Aromatic Resonance Effects on Ketones

Concept.   You will optimize the structure of a conjugated ketones by comparison to a model system. You will then examine the bond lengths and bond orders of the ketones, in order to look for effects of aromatic resonance contributions.

Procedure.   Build and optimize the following cyclic ketones using the AM1 and 6-31G* method. Record the C=O bond lengths and orders, and the Mulliken charges on the C=O bond. Use resonance arguments to try to explain the trends.

Literature.   Compare to any known geometric, dipole, or THEOCHEM data.