

## 2'-脱氧腺苷-5'-磷酸与羟基自由基反应所形成的自由基

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## Radicals Created from the Reactions of 2'-Deoxyadenosine-5'-monophosphate with Hydroxyl Radical

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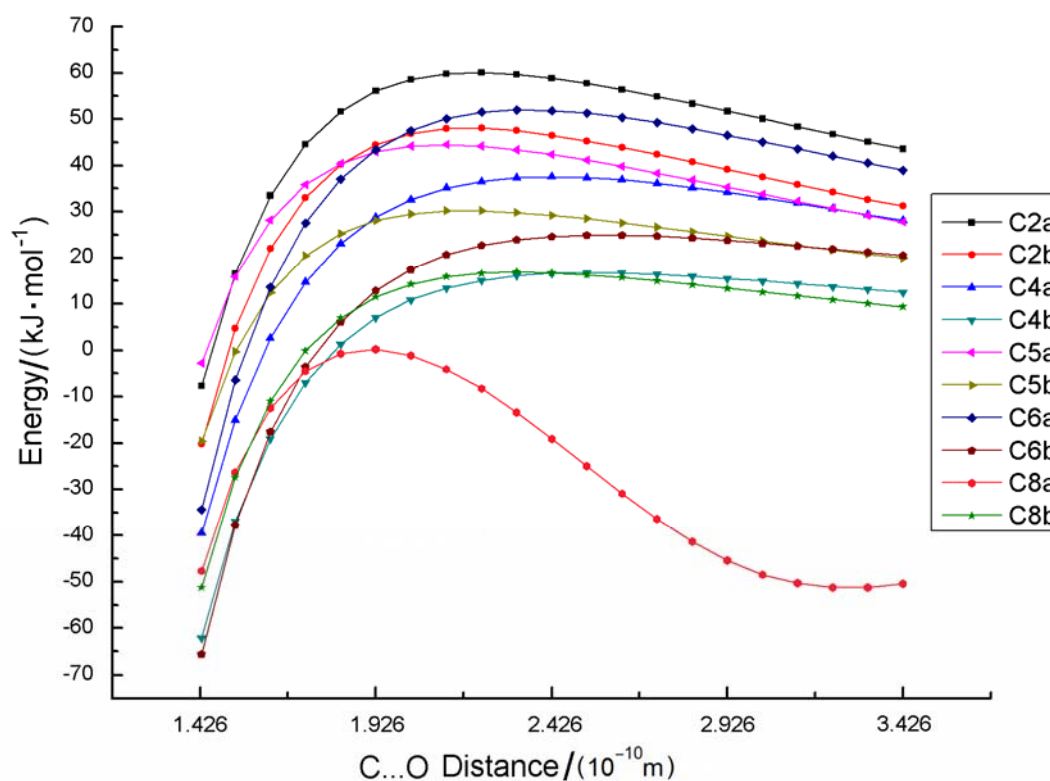
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In addition reactions (1),  $\text{HO}\cdot + \text{dAMP} \rightarrow (\text{dAMPOH})\cdot$ , an  $\text{HO}\cdot$  free radical will move close to all of C atoms of purine ring of dAMP before generating  $(\text{dAMPOH})\cdot$  radical. Therefore, it is reasonable to assume that the O atom of  $\text{HO}\cdot$  approaches to C atoms of purine base of dAMP along the C ... O line that is perpendicular to the base ring from two sides of the base.

On the basis of the orientation of  $\text{HO}\cdot$  and C atoms of base ring, we evaluated the variation of electrostatic interaction energies<sup>1,2</sup> between the C atoms of purine ring of dAMP and the O atom of  $\text{HO}\cdot$  with the C ... O distance. The electrostatic interaction energies with respect to the C ... O distance in the formations of the ten possible  $(\text{dAMPOH})\cdot$  radicals are depicted in Fig. 1S. The C ... O distance value of 142.6 pm is the bond length of C-O single bond.



**Fig.1S** Electrostatic interaction energies with respect to the C ... O distance in which the C ... O line is perpendicular to the base ring

## References

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