Spectroscopic characterization of diversity of amorphous carbonaceous C_{60} clusters.

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The nature of the carbonaceous carrier of the infrared (IR) emission spectra of planetary and proto-planetary nebulae is still an open question. This requires more studies on the interplay between the structural properties of carbon-based compounds and spectroscopic signatures. The recent observation of C_{60} buckminsterfullerene in space notably suggests that carbon clusters of similar size may also be relevant.

In the settings of the PACHYNO project[1] (Probing the diversity of Astrophysically relevant Carbon and Hydrogen NaNO particules) which involves the collaboration between the LCPQ, the ISMO and the LiPHY (France), we determine the characteristics of pure carbon compounds. A broad statistical samples of C_{60} isomers were computationally determined without any bias using a reactive force-field. This sample was locally optimized at ”Self-Consistent Charge Density Functional Tight Binding” (SCC-DFTB) level and was followed by IR harmonic spectra analysis at the same level of theory.

During this talk, I will present the results of our analysis. Four main structural families were determined. We compute for each of these families of structures their corresponding IR emission spectra. Also we compare our results with astronomical data. This indicates that the presence of the defined family can possibly contribute in the plateau observed in the region of 6-9µm. This work is a part of larger study and the exploration of hydrogenated carbonaceous compounds will be the next steps of our study.

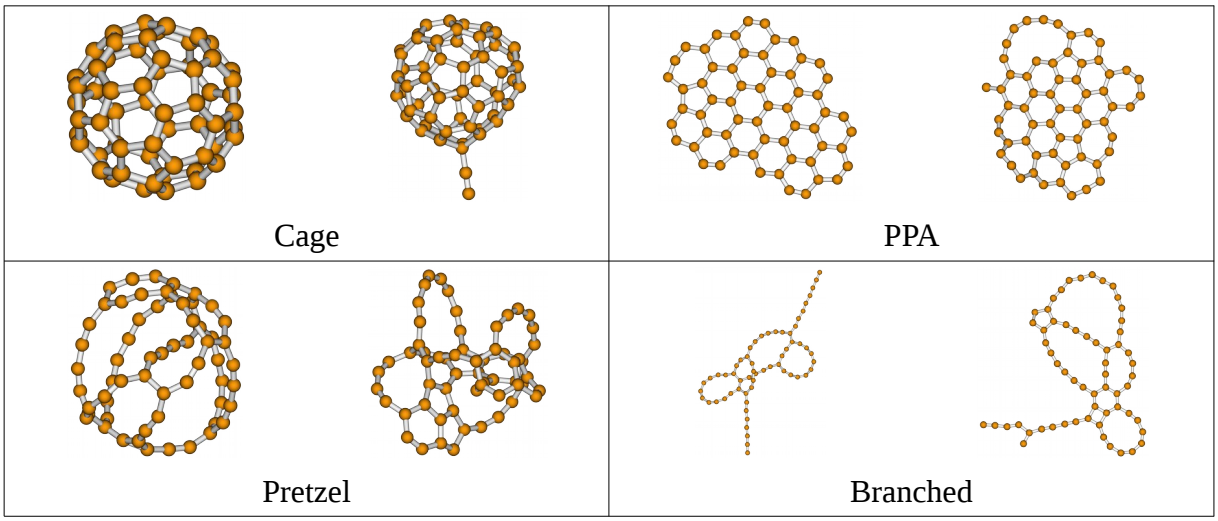

Figure 1: Determined families for carbonaceous structures of C_{60} at SCC-DFTB level.

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References

[1] ANR PACHYNO, ANR-16-CE29-0025-02