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Structure prediction using global optimization and data mining in new Ce-O-N compounds

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Stable and metastable modifications inside of an ionic Ce-O-N compound with the compositions Ce_2ON_2 and $\text{Ce}_3\text{O}_3\text{N}$ have been identified. The Ce_2ON_2 has been found as a best candidate with Ce^{4+} charge, even in the extreme conditions, [1,2] while $\text{Ce}_3\text{O}_3\text{N}$ system is predicted for Ce^{3+} ions. Structure candidates for both compositions have been obtained after exploring the energy landscape for different pressure values and using empirical potentials.

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