Supporting Information for:

The strongest dative bond in main-group compounds. Theoretical study of $OAeF^-$ (Ae = Be – Ba)

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Table S1

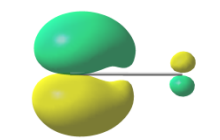
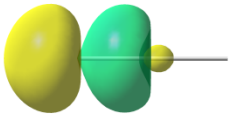
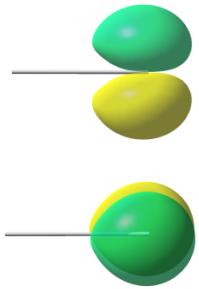
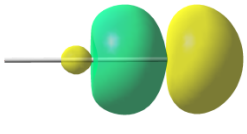
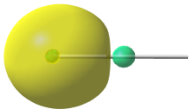
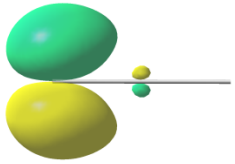
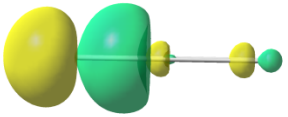
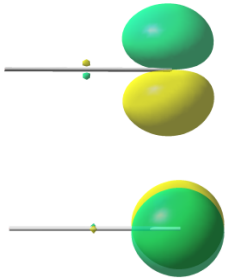
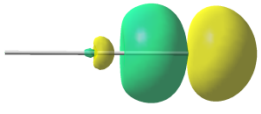
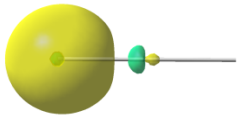
Figures S1 and S2

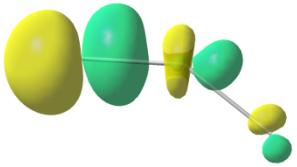
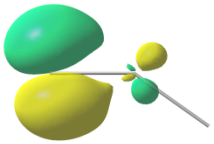
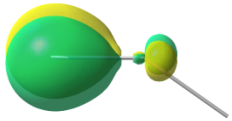
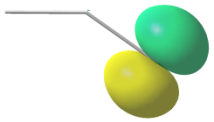
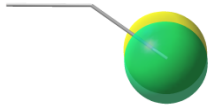
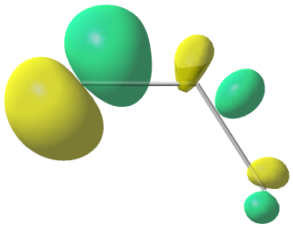
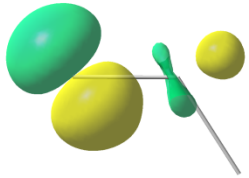
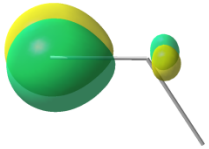
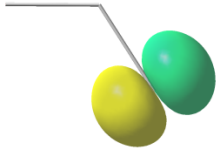
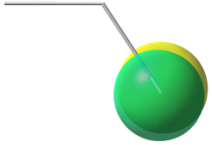
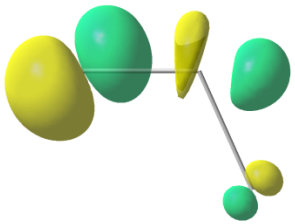
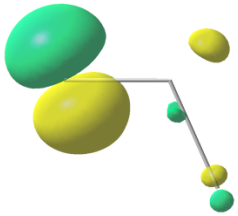
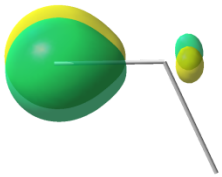
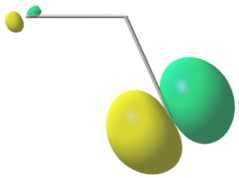
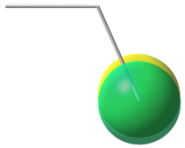
Table S1: EDA-NOCV results of $OAeF^-$ using OAe^- (D) and F (D) in the electronic doublet states as interacting fragments. All molecules are calculated at the equilibrium geometries except for the linear structure of $OBaF^-$. The calculations were carried out at the BP86/DZP level using BP86/def2-TZVPP optimized geometries. Energy values are given in kcal mol^{-1}.

Fragments	OBe^- (D) + F(D)	OMg^- (D) + F(D)	OCa^- (D) + F(D)	OSr^- (D) + F(D)	OBa^- (D) + F(D)	OBa^- (D) + F(D)
Structure	linear	linear	bent	bent	bent	linear
ΔE_{int}	-157.9	-138.9	-124.6	-120.5	-121.1	-113.5
ΔE_{Pauli}	200.6	128.5	85.3	55.8	54.1	49.2
ΔE_{elstat}[a]	-94.0 (26.2%)	-69.2 (25.9 %)	-49.9 (23.8%)	-28.8 (16.3 %)	-28.5 (16.3%)	-26.9 (16.5 %)
ΔE_{orb}[a]	-264.5 (73.8%)	-198.2 (74.1 %)	-160.0 (76.2%)	-147.4 (83.7 %)	-146.7 (83.7%)	-135.7 (83.5 %)

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb}$

Fig.S1: The five energetically highest-lying occupied MOs of $OAeF^-$ (Ae = Be-Ba) at the BP86/def2-TZVPP level of theory. (Isovalue 0.05e/au^3).

OAeF-	HOMO	HOMO-1	HOMO-2	HOMO-3	HOMO-4
$OBeF^-$					
	ε= 0.809 eV	ε= -0.103 eV	ε= -3.569 eV	ε= -4.749 eV	ε= -13.885 eV
$OMgF^-$					
	ε= 0.883 eV	ε= 0.212 eV	ε= -3.248 eV	ε= -3.889 eV	ε= -13.513 eV

$OCaF^-$					
	ε= 1.241 eV	ε= 0.999 eV	ε= 0.970 eV	ε= -2.209 eV	ε= -2.227 eV
$OSrF^-$					
	ε= 0.907 eV	ε= 0.730 eV	ε= 0.719 eV	ε= -1.937 eV	ε= -1.983 eV
$OBaF^-$					
	ε= 1.006 eV	ε= 0.672 eV	ε= 0.581 eV	ε= -1.575 eV	ε= -1.633 eV

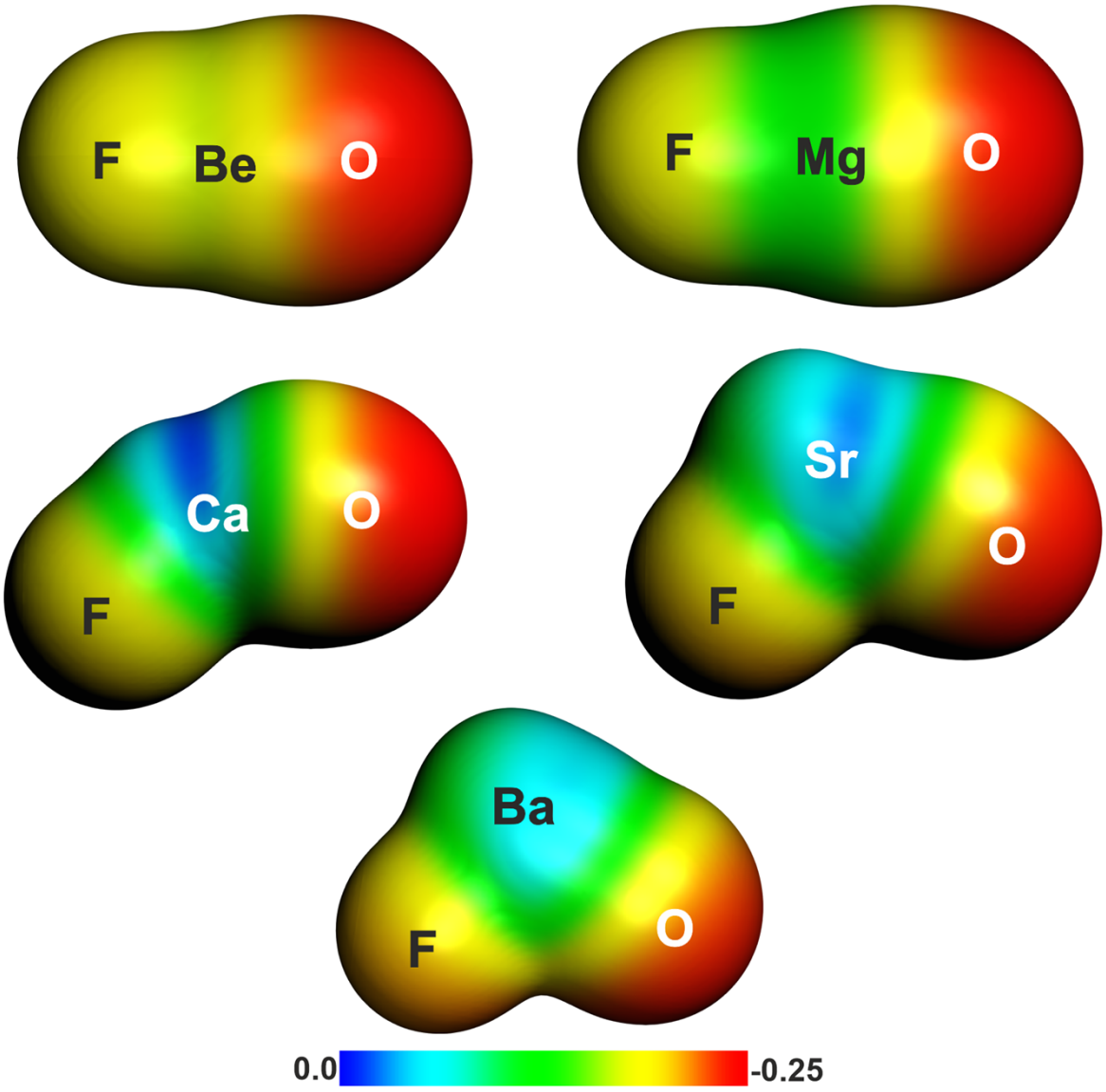


Fig.S2: Plot of molecular electrostatic potentials of $OAeF^-$ systems at the BP86/TZP level of theory, computed with value of 0.001 au for the contour of the electronic density.