Supplementary Material:

Short range parameters of the form: $V(r) = A\exp(-r/\rho) - Cr^{-6}$

Species	A (eV)	ρ (Å)	C (eVÅ^{-6})
Ba^{2+}-F^-	589.94	0.3748	0.018
Ca^{2+}-F^-	910.36	0.3135	2.490
F^-- F^-	1240.73	0.2795	22.900

Calculated lattice parameters, r_{lat} (Å), elastic constants, EC (10^{11}dyne/cm^2) and activation energies, E_{act} (eV), for fluoride ion mobility in pure CaF_2 and BaF_2; experimental values are presented as a comparison.

		CaF_2		BaF_2	
		Calculated	Experiment	Calculated	Experiment
r_{lat}		5.44	5.46	6.17	6.20
EC	C_{11}	17.17	16.42	8.87	9.20
	C_{12}	3.59	4.40	2.21	4.16
	C_{44}	3.58	3.37	2.20	2.57
E_{act}		1.2	1.31 Ref. [1]	1.1	1.04 Ref. [1]

References:

[1]   Ziraps, V., Kulis, P., Tale, I. And Viespals, A. Ion diffusion-controlled processes in fluoride crystals. Radiation Measurements 33, 633-636 (2001).