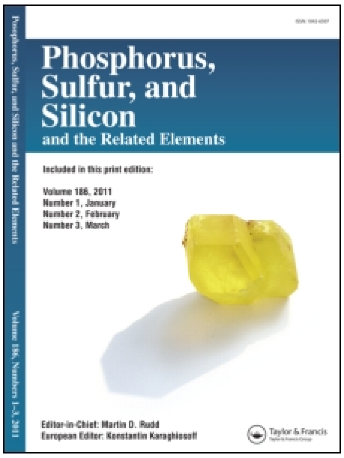

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On The Electronic Structures of Metaphosphate $PX_3^{(-)}$ and Metaphosphite $PX_2^{(-)}$ Anions, X = CH_2, SIH_2, NH, PH, O, S

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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, 1 (X = O)[1] in the gas phase, this species has been the subject of detailed discussion. Structural investigations are hitherto

$$AX_3^{(-)} \qquad\qquad AX_2^{(-)}$$

1 2

known on 1 (X =CR_2, R = $SiMe_3$)[2] and recently on the imino derivative, 1 (R = NR)[3]. On the whole series of metaphosphates, 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 reported[4]. They reveal for the metaphosphates various symmetry coupled distortions from total planarity in 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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