Formation of Atmospheric Molecular Clusters from Organic Waste Products and Sulfuric Acid Molecules: a DFT Study (Supporting Information)

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Here are reported the energetic data of cluster formation calculated at the ωB97X-D/aug-pcseg-1 (Table S1) and ωB97X-D/def2-SVPD (Table S2) levels of theory. Discussion about these results are to be found in the section 3.3 of the main paper.

In addition, geometries of the clusters optimized at the ωB97X-D/6-31++G(d,p), ωB97X-D/aug-pcseg-1 and ωB97X-D/def2-SVPD levels of theory can be found in separate text files, formatted in the standard XYZ format.

Table S1: Energetic data of cluster formation calculated at the ωB97X-D/aug-pcseg-1 level of theory. All values are given in kcal mol^{-1}.

Configurations	ΔE	ΔH	ΔG	ΔE^*	ΔG^*	$\Delta E^\dagger$	$\Delta G^\dagger$
$C_8H_7N + H_2SO_4$	−15.1	−16.2	−3.7				
$C_8H_7N + 2\,H_2SO_4$	−32.5	−34.7	−8.9	−15.1	−2.7	−17.4	−5.2
$C_9H_9N + H_2SO_4$	−15.9	−17.0	−4.2				
$C_9H_9N + 2\,H_2SO_4$	−33.3	−35.4	−9.6	−15.9	−3.4	−17.4	−5.4
$C_9H_9NO_2 + H_2SO_4$ (1)	−16.3	−17.2	−4.1				
$C_9H_9NO_2 + H_2SO_4$ (2)	−13.5	−14.5	−2.6				
$C_9H_9NO_2 + H_2SO_4$ (3)	−12.1	−13.1	−1.3				
$C_9H_9NO_2 + 2\,H_2SO_4$ (1)	−40.6	−42.8	−14.9	−23.2	−8.7	−24.4	−10.8
$C_9H_9NO_2 + 2\,H_2SO_4$ (2)	−38.5	−40.7	−13.7	−21.1	−7.5	−22.2	−9.5
$C_9H_9NO_3 + H_2SO_4$ (1)	−19.9	−20.9	−8.4				
$C_9H_9NO_3 + H_2SO_4$ (2)	−16.4	−17.3	−4.2				
$C_9H_9NO_3 + 2\,H_2SO_4$ (1)	−41.1	−43.2	−15.0	−23.6	−8.8	−21.2	−6.6
$C_9H_9NO_3 + 2\,H_2SO_4$ (2)	−36.4	−38.6	−12.9	−19.0	−6.7	−16.5	−4.5
$C_9H_9NO_3 + 2\,H_2SO_4$ (3)	−39.3	−41.5	−14.0	−21.9	−7.8	−19.5	−5.7
$C_9H_9NO_3 + 2\,H_2SO_4$ (4)	−38.5	−40.6	−12.6	−21.1	−6.4	−18.6	−4.3
$C_9H_9NO_3 + 2\,H_2SO_4$ (5)	−37.0	−39.3	−11.7	−19.6	−5.5	−17.2	−3.4
$2\,H_2SO_4$	−17.4	−18.5	−6.2				
$3\,H_2SO_4$	−34.4	−36.5	−11.5	−17.0	−5.4		

Table S2: Energetic data of cluster formation calculated at the ωB97X-D/def2-SVPD level of theory. All values are given in kcal mol^{-1}.

Configurations	ΔE	ΔH	ΔG	ΔE^*	ΔG^*	$\Delta E^\dagger$	$\Delta G^\dagger$
$C_8H_7N + H_2SO_4$	−15.0	−16.0	−3.7				
$C_8H_7N + 2\,H_2SO_4$	−32.9	−34.9	−9.7	−14.6	−2.5	−17.9	−6.0
$C_9H_9N + H_2SO_4$	−15.7	−16.8	−4.1				
$C_9H_9N + 2\,H_2SO_4$	−33.4	−35.4	−9.8	−15.1	−2.7	−17.6	−5.7
$C_9H_9NO_2 + H_2SO_4$ (1)	−16.9	−17.7	−5.1				
$C_9H_9NO_2 + H_2SO_4$ (2)	−14.3	−15.2	−3.5				
$C_9H_9NO_2 + H_2SO_4$ (3)	−12.8	−13.8	−1.8				
$C_9H_9NO_2 + 2\,H_2SO_4$ (1)	−42.4	−44.5	−16.7	−24.0	−9.6	−25.4	−11.6
$C_9H_9NO_2 + 2\,H_2SO_4$ (2)	−39.8	−42.0	−15.1	−21.5	−7.9	−22.9	−10.0
$C_9H_9NO_3 + H_2SO_4$ (1)	−20.7	−21.8	−9.1				
$C_9H_9NO_3 + H_2SO_4$ (2)	−16.8	−17.6	−5.0				
$C_9H_9NO_3 + 2\,H_2SO_4$ (1)	−42.8	−44.9	−17.1	−24.5	−10.0	−22.1	−8.0
$C_9H_9NO_3 + 2\,H_2SO_4$ (2)	−38.7	−41.0	−15.1	−20.4	−8.0	−18.0	−6.0
$C_9H_9NO_3 + 2\,H_2SO_4$ (3)	−40.1	−42.4	−14.7	−21.8	−7.5	−19.4	−5.6
$C_9H_9NO_3 + 2\,H_2SO_4$ (4)	−39.0	−41.1	−13.3	−20.7	−6.2	−18.3	−4.3
$C_9H_9NO_3 + 2\,H_2SO_4$ (5)	−38.3	−40.5	−13.1	−20.0	−5.9	−17.6	−4.0
$2\,H_2SO_4$	−18.3	−19.4	−7.1				
$3\,H_2SO_4$	−36.3	−38.5	−13.5	−18.0	−6.4		