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Correction: Resolving the anomalous infrared spectrum of the MeCN–HCl molecular cluster using *ab Initio* molecular dynamics

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Correction for 'Resolving the anomalous infrared spectrum of the MeCN–HCl molecular cluster using *ab Initio* molecular dynamics' by Nicolai Bork *et al.*, *Phys. Chem. Chem. Phys.*, 2014, **16**, 24685–24690.

In our original manuscript, we wrote about and discussed the angular distribution of the H–N–Cl angle from a Molecular Dynamics (MD) simulation trajectory. We stated that the global energy minimum conformation of 180 degrees was essentially unpopulated, and that the most populated value of the H–N–Cl angle was 162 degrees. With this comment, we stress that it is not a surprise that the global energy minimum conformation is almost unpopulated. This is a geometrical consequence, as the volume element, $\sin(\theta)$, goes to zero, when θ goes to 180 degrees, where θ is the angle defined by the three atoms. If the population from the MD simulation, shown in Fig. 3 of the article, is divided by the volume element associated with the H–N–Cl coordinate, the maximum in the ensuing probability is shifted towards the global energy minimum, as expected. The simulation of the IR spectrum and the conclusions drawn from this simulation, which is the main focus of our manuscript, are unaffected.

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The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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