Supplementary Materials: Regulation of Ionic Bond in Group IIB Transition Metal Iodides

Zhenzhen Xu(徐真真)[1], Jianfu Li(李建福)[1*], Yanlei Geng(耿延雷)[1], Zhaobin Zhang(张钊斌)[1], Yang Lv(吕阳)[1], Chao Zhang(张超)[1], Qinglin Wang(王庆林)[2], and Xiaoli Wang(王晓丽)[1*]

[1]School of Physics and Electronic Information, Yantai University, Yantai 264005, China;

[2]Shandong Key Laboratory of Optical Communication Science and Technology, School of Physics Science & Information Technology, Liaocheng University, Liaocheng 252059, China

*Corresponding authors. Email: jianfuli@ytu.edu.cn; xlwang@ytu.edu.cn

Table S1 Structural details for the compounds.

Structure	Pressure (GPa)	Lattice parameters		Wyckoff positions (fractional)				
				atoms	site	x	y	z
ZnI_2-122 (*I*-42*d*)	0	a=6.706 b=6.706 c=11.352	α=90.000 β=90.000 γ=90.000	Zn1 I1	4b 8d	1.000 1.250	1.000 1.278	0.500 0.875
ZnI_2-186 ($P6_3mc$)	10	a=3.830 b=3.830 c=12.213	α=90.000 β=90.000 γ=120.000	Zn1 I1 I3	2b 2b 2a	0.333 0.333 -0.000	0.667 0.667 1.000	0.999 0.368 0.633
HgI-139 (*I*4/*mmm*)	0	a=5.262 b=5.262 c=11.805	α=90.000 β=90.000 γ=90.000	Hg1 I1	4e 4e	0.000 0.000	0.000 0.000	0.113 0.346
HgI-221 (*Pm*-3*m*)	20	a=3.598 b=3.598 c=3.598	α=90.000 β=90.000 γ=90.000	Hg1 I1	1a 1b	0.000 0.500	0.000 0.500	0.000 0.500
HgI_2-137 (*P*4/*nmc*)	0	a=4.523 b=4.523 c=13.464	α=90.000 β=90.000 γ=90.000	Hg1 I1	2b 4d	0.000 0.000	1.000 0.500	0.500 0.631
HgI_2-186 ($P6_3mc$)	10	a=4.017 b=4.017 c=12.498	α=90.000 β=90.000 γ=120.000	Hg1 I1 I3	2b 2b 2a	0.333 0.333 0.000	0.667 0.667 0.000	0.999 0.357 0.643
HgI_2-139 (*I*4/*mmm*)	30	a=3.508 b=3.508 c=10.830	α=90.000 β=90.000 γ=90.000	Hg1 I1	2a 4e	0.000 -0.000	0.000 0.000	0.000 0.655

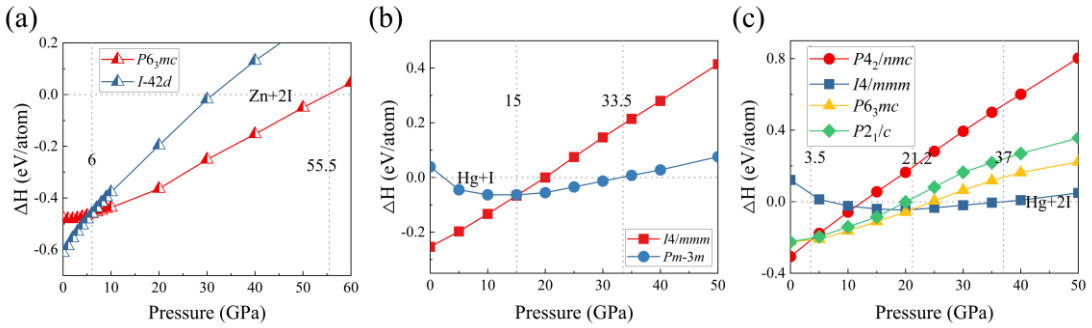

Fig. S1. The enthalpy difference of the compounds relative to the constituent elements as a function of pressure. (a) ZnI_2, (b) HgI, (c) HgI_2.

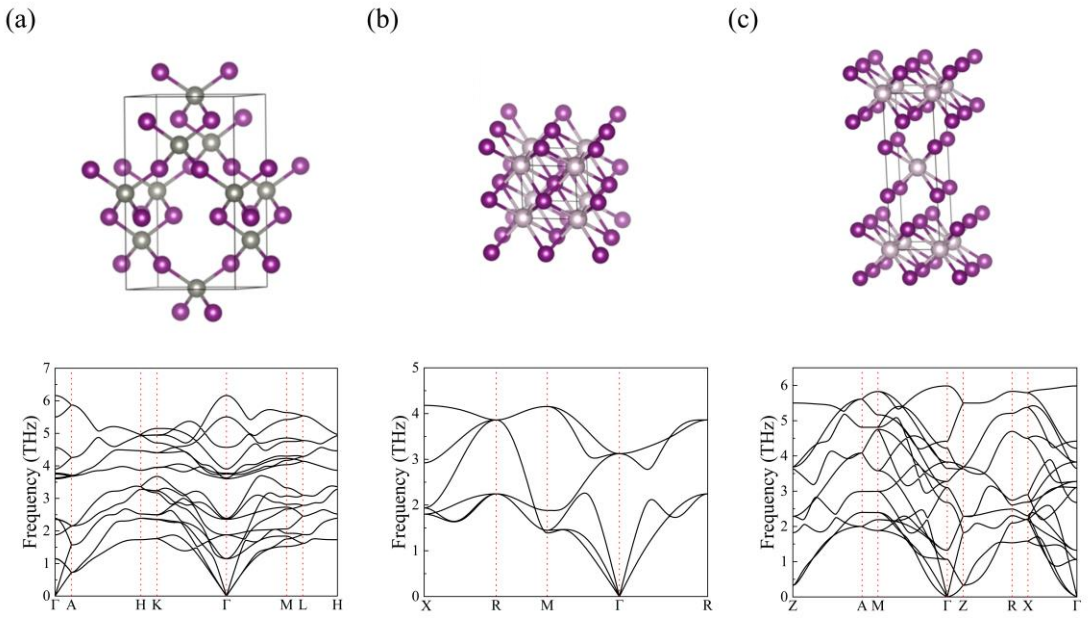

Fig. S1. Structures of new three stable phases (top of the Figure) and the corresponding calculated phonon spectra (bottom of the Figure). (a) 0 GPa, *I*-42*d*-ZnI_2, (b) 20 GPa, *Pm*-3*m*-HgI, (b) 30 GPa, *I*4/*mmm*-HgI_2.

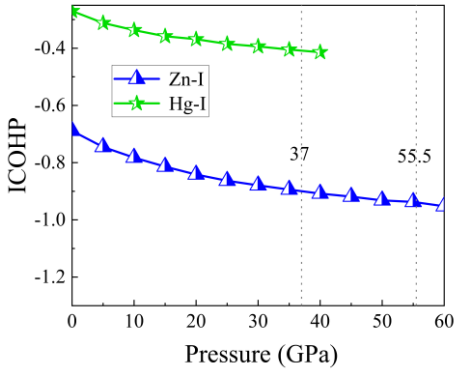

Fig. S2. The calculated changes of ICOHP in compressed conditions, the blue line represents the Zn-I atomic pair in *P*6$_3$*mc*-ZnI_2 structure, and the green line represents the Hg-I atomic pair in *I*4/*mmm*-HgI_2 structure.