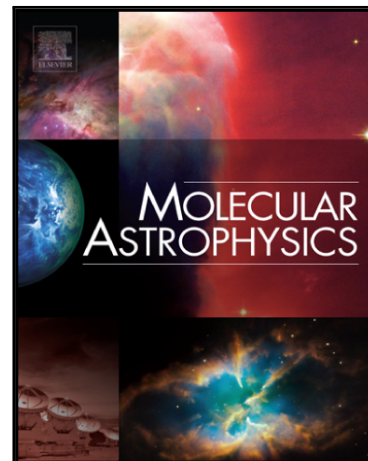


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First-principles study of the formation of glycine-producing radicals from common interstellar species

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*First-principles study of the formation of glycine-producing radicals from common interstellar species*

A short title: glycine radical formation

Keywords: density functional theory, origin, amino acid, ISM, chemical reaction, reaction mechanism

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## ABSTRACT

Glycine, the simplest amino acid, has been intensively searched for in molecular clouds, and the comprehensive clarification of the formation path of interstellar glycine is now imperative. Among all the possible glycine formation pathways, we focused on the radical pathways revealed by Garrod (2013). In the present study, we have precisely investigated all the chemical reaction steps related to the glycine formation processes based on state-of-the-art density functional theory (DFT) calculations. We found that two reaction pathways require small activation barriers ( $\Delta E^\ddagger \leq 7.75$  kJmol<sup>-1</sup>), which demonstrates the possibility of glycine formation even at low temperatures in interstellar space if the radical species are generated. The origin of carbon and nitrogen in the glycine backbone and their combination patterns are further discussed in relation to the formation mechanisms. According to the clarification of the atomic correspondence between glycine and its potential parental molecules, it is shown that

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