Title:	Cation-π interaction: To stack or to spread
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Abstract:	The interaction between different cations and certain aromatic dimers (benzene, naphthalene, anthracene) and heteroaromatic dimers (pyridine, pyrazine, sym-triazine and sym-tetrazine) has been investigated employing the MP2 level of theory with the 6-31G** and 6-311++G** basis sets. The trend in the stabilization energy for aromatic dimers is found to be: (anthracene)2-cation> (naphthalene)2-cation>(benzene)2-cation. In all three cases, the cation remains sandwiched between the rings. In the case of the heteroaromatic systems, on the other hand, the cation prefers to interact with the nitrogen atom of the ring. These results can be rationalized by molecular electrostatic potential maps for the systems under consideration. In addition, these results are in conformity with the available cation aromatic database.
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