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[1] Normandie Univ, ENSICAEN, UNICAEN, CNRS/IN2P3, LPC Caen, 14000 Caen, France
[2] CIMAP, CEA-CNRS-ENSICAEN-UNICAEN, Normandie Université, BP5133, F-14050 Caen Cedex 04, France
[3] Department of Chemistry, Tokyo Metropolitan University, 1-1 Minamiosawa, Hachiouji-shi, Tokyo 192-0397, Japan

Synopsis The Coulombic explosion of multi-charged $(CO)_3^{q+}$ molecular ions produced in low energy collisions with Ar^{9+} projectiles was investigated using recoil ion momentum spectrometry (RIMS). A preliminary analysis of the data clearly shows a dominant triangular cyclic structure. Events that may correspond to a linear chain are also observed, but the latter could as well originate from false coincidences, associated to the fragmentation of dimers. A careful analysis of this source of background is proposed to disentangle trimer fragmentation events from false coincidences.

Direct observation of weakly bound structures, such as small molecular clusters, remains an experimental challenge. Infrared (IR) spectroscopy, combined with calculations of intermolecular potential surfaces, has for long been the only way to access such structures. In the last decade, a new technique providing more direct measurements has been developed: by Coulomb exploding the cluster, all momentum vectors of the charged ions or molecular ions can be measured in coincidence, giving access to the initial 3D relative position prior dissociation. A nice illustration of this technique, called "Coulomb imaging", can be found in [1], where such measurements were performed to determine the geometry of argon and neon dimer, trimer, and tetramer.

Our study focuses on the structure of molecular CO trimers. Few experimental results from IR spectroscopy were made available for this structure, as the $(CO)_3$ transitions were found partly overlapped and obscured by those of $(CO)_2$. The work from Rezaei and collaborators [2] has previously shown a strong evidence for a planar, cyclic and C-bonded structure of the trimer. But satellite peaks and other spectroscopic features remained unexplained. This shortcoming called for a new investigation of the structure of $(CO)_3$ using a completely different and independent technique.

In the present experiment, Coulomb explosion is induced by collisions between a supersonic gas jet, providing the $(CO)_3$ molecular trimers, and Ar^{9+} ions delivered by the low energy beam line of the GANIL/ARIBE facility. The fragments momenta are measured using a COLTRIMS setup. A clean data selection is first achieved by imposing momentum conservation laws to the fragments resulting from Coulomb explosion. The momentum vectors of the fragments are then further analyzed to infer the geometry of the trimer.

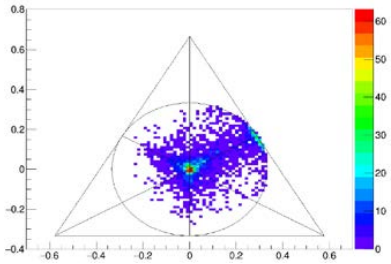

Figure 1. Dalitz plot obtained for the fragmentation of $(CO)_3^{3+}$ in three singly charged $(CO)^+$ fragments.

The plot of Fig. 1 clearly shows two distinct contributions. The dominant one, in the center, can be associated to a regular triangular structure. The weaker contribution, visible on the right edge of the Dalitz plot, could either indicate a linear structure or originate from false coincidences between a dissociating dimer and a monomer. A careful analysis of the background has been performed to quantify this possible contribution.

References

[1] Ulrich B *et al* 2011 *J. Phys. Chem. A* **115** 6936
[2] Rezaei M *et al* 2013 *J. Chem. Phys.* **138** 071102

* E-mail: flechard@lpccaen.in2p3.fr