski, M. Derzsi, A. Budzianowski, Z. Jagličić, W. Koźmiński, Z. Mazej, W. Grochala, , *Eur. J. Inorg. Chem.*, 2010, 2919.