Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Theoretical Gas to Liquid Shift of 15N Isotropic Nuclear Magnetic Shielding in Nitromethane using Ab Initio Molecular Dynamics and GIAO / GIPAW Calculations.

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Figure S1 Variation of ^{15}N chemical shielding of nitromethane calculated using 6-311++g(d,p) basis sets.

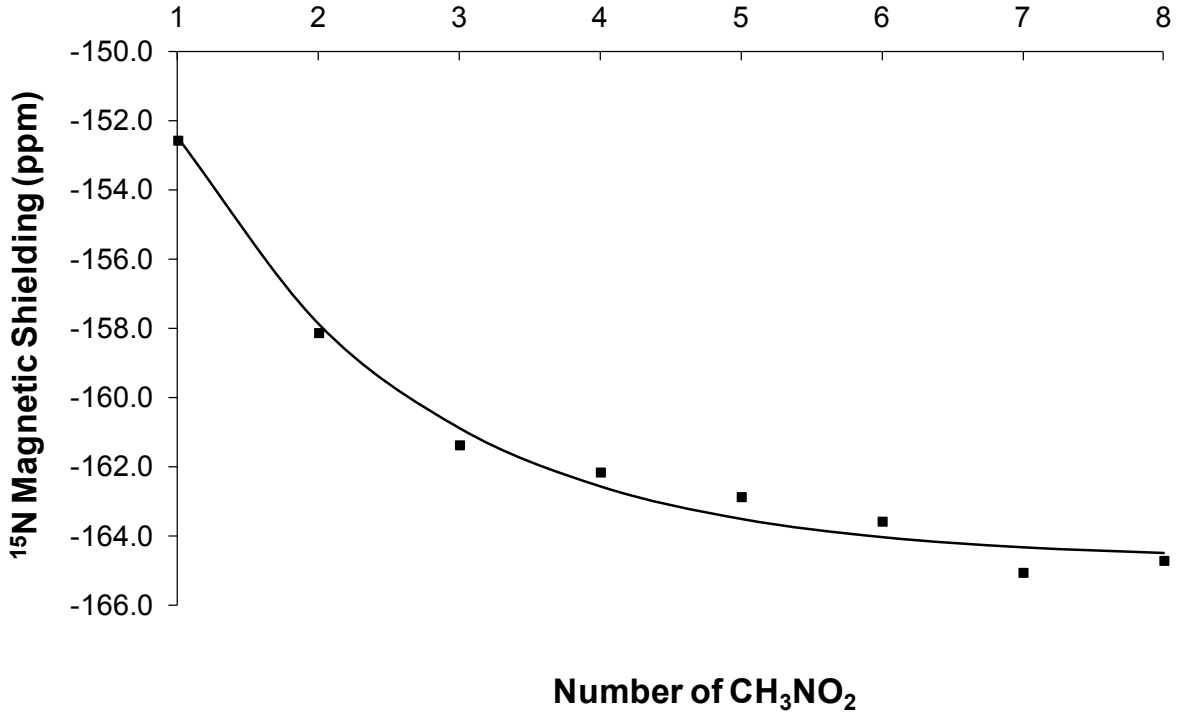

Figure S2. Selected radial distribution functions for nitromethane. Molecular Dynamics within Periodic Boundary Conditions using 8 molecules (Solid line) and 20 molecules (dash line).

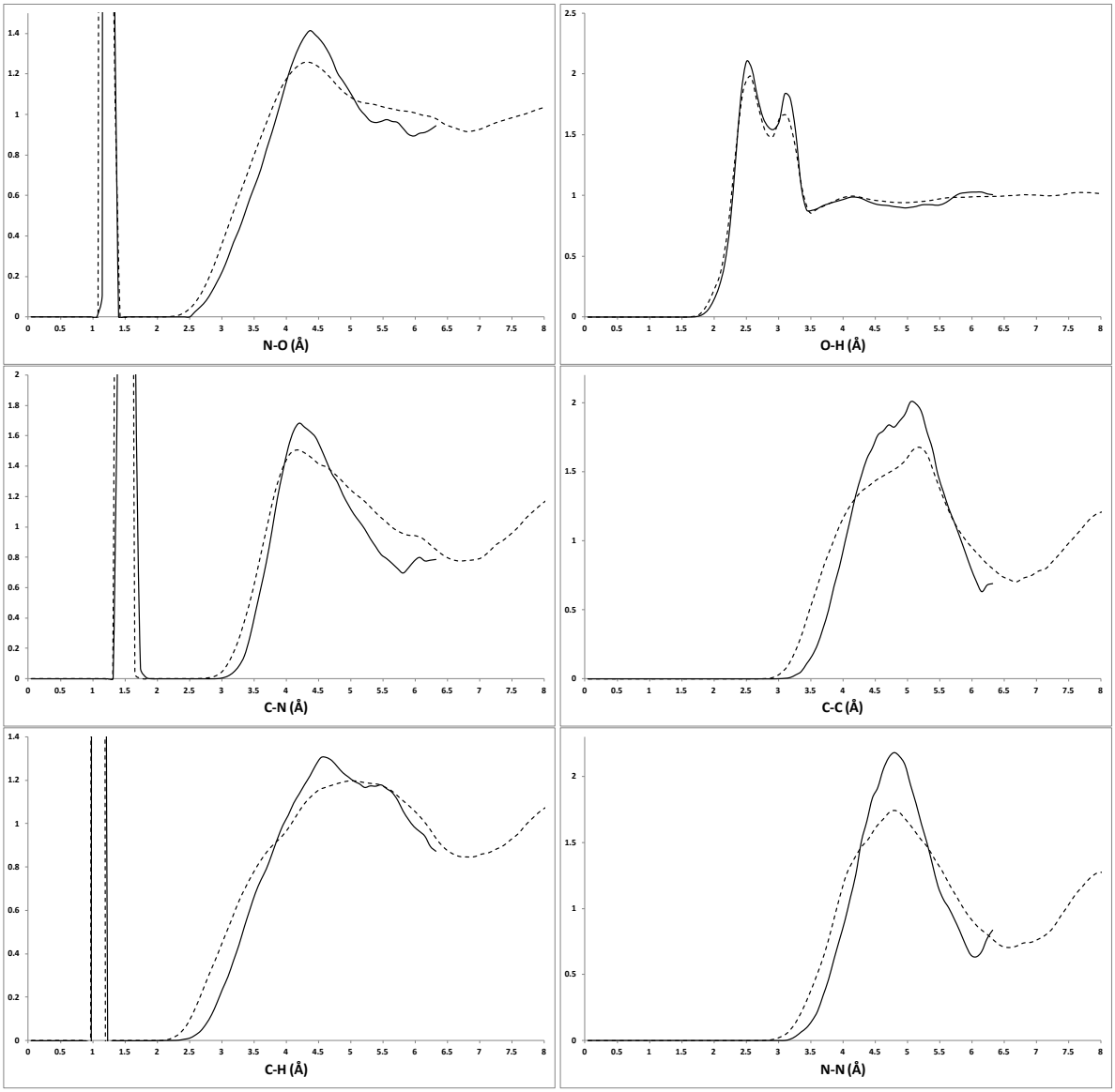

Figure S3. ^{15}N shielding average evolution as a function of the number of structures. The structures used for the NMR calculations were extracted from dynamic simulations performed in several conditions.