

ADDITIONS AND CORRECTIONS

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Maciej Bobrowski, Adam Liwo,* and Kimihiko Hirao:
Theoretical Study of the Energetics of the Reactions of Triplet
Dioxygen with Hydroquinone, Semiquinone, and Their Proton-
ated Forms: Relation to the Mechanism of Superoxide Genera-
tion in the Respiratory Chain

Page 3543. This is a correction of Figures 3 and 5 of the
paper. The geometric parameters in Figure 3 corresponded to
the smaller 6-31G(d) basis set and not to the 6-31+G(d) basis
set, and there were some typos in the charges shown in both
figures. These errors have been fixed in this Correction.

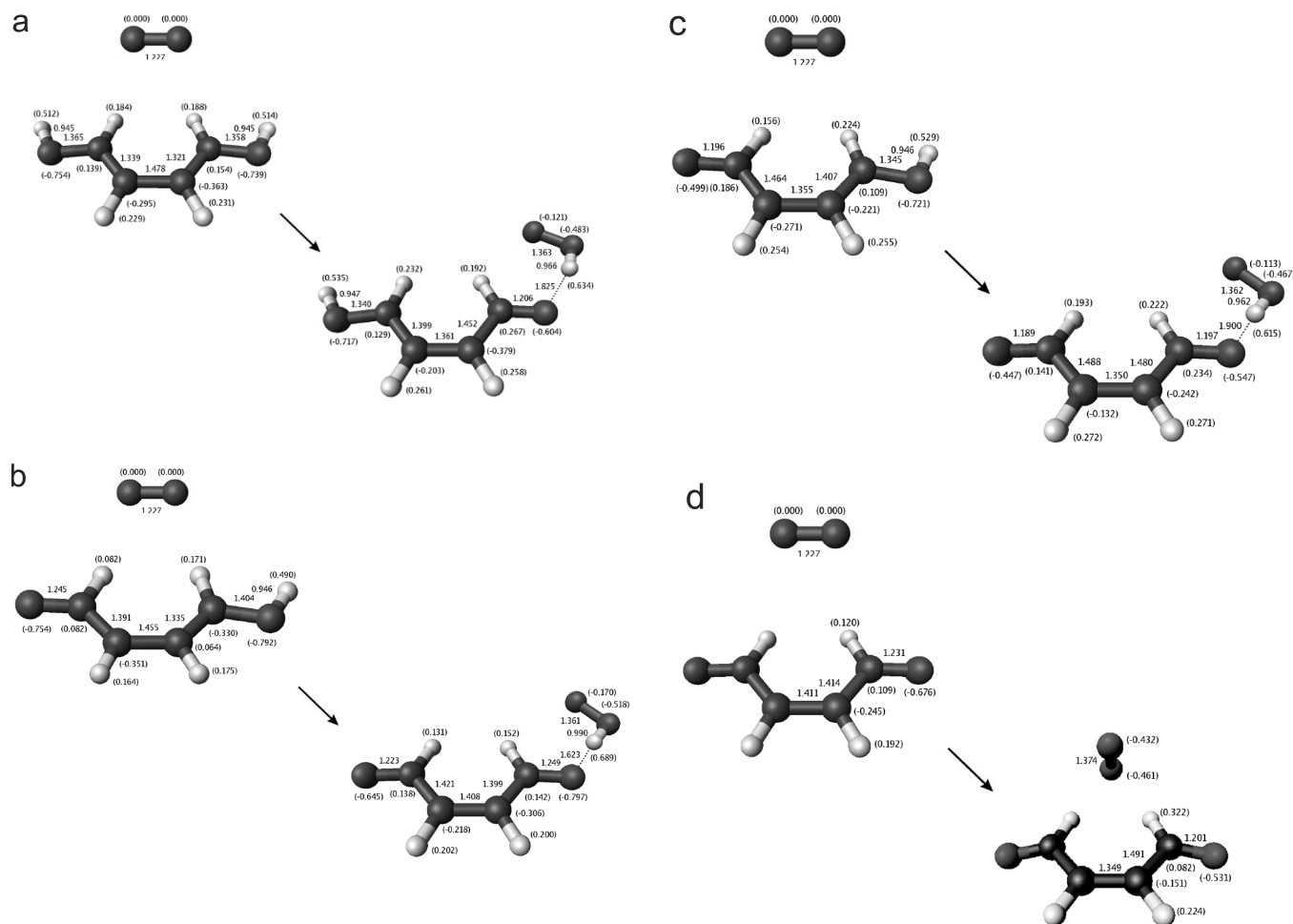


Figure 3. MRMP/CASSCF/6-31+G(d)-optimized geometries and partial atomic charges of the substrates and the products of reactions (a) 1, (b) 2, (c) 3, and (d) 4 for *cis*-1,3-but-1,4-dione. The pictures have been drawn with MOLMOL.⁵⁹

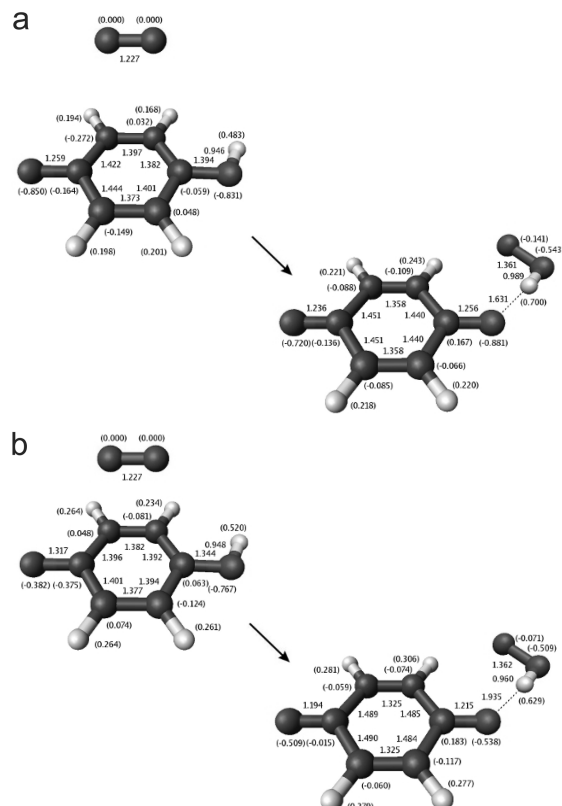


Figure 5. MRMP/CASSCF/6-31+G(d)-optimized geometries and partial atomic charges of the substrates and the products of reactions (a) **2** (b) and **3** for *p*-benzoquinone. The pictures have been drawn with MOLMOL.⁵⁹

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