Supporting Information

Thermochemistry of Multiferroic Organic - Inorganic Hybrid Perovskites $[(CH_3)_2NH_2][M(HCOO)_3]$ (M = Mn, Co, Ni and Zn)

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SI 1. Structural parameters of [DMA-Zn-F] obtained by Rietveld refinement

Structure data
Structure and profile data

Formula sum	$Zn_{6.00}C_{30.00}H_{65.88}O_{36.00}N_{5.94}$
Formula mass/ g/mol	1478.1890
Density (calculated)/ g/cm^3	1.8882
F(000)	755.4600
Weight fraction/ %	100.000000
Space group (No.)	R -3 c (167)
Lattice parameters	
a/ Å	8.204(1)
b/ Å	8.204(1)
c/ Å	22.295(3)
alpha/ °	90
beta/ °	90
gamma/ °	120
V/ 10^6 pm^3	1299.79900

Occupancy, atomic fractions and atomic coordinates

Atom	Wyck.	s.o.f.	x	y	z
Zn1	6b	1.000000	0.000000	0.000000	0.000000
C1	18e	1.000000	0.544300	0.000000	0.250000
H1	18e	1.000000	0.429700	0.000000	0.250000
O1	36f	1.000000	0.217270	0.009030	0.053780
N1S	18e	0.330000	0.086300	0.000000	0.250000
H1S1	36f	0.170000	0.103000	0.203900	0.250000
H1S2	36f	0.170000	0.103000	0.203800	0.250000
C1S	12c	1.000000	0.000000	0.000000	0.195000
H1S3	36f	0.330000	0.000000	0.076800	0.161800
H1S4	36f	0.330000	0.012200	0.123800	0.192700
H1S5	36f	0.330000	0.123900	0.012300	0.192700

SI 2. Structural parameters of [DMA-Mn-F] obtained by Rietveld refinement

Structure and profile data	
Formula sum	$C_{30.00}H_{65.88}N_{5.94}Mn_{6.00}O_{36.00}$
Formula mass/ g/mol	1415.5370
Density (calculated)/ g/cm^3	1.7081
F(000)	725.4600
Weight fraction/ %	100.000000
Space group (No.)	R -3 c (167)
Lattice parameters	
a/ Å	8.331(1)
b/ Å	8.331(1)
c/ Å	22.888(4)
alpha/ °	90
beta/ °	90
gamma/ °	120
V/ 10^6 pm^3	1375.89000

Occupancy, atomic fractions and atomic coordinates

Atom	Wyck.	s.o.f.	x	y	z
C2	12c	1.000000	0.000000	0.000000	0.197120
H2A	36f	0.330000	0.125600	0.021100	0.186400
H2B	36f	0.330000	0.087500	0.038500	0.160400
H2C	36f	0.330000	0.133900	0.046800	0.197900
N1	18e	0.330000	0.087800	0.000000	0.250000
H1A	36f	0.170000	0.103300	0.214800	0.250000
H1B	36f	0.170000	0.103200	0.214700	0.250000
Mn1	6b	1.000000	0.000000	0.000000	0.000000
O1	36f	1.000000	0.220870	0.010180	0.054330
C1	18e	1.000000	0.548770	0.000000	0.250000
H1	18e	1.000000	0.437370	0.000000	0.250000

SI 3. Structural parameters of [DMA-Ni-F] obtained by Rietveld refinement

Formula sum	$C_{30.00}H_{65.88}N_{5.94}Ni_{6.00}O_{36.00}$
Formula mass/ g/mol	1438.1090
Density (calculated)/ g/cm^3	1.9023
F(000)	743.4600
Weight fraction/ %	100.000000
Space group (No.)	R -3 c (167)
Lattice parameters	
a/ Å	8.138(3)
b/ Å	8.138(3)
c/ Å	21.952(8)
alpha/ °	90
beta/ °	90
gamma/ °	120
V/ 10^6 pm^3	1255.15900

Occupancy, atomic fractions and atomic coordinates

Atom	Wyck.	s.o.f.	x	y	z
C2	12c	1.000000	0.000000	0.000000	0.194590
H2A	36f	0.330000	0.117900	0.001300	0.190200
H2B	36f	0.330000	0.083300	0.015100	0.161600
H2C	36f	0.330000	0.128600	0.025800	0.194300
N1	18e	0.330000	0.086900	0.000000	0.250000
H1A	36f	0.170000	0.102900	0.214400	0.250000
H1B	36f	0.170000	0.103500	0.214700	0.250000
Ni1	6b	1.000000	0.000000	0.000000	0.000000
O1	36f	1.000000	0.213840	0.006190	0.053270
C1	18e	1.000000	0.539770	0.000000	0.250000
H1	18e	1.000000	0.425570	0.000000	0.250000