

Abstract Submitted
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Cs in high oxidation states and as a p-block element MAOSHENG MIAO, University of California Santa Barbara — A long time doctrine rooted in the atomic shell model states that the atoms maintain a complete inner shell while interacting with other atoms. Therefore, group IA elements, for example, are invariably stable in the +1 charge state because the p electrons of their inner shells do not react with other chemical species. This general rule governs our understanding of the structures and reactions of matter and has never been challenged. In this work, I will show for the first time a striking result that while mixing with fluorine under pressure, Cs atoms will share their 5p electrons and become oxidized to a higher charge state. It forms stable CsF_n compounds, consisting of neutral or ionic CsF_n molecules. Their geometry and bonding resemble isoelectronic XeF_n molecules, showing that Cs chemically behaves like a p-block element. The stability of these remarkable compounds will change the understanding of the periodic table and chemistry of elements. The work was done by using an automatic crystal structure search based on particle swarm optimization algorithm and the first principles total energy calculations.

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