# Document details - Density Functional Theory Analysis of Ground State and Evaluation of Transition Probability Parameters for Carbon Mono-Fluoride Molecule





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## Density Functional Theory Analysis of Ground State and Evaluation of Transition Probability Parameters for Carbon Mono-Fluoride Molecule(Article)

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### Abstract

In view of astrophysical application, the ground state molecular parameters such as bond length, dipole moment, rotational constant, harmonic frequency, IR intensity, vibrational temperature of the astrophysically significant diatomic molecule of carbon mono-fluoride (CF) were derived using B3LYP hybrid density functional theory with three basis sets of 3-21G, 6-31G, and 6-311G. The computed data were collectively compared with the values reported in the literature. It was found that the vibrational temperature obtained using the density functional theory approach resembles the favorable temperature for the formation of the CF molecule in an interstellar medium. The transition probability parameters, namely Franck–Condon factors and r-centroids were evaluated for A–X, B–X, and D–X band systems of the CF molecule, using a more reliable numerical integration procedure. The molecular parameters of ground state obtained in the present study was compared with the reported values for better justification. The results of Franck–Condon factors and r-centroids were also discussed in view of astrophysical application. © 2022, Springer Science+Business Media, LLC, part of Springer Nature.

### Author keywords

astrophysical significance | carbon mono-fluoride molecule | density functional theory | Franck–Condon factor | r-centroid

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