

Supporting Information

DFT Studies on the Al-Speciation and Its Structure in Aqueous Aluminum Sol Formed by Aluminum Formoacetate

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Table S1: Gibbs free energy of isomers for aluminum formoacetate in aqueous solution

Species	Gibbs free energy/hartree	ΔG / kJ·mol ⁻¹
Al-1	-736.235068	0.0
Al-2	-736.225577	24.9
Al-3	-736.217557	46.0
Al-4	-736.195249	104.6

Table S2: Gibbs free energies of Al-1 and its dimerization products in aqueous solution

Species	Gibbs free energy/hartree	ΔG / kJ·mol ⁻¹
Al-1+ Al-1	-1472.470136	0.0
P-Al-1-IM1	-1472.478688	-22.5
i-P-Al-1-IM1 (isomer)	-1472.519250	-129.0
d-Al-1 (isomer)	-1472.523035	-139.0

Table S3: Gibbs free energies of d-Al-1 and its polymerization products in aqueous solution

Species	Gibbs free energy/hartree	ΔG / kJ·mol ⁻¹
d-Al-1+ d-Al-1	-2945.046070	0.0
P-d-Al-1-IM1	-2945.047057	-2.6
i-P-d-Al-1-IM1 (isomer)	-2945.077119	-81.6

Table S4: Gibbs free energies of isomers for aluminum formoacetate in acidic aqueous solution

Species	Gibbs free energy/hartree	ΔG / kJ·mol ⁻¹
Al-1-H (a)	-736.622972	0.0
Al-1-H (b)	-736.623484	-1.3
Al-1-H (c)	-736.639092	-42.3

Table S5: Gibbs free energies of hydrolysis product H-3H₂O-IM3 and its polymerization products in aqueous solution

Species	Gibbs free energy/hartree	ΔG / kJ·mol ⁻¹
H-3H ₂ O-IM3-1 + H-3H ₂ O-IM3-1	-1552.418844	0.0
P-H-3H ₂ O-IM3-1-IM4	-1552.423606	-12.5
d-Al-1-H-1(isomer)	-1552.453120	-90.0
d-Al-1-H-2 (isomer)	-1552.445321	-69.5

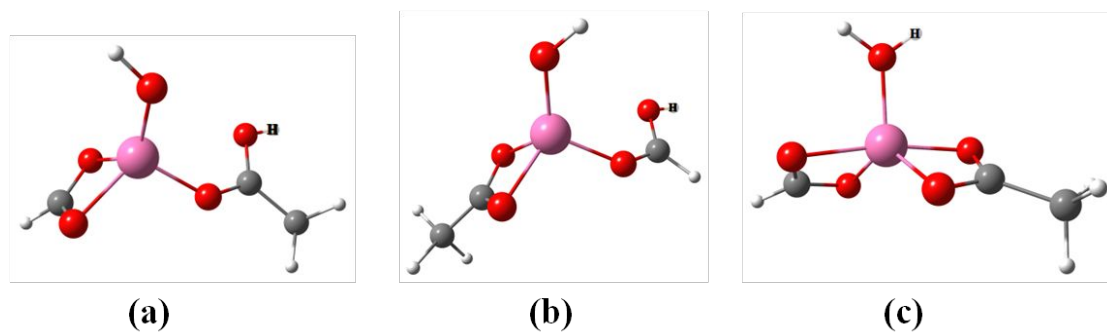


Figure S1. Optimized structures of isomers for Al-1-H in aqueous solution.

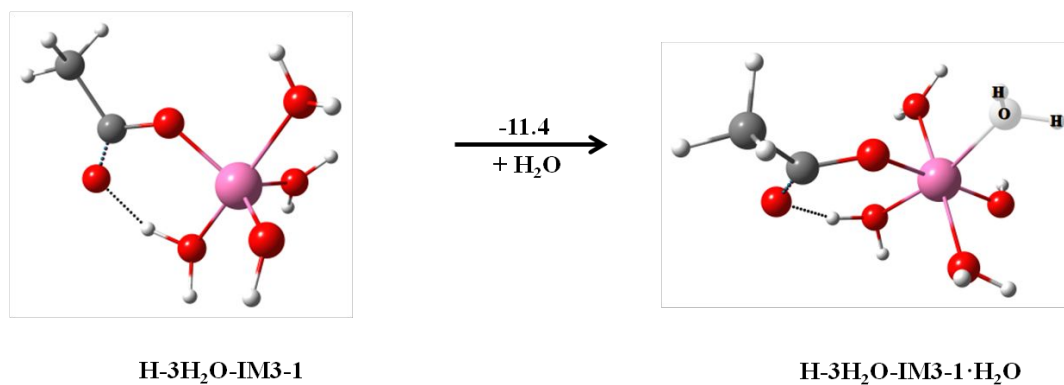


Figure S2. Optimized structures and relative energies of H-3H₂O-IM3-1·H₂O in aqueous solution.