

SUPPORTING INFORMATION

Solid-State Principles Applied to Organic-Inorganic Perovskites: New Tricks for an Old Dog

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SI-Table 1. The calculated effective radii $r_{eff} = r_{mass} + r_{ion}$ for different anions and amine based cations and corresponding tolerance factors (α) of lead iodides and manganese formates; h_{Xeff} and r_{mass} were calculated by using reported room temperature crystallographic data. In case where differences between the reported structures were observed, an average value was calculated and the error estimated to 6%.*

Cation		r_{mass}	r_{ion}	r_{Aeff}	Reference	α A-PbI ₃	α A-Mn(HCOO) ₃
#1	Ammonium	0	146	146	1	0.76(3)	0.65(1)
#2	Hydroxylammonium	70	146	216	2	0.90(9)	0.81(2)
#3	Hydrazinium	71	146	217	3	0.91(2)	0.81(4)
#4	Methylammonium	71	146	217	4,5	0.91(2)	0.81(4)
#5	Azetidinium	204	146	250	4,6	0.98(0)	0.89(1)
#6	Formamidinium	107	146	253	5,7	0.98(7)	0.89(7)
#7	Imidazolium	107	146	258	8,9, 10	0.99(7)	0.90(9)
#8	Dimethylammonium	126	146	272	4,11,12	1.02(6)	0.94(1)
#9	Ethylammonium	128	146	274	4	1.03(0)	0.94(6)
#10	Guanidinium	132	146	278	13	1.03(9)	0.95(5)
#11	Tetramethylammonium	146	146	292	14,15	1.06(8)	0.98(7)
Anion							
Iodide, I ⁻		0	220	$r_{Xeff} = 220$	1		
Cyanide, CN ⁻		0	146	$r_{Xeff} = 146$ $h_{Xeff} = 395$	16,8		
Formate**, HCOO ⁻		-	-	$r_{Xeff} = 136$ $h_{Xeff} = 447$	4,11,17		
Azide, N ₃ ⁻		0	146	$r_{Xeff} = 146$ $h_{Xeff} = 447$	13,18,19		

* The effective height of the azide anion shows a larger flexibility than the other bridging anions (426 pm - 494 pm) .

** The effective radius of the cylinder for the formate anion was estimated to be equal the ionic radius of oxygen.

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