The benzene dimer cation is a model system for ionized π-stacked aromatic molecules, which are thought to play an important role in charge transfer and localization processes in biological systems (e.g. DNA). Using the EOM-IP method, we characterized the ten lowest states of the benzene dimer cation and determined important relaxation coordinates (scans along the interfragment distance are shown on the right). An important feature in the electronic spectrum of the ionized π-stacked aromatics (see the stick spectrum on the right) is the appearance of strong charge-resonance bands, which are unique to the dimer and are very sensitive to its geometry. These transitions can be used as a probe for dimer formation and dynamics.

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