

OP-9

BAY QUINONES – ELECTRONIC PROPERTIES AND STABILITY

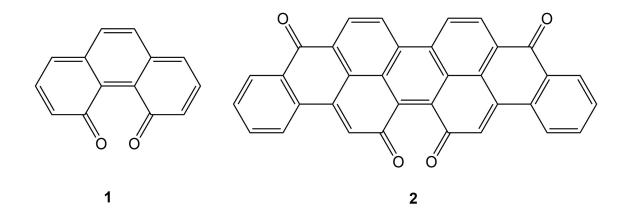
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Bay quinones have carbonyl groups pointing into the congested space of a bay region of their hydrocarbon skeleton. The parent bay quinone, phenanthrene-4,5-quinone **1**, has never been synthesized, in spite of several attempts.^[1-3] In this contribution, we report on our experiments aimed at generating **1** via low temperature electrochemical synthesis and matrix isolation spectroscopy. We will also report on the electrochemical synthesis of the larger homologue violanthrone-16,17-quinone **2**, and on the results of quantum chemical calculations revealing structure-property relationships in this little-explored class of compounds. Very low-lying, thermally populated triplet excited states were found to be a factor contributing to the very limited stability of **1** and derivatives.



REFERENCES

- [1] M. S. Newman, R. L. Childers, J. Org. Chem. 1967, 32, 62–66.
- [2] M. S. Newman, H. M. Dali, J. Org. Chem. 1977, 42, 734–736.
- [3] F. R. Hewgill, J. M. Stewart, J. Chem. Soc. Chem. Commun. 1984, 1419–1420.