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Pressure-stabilized lithium cesides with cesium anions beyond the -1 state JORGE BOTANA, Beijing Computational Science Research Centre, Beijing 10084, China., MAO-SHENG MIAO, Materials Research Laboratory, University of California, Santa Barbara, California Q3 93106-5050, USA. — Main group elements usually assume a typical oxidation state while forming compounds with other species that depends on the occupation of the outermost orbital. Group I elements are usually in the +1 state in inorganic materials. Our recent work on Cs-F compounds reveals that pressure may make the inner shell 5p electrons of Cs reactive, causing Cs to expand beyond the +1 oxidation state. In our study, we have found that pressure can cause large electron transfer from light alkali metals such as Li to Cs, causing Cs to become anionic with a formal charge much beyond -1. Li and Cs only form alloys at ambient conditions, but by studying the thermodynamic stability of the intermetallic compounds $\mathrm{Li}_n\mathrm{Cs}_m$ (n=1-5, m=1; n=1,m=1-4), we have found that some $\mathrm{Li}_n\mathrm{Cs}$ (n=1,3,4,5) compounds become stable under pressures higher than 100 GPa. Once formed, these compounds exhibit interesting structural features, including capped cuboids and dimerized icosahedra. Finally, we have also found superconductivity in metastable LiCs and that the unusual anionic state of Cs has a strong effect on the transition temperature.

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