Intermolecular interactions in 3-aminopropyltrimethoxysilane , N-methyl-3-aminopropyltrimethoxysilane and 3-aminopropyltriethoxysilane: Insights from computational spectroscopy

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Electronic Supplementary Material

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Table S1– Calculated energies of the relevant optimized structures.

Electronic energies at the M062X /6-311+g(d,p) level, without basis set superposition error (BSSE) and zero-point vibrational energy correction (ZVPE).

Dimerization energy = Dimer energy – 2x(Monomer energy); Trimerization energy = Trimer energy – 3x(Monomer energy).

	Total Energy (Hartree)	**Dimerization Energy** (kJ/mol)	**Trimerization Energy** (kJ/mol)
APTS			
Monomer	-808.8205587750		
Dimer HH	-1617.6545797600	-35.3	
Dimer HT	-1617.6545398400	-35.2	
Trimer HH	-2426.4883394300		-70.0
Trimer HT	-2426.4951220900		-87.8
MAPTS			
Monomer	-848.1149860590		
Dimer HH	-1696.2449267600	-39.3	
Dimer HT	-1696.2456762900	-41.2	
Trimer HH	-2544.3746790900		-78.0
Trimer HT	-2544.3830622900		-100.0
APTES			
Monomer	-926.7458436300		
Dimer HH	-1853.5078134200	-42.3	
Dimer HT	-1853.5099502100	-47.9	
Trimer HH	-2780.2697646400		-84.6
Trimer HT	-2780.2799148600		-111.3

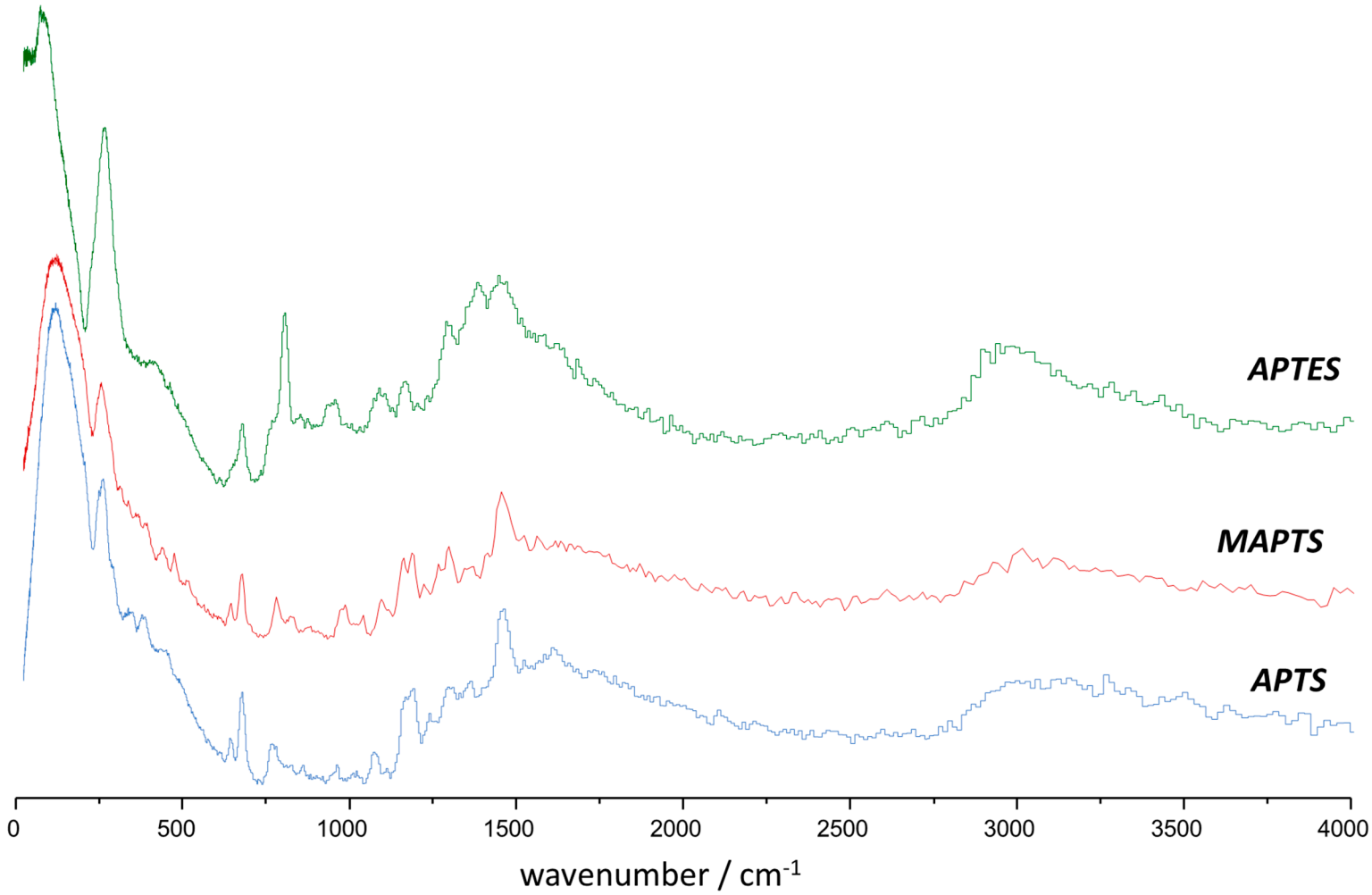


Figure S1. *INS spectra of APTS, MAPTS, and APTES up to 4000 cm^{-1}.*

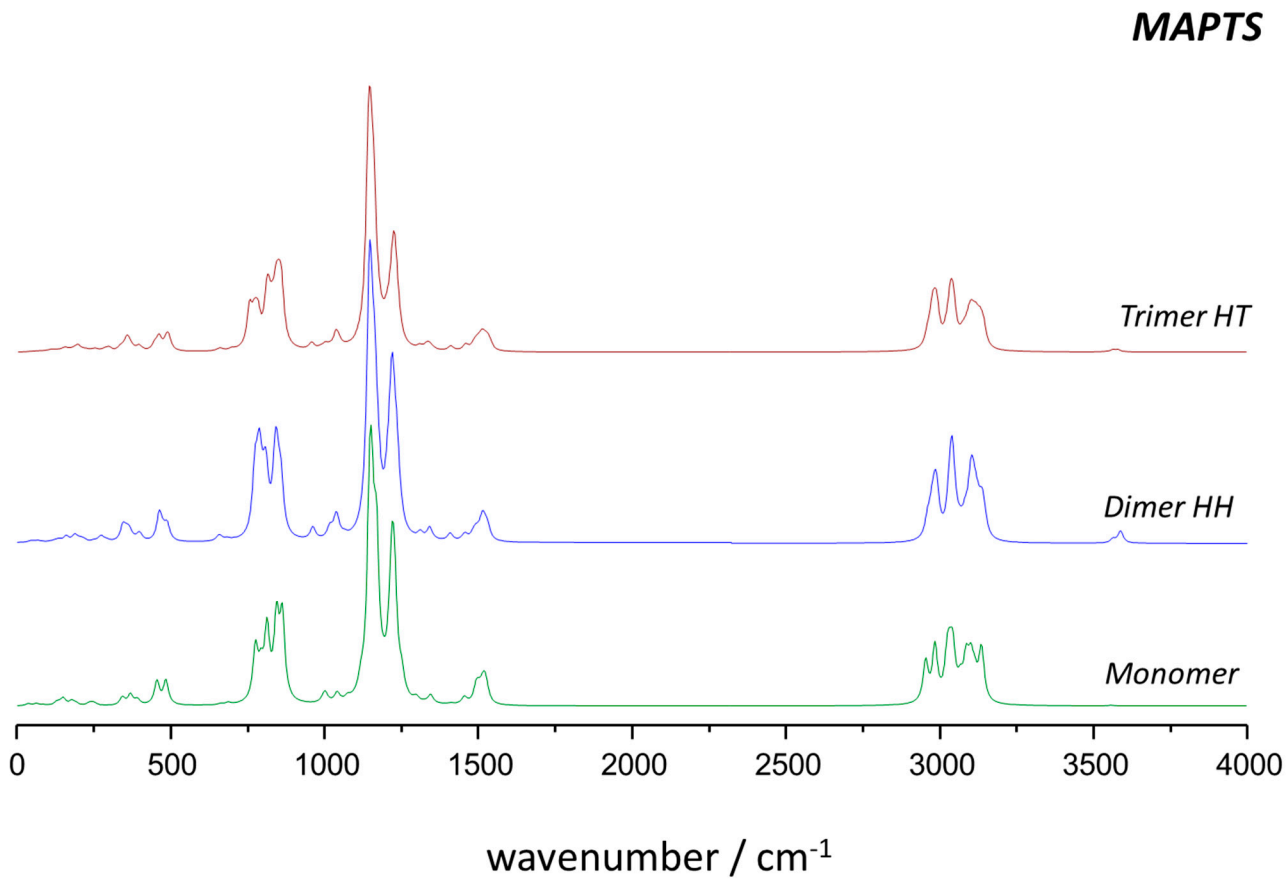


Figure S2. *Calculated infrared spectra of MAPTS, up to 4000 cm^{-1}. Calculated spectra in coloured lines, from bottom: monomer (green), head-to-head dimer (blue), head-to-tail trimer (red).*

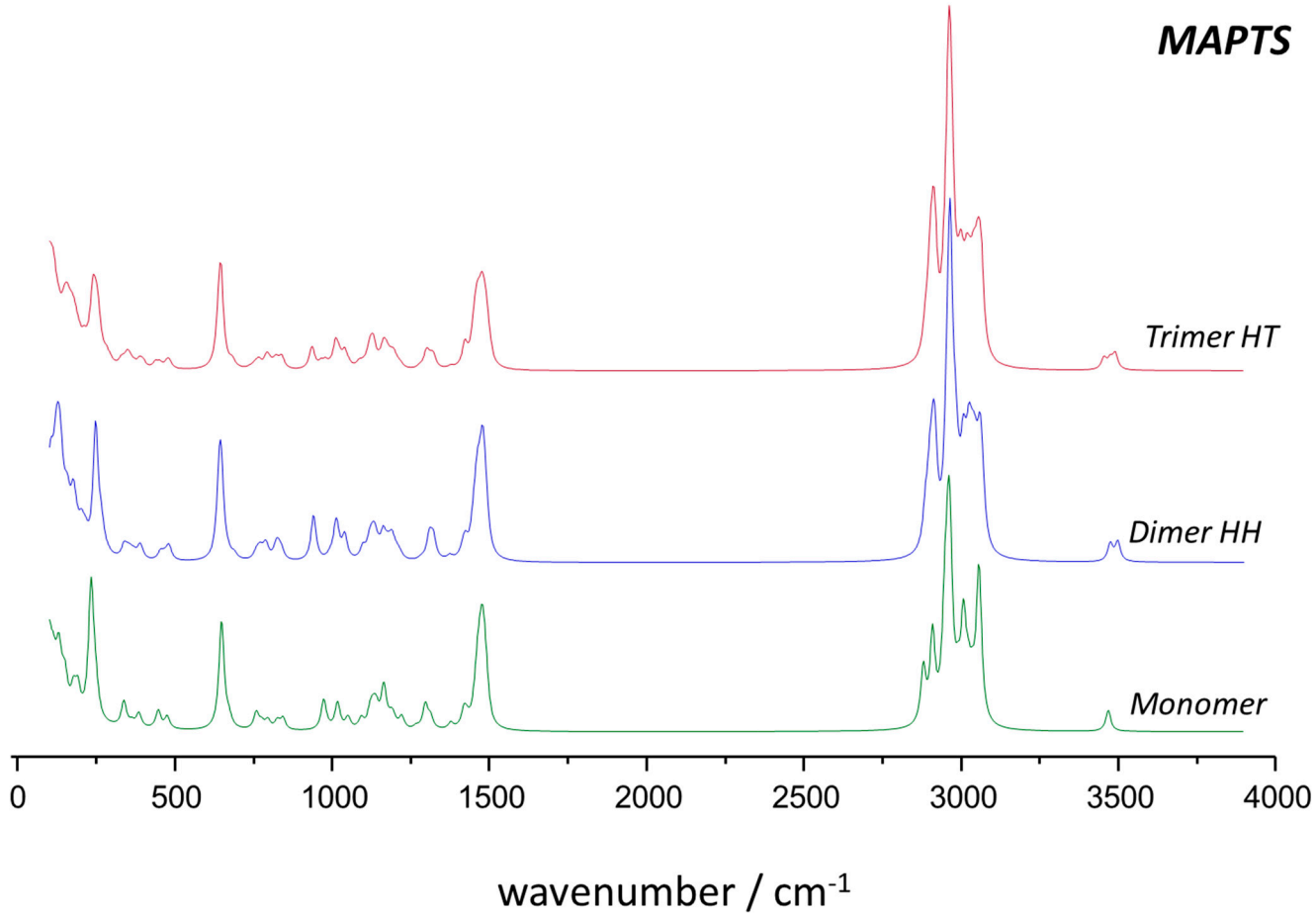


Figure S3. *Calculated Raman spectra of MAPTS, up to 4000 cm^{-1}. Calculated spectra in coloured lines, from bottom: monomer (green), head-to-head dimer (blue), head-to-tail trimer (red).*

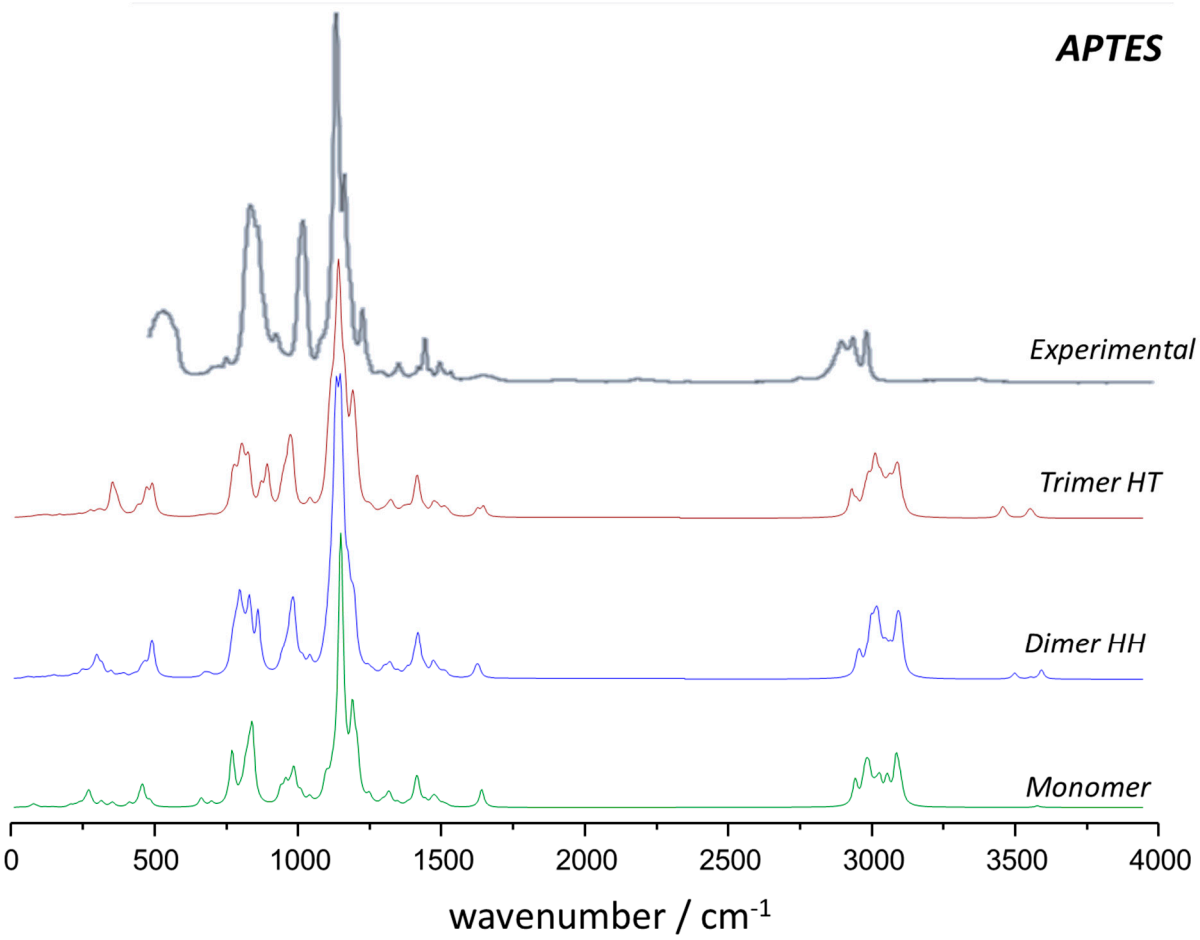


Figure S4. *Experimental and calculated infrared spectra of APTES. Top line: experimental spectrum, up to 4000 cm^{-1}. Calculated spectra in coloured lines, from bottom: monomer (green), head-to-head dimer (blue), head-to-tail trimer (red).*

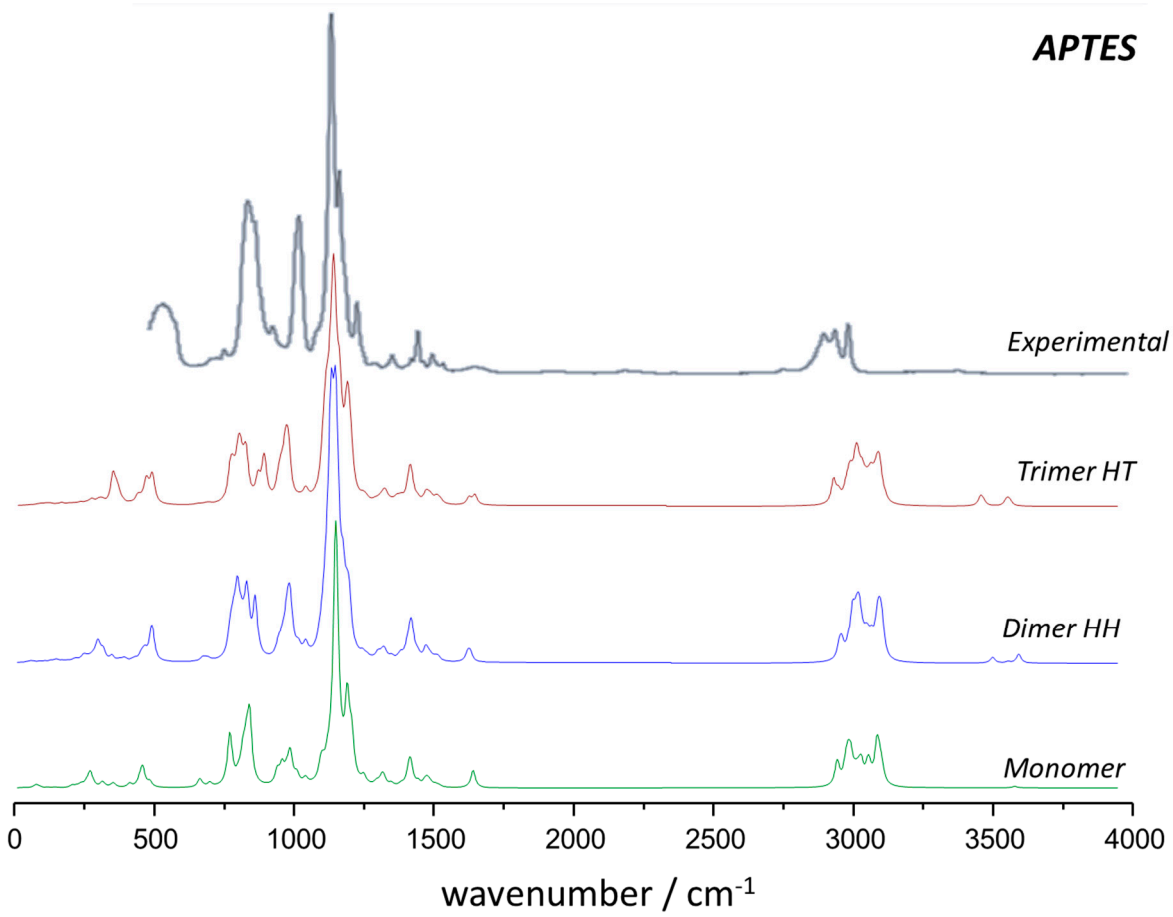


Figure S5. *Experimental and calculated infrared spectra of APTES. Top line: experimental spectrum, up to 4000 cm^{-1}. Calculated spectra in coloured lines, from bottom: monomer (green), head-to-head dimer (blue), head-to-tail trimer (red).*