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Atmospheric new particle formation enhanced by tricarboxylic acids

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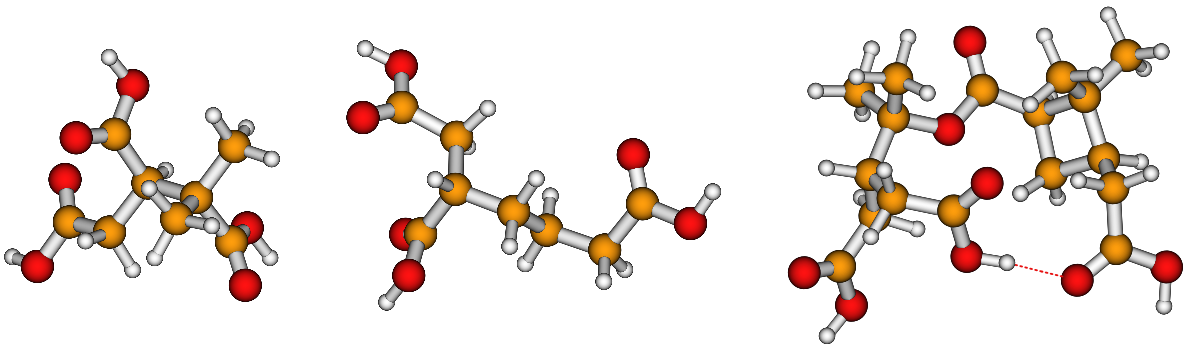
S1 Supporting Data and Structures

The coordinates of the calculated structures and the associated thermochemistry are available in the Atmospheric Cluster Database at:

https://github.com/elmjonas/ACDB.git

The datasets for this work can be found under the Articles/pedersen26_organics folder.

S2 Monomer geometries



MBTCA CHA PDPE

Figure S1: The monomer geometries lowest in free energy at the DLPNO-CCSD(T_0)/aug-cc-pVTZ//ωB97X-D/6-31++G(d,p) level of theory with a quasi-harmonic threshold of 100 cm^{-1}, at 298.15 K and 1 atm. Orange is carbon and red is oxygen.

S3 Cluster radii

Table S1: The radii of the clusters presented in figure 4 and 6. The radius is determined by the sphere whose volume equals that of an ellipsoid fitted to the structure, where the ellipsoid's shape is derived from the spatial spread of the atoms (the eigenvectors of the covariance matrix) and its scale from the maximum distance across the structure.

Cluster	Cluster radius [Å]
$(SA)_1(DMA)_1(MBTCA)_1$	3.63
$(SA)_1(DMA)_1(CHA)_1$	3.67
$(SA)_1(DMA)_1(PDPE)_1$	4.37
$(SA)_2(DMA)_2(MBTCA)_1$	4.11
$(SA)_2(DMA)_2(CHA)_1$	4.22
$(SA)_2(DMA)_2(PDPE)_1$	4.65
$(SA)_1(DMA)_1(MBTCA)_2$	4.04
$(SA)_1(DMA)_1(CHA)_2$	4.29
$(SA)_1(DMA)_1(PDPE)_2$	4.92
$(SA)_2(DMA)_2(MBTCA)_2$	4.60
$(SA)_2(DMA)_2(CHA)_2$	4.92
$(SA)_2(DMA)_2(PDPE)_2$	5.39