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New Alkaline Earth Rich Binary Indides: Ca_2In, $Sr_{28}In_{11}$ and Sr_5In_3

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The new binary alkaline earth rich indides Ca_2In (orthorhombic, space group *Pnma*, $a = 727.5(2)$, $b = 537.1(2)$, $c = 999.0(3)$ pm, $Z = 4$, $R1 = 0.0252$, Co_2Si structure type) and $Sr_{28}In_{11}$ (orthorhombic, space group *Imm*2, $a = 582.6(3)$, $b = 6687.8(9)$, $c = 823.5(6)$ pm, $Z = 2$, $R1 = 0.0571$, $Ca_{28}Ga_{11}$ structure type) have been synthesized from stoichiometric melts of the elements. Both crystal structures exhibit isolated In atoms coordinated by seven to ten alkaline earth atoms. In the crystal structure of Sr_5In_3 (tetragonal, space group $I4/mcm$, $a = 874.4(3)$, $c = 1642.9(8)$ pm, $Z = 4$, $R1 = 0.0347$, Cr_5B_3 structure type) isolated In atoms coexist with In_2 dumbbells exhibiting short In-In contacts (284.4 pm). The electronic structures of the less elaborate compounds Ca_2In and Sr_5In_3 are discussed in comparison with those of the closely related, nominally electron precise Zintl compounds Ca_2Sn and Sr_5Sn_3.

Key words: Indides, Alkaline Earth, Crystal Structure, Band Structure Calculation