

Supporting Information

for

**Direct Formation of the C5'-Radical in the Sugar-Phosphate
Backbone of DNA by High Energy Radiation**

by

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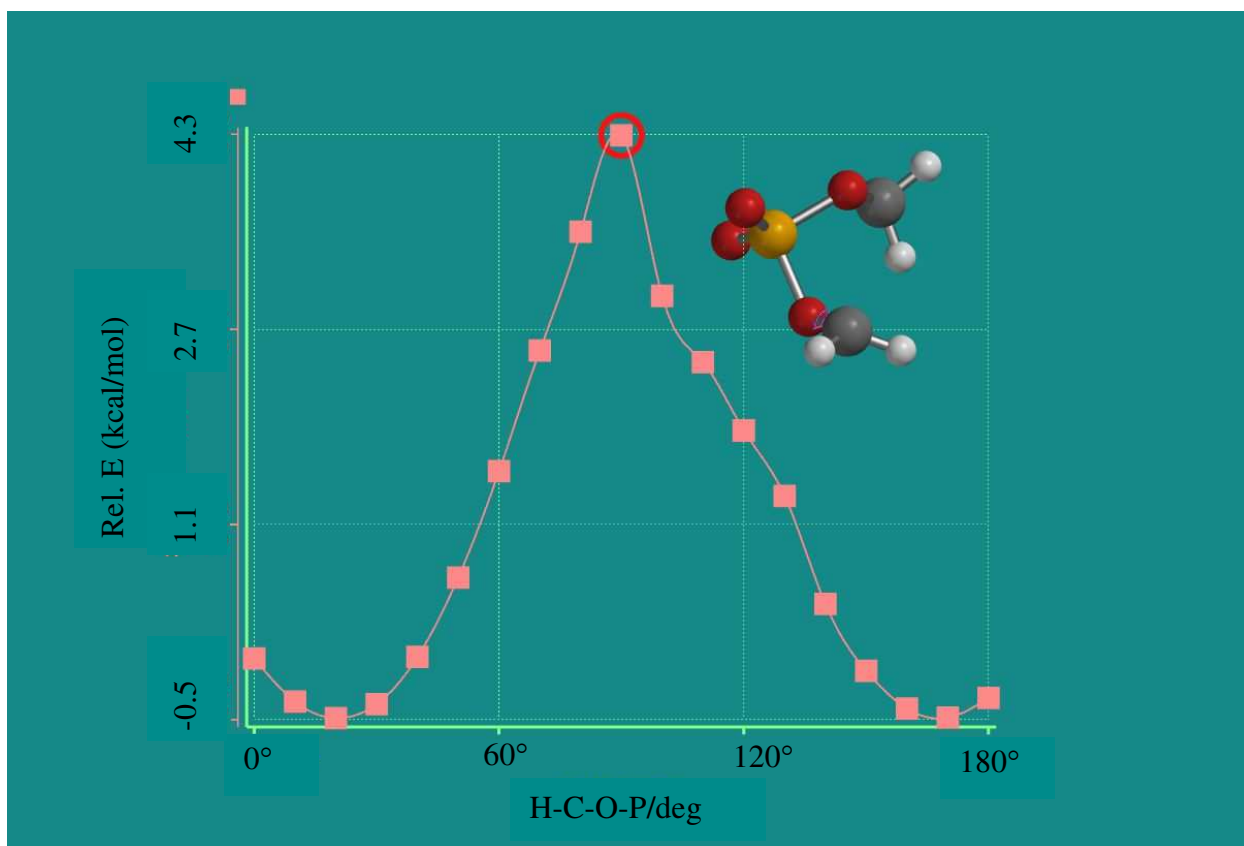


Figure S1. The optimized geometry of the highest energy conformation of $\text{CH}_3\text{OP}(\text{O}_2^-)\text{OCH}_2\bullet$ in the gas phase obtained by employing DFT/B3LYP/6-31G(d) method. The potential energy surface of various conformations of $\text{CH}_3\text{OP}(\text{O}_2^-)\text{OCH}_2\bullet$ was obtained by stepwise (each step = 10°) gradual increase of the dihedral angle H-C-O-P from 0° to 180° in 18 steps.

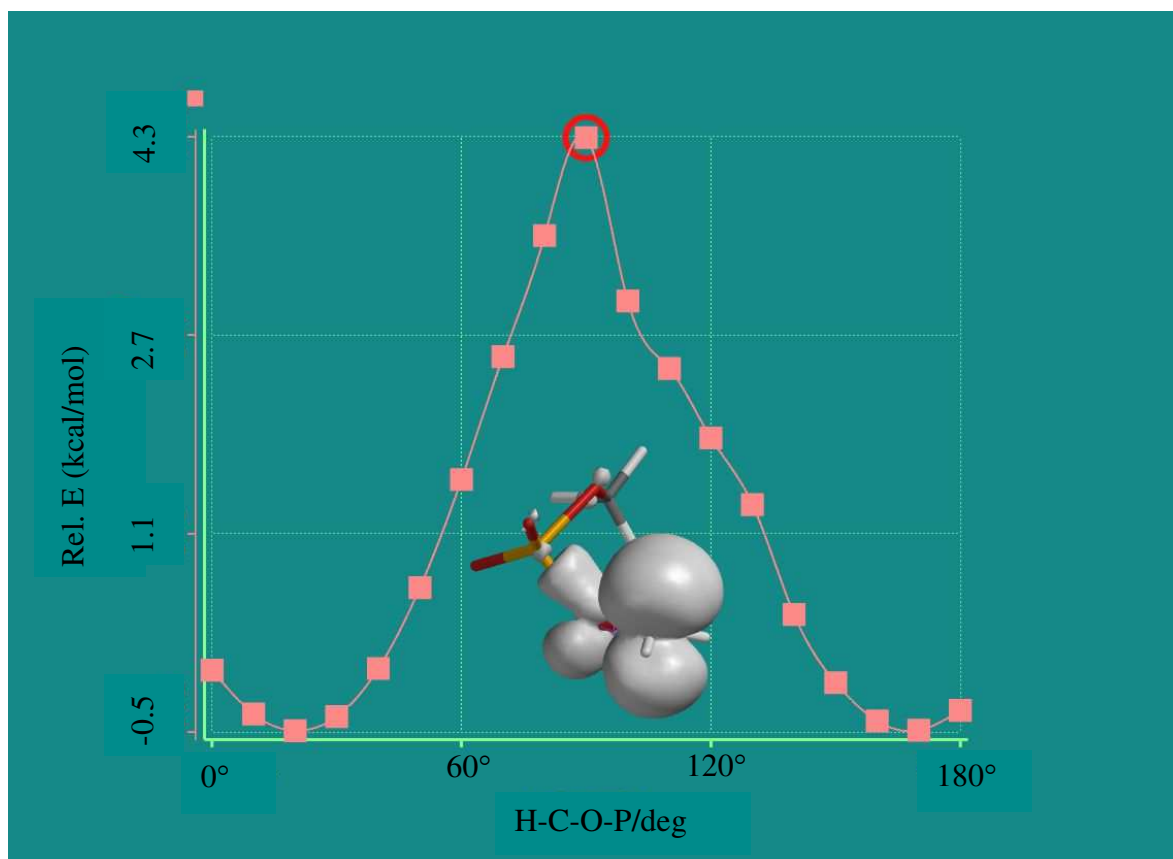


Figure S2. The spin density distributions in the optimized geometry of the highest energy conformation of $\text{CH}_3\text{OP}(\text{O}_2^-)\text{OCH}_2\bullet$ in the gas phase obtained by employing DFT/B3LYP/6-31G(d) method. The potential energy surface of various conformations of $\text{CH}_3\text{OP}(\text{O}_2^-)\text{OCH}_2\bullet$ was obtained by stepwise (each step = 10°) gradual increase of the dihedral angle H-C-O-P from 0° to 180° in 18 steps. A 40 G beta phosphorous coupling is found at the maximum in energy.

The complete reference 36(b):

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