molecular vibrational constants and chemical bonding in the cyclic oxocarbon dianions Cnon-2(n=3, 4 and 5)

Campos-Vallette, M.

Figueroa, K. A.

By means of an ab initio force field and the mean amplitudes of vibration of the cyclic oxocarbon dianions Cn0nwith n= 3, 4 and 5, it has been found that the ground-state aromaticity order in the series is: deltate (n=3) > squarate (n=4) > croconate (n=5) ion. The reactivity of these molecules with respect to an electrophilic attack follows the order croconate > squarate > deltate ion. © 1988, Taylor & Francis Group LLC, All rights reserved.