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Crystal structure and electrical characterisation of Bi_2NbO_5F: An Aurivillius oxide fluoride

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Bond Valence Sum calculations for Bi^{3+} and Nb^{5+} cation sites in Bi_2NbO_5F from refinements of NPD data collected at 295 K in space groups *I*4/*mmm* and *Aea*2

		*I*4/*mmm*	*Aea*2
Bi	O(1) = F	**2.89**	**3.00**
	O(2) = F	2.70	2.91
	O(3) = F	2.45	2.55
Nb	O(1) = F	5.66	4.48
	O(2) = F	4.72	**4.89**
	O(3) = F	**5.24**	5.32
X	O(1) = F	1.59	1.49
	O(2) = F	**1.10**	**1.12**
	O(3) = F	1.85	1.89

Bond Valence Sum calculations for Bi^{3+} and Nb^{5+} cation sites in Bi_2NbO_5F from refinements of NPD data collected at 295 K in space group $Pca2_1$

	Anion Site Occupies by F								
	O(1)	O(2)	O(3)	O(4)	O(5)	O(6)	ap.	eq.	fl.
Bi(1)	2.98	2.98	2.52	2.98	2.97	2.86	2.92	2.75	2.98
Bi(2)	3.09	2.74	3.22	3.20	3.21	3.22	3.10	2.93	3.15
average Bi	3.04	2.86	2.87	3.09	3.09	3.04	**3.01**	2.84	3.07
Nb	5.03	5.26	5.26	4.91	4.80	5.09	**5.06**	5.26	4.86