Electronic Supplementary Information (ESI)

Pressure-induced phase transitions of lead iodide

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Table SI Structure information and enthalpies relative to the ground-state structure of low-lying structures form the structure search at 10 GPa.

Symmetry	*Z*	Lattice (Å, º)	Atom	X	Y	Z	Enthalpy (meV)	
							PBE	PBE+SOC
P*nma*	4	a=8.45 b=4.06 c=10.60	Pb (4c) I1 (4c) I2 (4c)	0.813 0.665 0.508	0.75 0.75 0.25	0.337 0.062 0.340	0	0
P*nma* α-$PbCl_2$	4	a=7.79 b=4.87 c=9.59	Pb (4c) I1 (4c) I2 (4c)	0.766 0.148 0.027	0.75 0.25 0.25	0.390 0.931 0.321	28	35
P*nma*	8	a=8.51 b=4.31 c=19.70	Pb1 (4c) Pb2 (4c) I1 (4c) I2 (4c) I3 (4c) I4 (4c)	0.250 0.723 0.960 0.637 0.635 0.515	0.25 0. 25 0.25 0.75 0.75 0.75	0.951 0.306 0.719 0.437 0.655 0.925	33	39
C2/*m*	4	a=12.57 b=4.03 c=10.76 β=137.33°	Pb (4i) I1 (4i) I2 (4i)	0.936 0.222 0.082	0.0 0.5 0.5	0.297 0.631 0.930	144	129
C*m*	6	a=14.990 b=4.024 c=11.935 β=129.60°	Pb1 (2a) Pb2 (2a) Pb3 (2a) I1 (2a) I2 (2a) I3 (2a) I4 (2a) I5 (2a) I6 (2a)	0.297 0.873 0.235 0.606 0.452 0.956 0.202 0.652 0.915	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	0.731 0.421 0.982 0.670 0.296 0.745 0.408 0.097 0.016	147	133
P*nma* FeF_2	4	a=15.46 b=4.06 c=6.14	Pb (4c) I1 (4c) I2 (4c)	0.394 0.450 0.724	0.25 0.25 0.25	0.250 0.749 0.525	415	400

Table SII Structure information and enthalpies relative to the ground-state structure of low-lying structures form the structure search at 50 GPa.

Symmetry	*Z*	Lattice (Å, º)	Atom	X	Y	Z	Enthalpy (meV)	
							PBE	PBE+SOC
I4/*mmm*	2	a=b=3.63 c=9.77	Pb (2b) I (4e)	0.5 0.0	0.5 0.0	0.0 0.161	0	0
F*mmm*	4	a=9.79 b=5.137 c=5.133	Pb (4a) I (8g)	0.5 0.839	0.5 0.5	0.5 0.5	9	1
P*nma*	4	a=7.87 b=3.39 c=9.89	Pb (4c) I1 (4c) I2 (4c)	0.312 0.005 0.339	0.75 0.25 0.25	0.163 0.141 0.926	213	218

Table SIII Structure information and enthalpies relative to the ground-state structure of low-lying structures form the structure search at 80 GPa.

Symmetry	*Z*	Lattice (Å, º)	Atom	X	Y	Z	Enthalpy (meV)	
							PBE	PBE+SOC
I*mmm*	2	a=9.01 b=3.10 c=4.04	Pb (2d) I (4f)	0.0 0.335	0.5 0.5	0.0 0.0	0	0
P-1	2	a=5.12 b=5.12 c=5.22 α=71.82° β=99.03° γ=119.97°	Pb (2i) I1 (2i) I2 (2i)	0.325 0.335 0.993	0.913 0.418 0.247	0.75 0.25 0.75	6	25
C*mmm*	4	a=13.26 b=4.51 c=3.77	Pb (4h) I1 (4g) I2 (2b) I3 (2d)	0.663 0.171 0.5 0.0	0.0 0.0 0.0 0.0	0.5 0.0 0.0 0.5	100	113
P-3*m*1	1	a=b=4.73 c=2.93 γ=110°	Pb (1b) I (2c)	0.0 2/3	0.0 1/3	0.5 0.792	136	125

Table SIV Structure information and enthalpies relative to the ground-state structure of low-lying structures form the structure search at 150 GPa.

Symmetry	*Z*	Lattice (Å, º)	Atom	X	Y	Z	Enthalpy (meV)	
							PBE	PBE+SOC
C2/*c*	4	a=4.84 b=8,45 c=5.72 β=125.68°	Pb (4e) I1 (4e) I2 (4e)	0.0 0.0 0.0	0.665 0.333 0.001	0.25 0.25 0.75	0	0
P1	4	a=5.67 b=5.68 c=6.21 α=102.85° β=103.21° γ=89.52°	Pb1 (1a) Pb2 (1a) Pb3 (1a) Pb4 (1a) I1 (1a) I2 (1a) I3 (1a) I4 (1a) I5 (1a) I6 (1a) I7 (1a) I8 (1a)	0.122 0.622 0.788 0.288 0.788 0.122 0.953 0.456 0.455 0.621 0.955 0.287	0.806 0.297 0.466 0.467 0.968 0.308 0.138 0.630 0.132 0.796 0.638 0.968	0.453 0.454 0.115 0.117 0.121 0.450 0.782 0.786 0.786 0.452 0.788 0.115	91	57
I4/*mmm*	2	a=b=2.89 c=11.37	Pb (2a) I (4e)	0.0 0.0	0.0 0.0	0.0 0.335	226	166