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On The Electronic Structures of Metaphosphate $PX_3^{(-)}$ and Metaphosphite $PX_2^{(-)}$ Anions, $X = CH_2, SiH_2, NH, PH, O, S$

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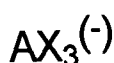
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ON THE ELECTRONIC STRUCTURES OF METAPHOSPHATE $PX_3^{(-)}$ AND METAPHOSPHITE $PX_2^{(-)}$ ANIONS, $X = CH_2, SiH_2, NH, PH, O, S$

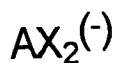
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Abstract Quantum chemical calculations at RHF/6-31+g(d,p) with electron correlation and vibrational energy corrections are reported on the metaphosphate and metaphosphite series, indicating a facile second-order Jahn Teller distortion of the planar geometries.

Since the first detection of the metaphosphate anion, $\underline{1}$ ($X = O$)¹ in the gas phase, this species has been the subject of detailed discussion. Structural investigations are hitherto



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known on $\underline{1}$ ($X = CR_2$, $R = SiMe_3$)² and recently on the imino derivative, $\underline{1}$ ($R = NR$)³. On the whole series of metaphosphates, $\underline{1}$ ($X = CH_2, SiH_2, NH, PH, O, S$) and corresponding metaphosphites, $PX_2^{(-)}$ quantum chemical investigations at RHF/6-31+g(d,p) level with MP4SDTQ and zero-point vibrational energy corrections are reported⁴. They reveal for the metaphosphates various symmetry coupled distortions from total planarity in $\underline{1}$, as the consequence of a second-order Jahn-Teller effect. Corresponding group transfer reactions relate the stabilities of the metaphosphates with respect to the metaphosphites.

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