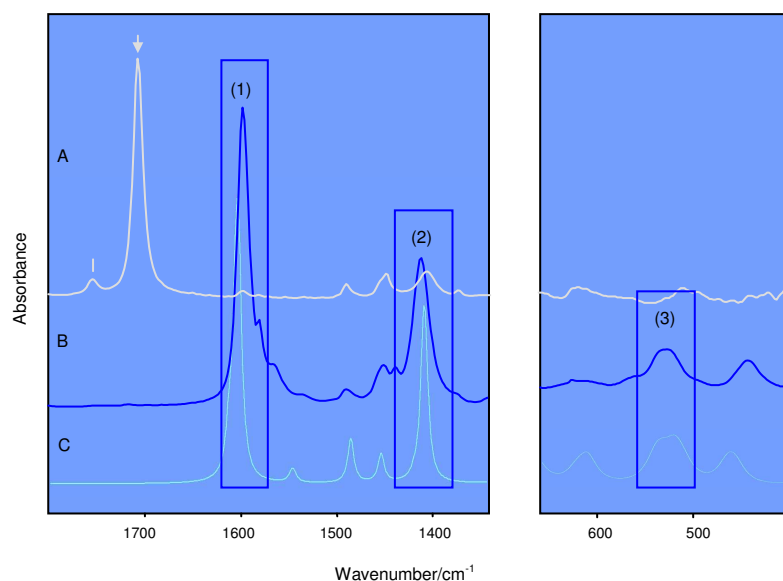
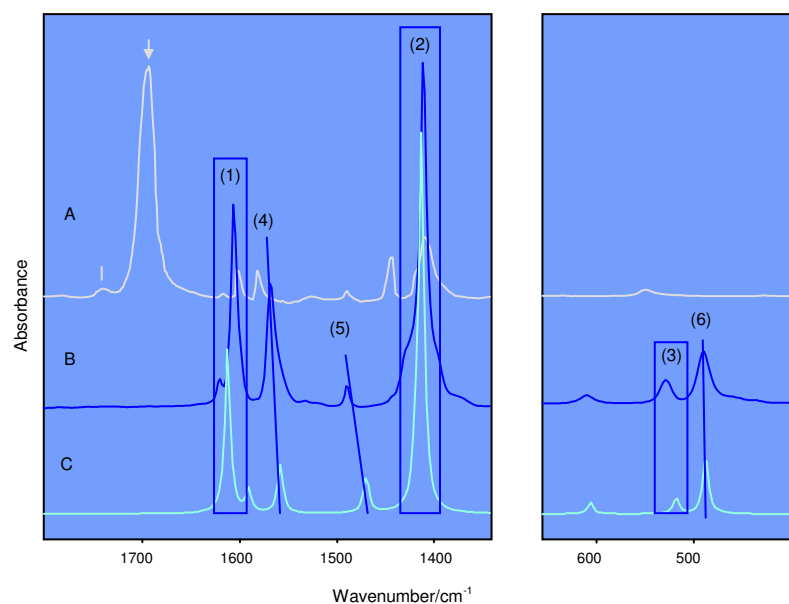


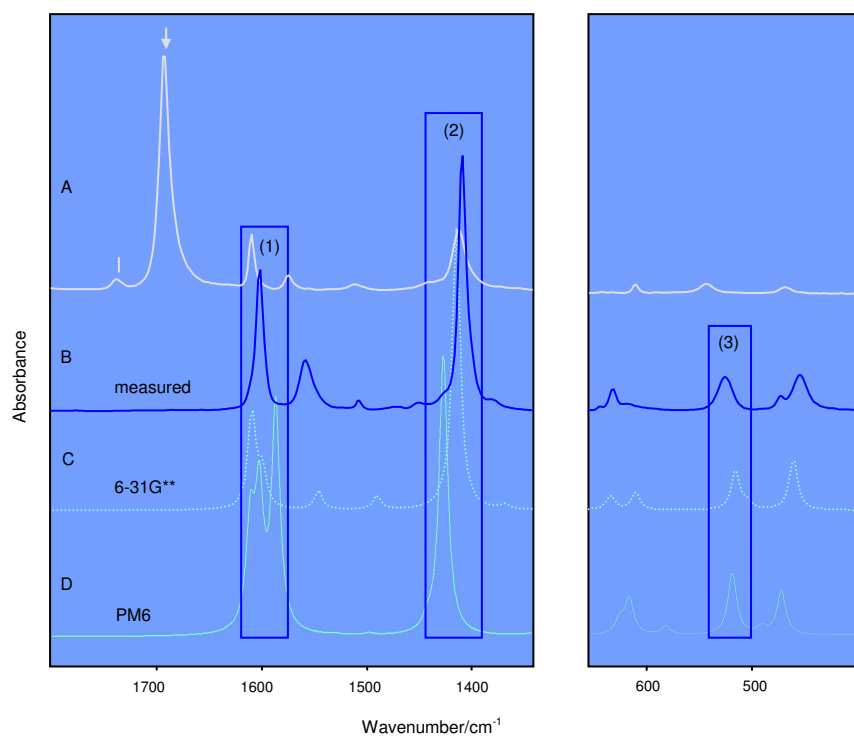
The vibrational spectra of A: adamantylcarboxylic acid, B: $\text{Zn}_4\text{O}(\text{1-adamantylcarboxylate})_6$, C: adamantylacetic acid, D: $\text{Zn}_4\text{O}(\text{1-adamantylacetate})_6$ dissolved in decane in the 1850–1350 cm^{-1} and 650–400 cm^{-1} ranges. Band assignation: $\nu_{\text{as}}\text{COO}^-$ 1591 cm^{-1} , 1595 cm^{-1} ; $\nu_{\text{s}}\text{COO}^-$ 1427 cm^{-1} , 1416 cm^{-1} ; $\nu_{\text{as}}\text{Zn}_4\text{O}$ 528 cm^{-1} and 529 cm^{-1} , $\nu\text{C=O}$: carboxylic acid dimer with grey arrow, monomeric carboxylic acid with grey line.



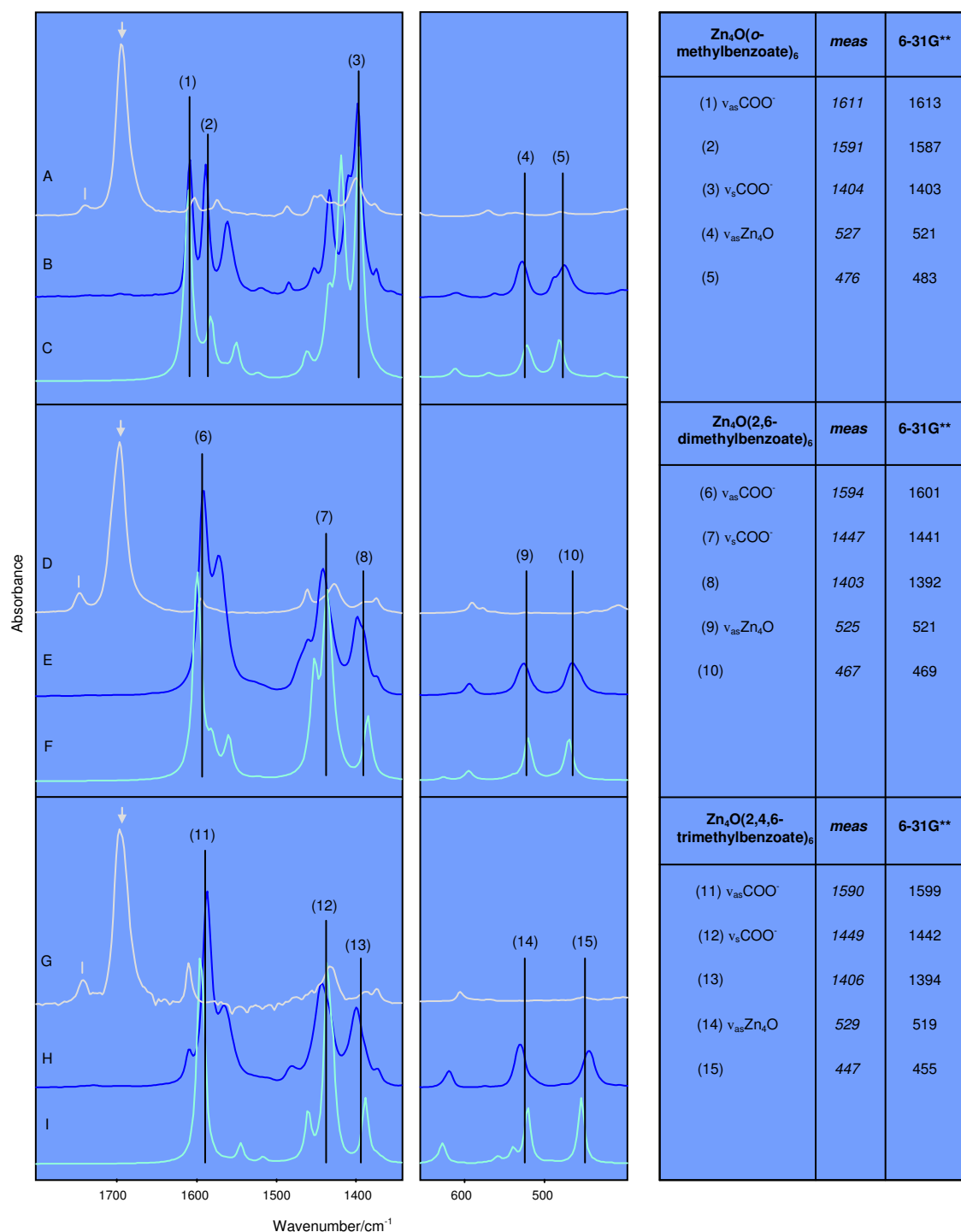
The experimental spectrum of 2-phenylbutanoic acid dissolved in C₂Cl₄ (trace A) and the measured and the PM6 simulated and scaled spectra of Zn₄O(2-phenylbutyrate)₆ (traces B – dissolved in C₂Cl₄ – and C) in the 1800–1350 cm⁻¹ and 650–400 cm⁻¹ range. Band assignment: $\nu_{as}\text{COO}^-$: (1), $\nu_s\text{COO}^-$: (2) and $\nu_{as}\text{Zn}_4\text{O}$: (3), $\nu\text{C=O}$: carboxylic acid dimer with grey arrow, monomeric carboxylic acid with grey line.



The experimental spectrum of benzoic acid dissolved in C_2Cl_4 (trace A) and the measured and the 6-31G** simulated and scaled spectra of $\text{Zn}_4\text{O}(\text{benzoate})_6$ (traces B – dissolved in C_2Cl_4 – and C) in the $1800\text{--}1350\text{ cm}^{-1}$ and $650\text{--}400\text{ cm}^{-1}$ range. Band assignment: $\nu_{\text{as}}\text{COO}^-$: (1), $\nu_{\text{s}}\text{COO}^-$: (2) and $\nu_{\text{as}}\text{Zn}_4\text{O}$: (3), (4), (5), (6), $\nu\text{C=O}$: carboxylic acid dimer with grey arrow, monomeric carboxylic acid with grey line.



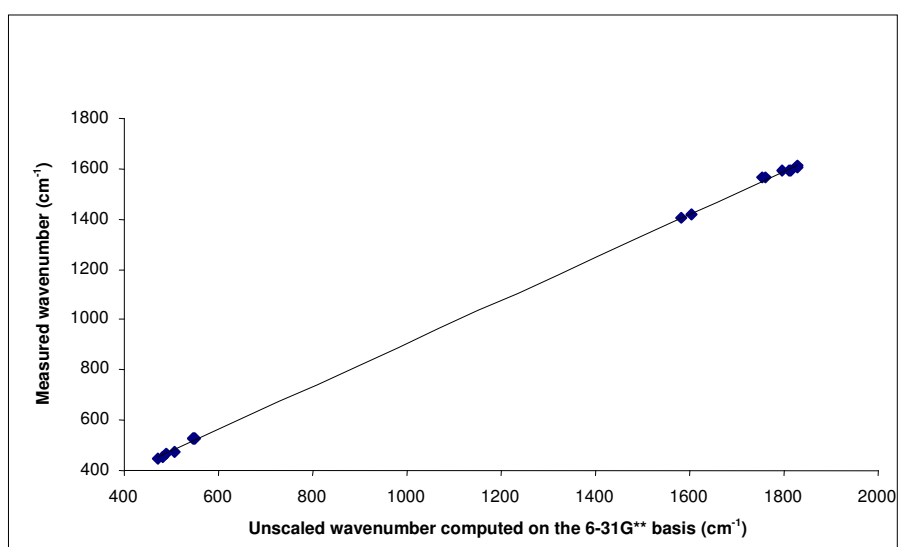
The experimental spectra of *para*-methylbenzoic acid and $\text{Zn}_4\text{O}(\textit{para}\text{-methylbenzoate})_6$ (traces A and B, respectively, both materials dissolved in C_2Cl_4) and the 6-31G** and the PM6 simulated and scaled spectra of $\text{Zn}_4\text{O}(\textit{para}\text{-methylbenzoate})_6$ (traces C and D, respectively) in the 1800–1350 cm^{-1} and 650–400 cm^{-1} range. Band assignment: $\nu_{\text{as}}\text{COO}^-$: (1), $\nu_{\text{s}}\text{COO}^-$: (2) and $\nu_{\text{as}}\text{Zn}_4\text{O}$: (3) $\nu\text{C}=\text{O}$: carboxylic acid dimer with grey arrow, monomeric carboxylic acid with grey line.



The experimental spectra of *ortho*-methylbenzoic acid and $\text{Zn}_4\text{O}(\textit{ortho}\text{-methylbenzoate})_6$ (traces A and B, respectively, both materials dissolved in C_2Cl_4), the 6-31G** simulated and scaled spectra of $\text{Zn}_4\text{O}(\textit{ortho}\text{-methylbenzoate})_6$ (trace C), the experimental spectra of 2,6-dimethylbenzoic acid and $\text{Zn}_4\text{O}(\text{2,6-dimethylbenzoate})_6$ (traces D and E, respectively, both materials dissolved in C_2Cl_4), the 6-31G** simulated and scaled spectra of $\text{Zn}_4\text{O}(\text{2,6-dimethylbenzoate})_6$ (trace F), the experimental spectra of 2,4,6-trimethylbenzoic acid and $\text{Zn}_4\text{O}(\text{2,4,6-trimethylbenzoate})_6$ (traces G and H, respectively, both materials dissolved in C_2Cl_4), the 6-31G** simulated and scaled spectra of $\text{Zn}_4\text{O}(\text{2,4,6-trimethylbenzoate})_6$ (trace I) in the 1800–1350 cm^{-1} and 650–400 cm^{-1} range. For band assignment, see the table, $\nu\text{C=O}$: carboxylic acid dimer with grey arrow, monomeric carboxylic acid with grey line.

Parameters used and obtained for and during calculating the scaling of wavenumbers computed on the 6-31G** basis

	Measured	6-31G** unscaled	6-31G** scaled
Zn ₄ O(<i>p</i> -methylbenzoate) ₆	1605	1827	1612
	1416	1603	1421
	525	545	516
	1563	1754	1550
	451	482	463
Zn ₄ O(<i>o</i> -methylbenzoate) ₆	1611	1828	1613
	1404	1582	1403
	527	550	521
	1591	1797	1587
	1565	1759	1554
Zn ₄ O(2,4,6-trimethylbenzoate) ₆	1590	1812	1599
	529	548	519
	447	473	455
Zn ₄ O(2,6-dimethylbenzoate) ₆	1594	1814	1601
	525	550	521
	467	490	469
parameters	0.8548	50.5016	
error	0.003218	4.2661	
R ²	0.9998		



Parameters used and obtained for and during calculating the scaling of wavenumbers computed by the PM6 method

	Measured	PM6 unscaled	PM6 scaled
Zn ₄ O(<i>p</i> -methylbenzoate) ₆	1605	1620	1590
	1416	1455	1433
	525	495	518
	451	446	471
Zn ₄ O(cyclohexylcarboxylate) ₆	1591	1631	1601
	1431	1438	1417
	515	495	518
Zn ₄ O(cyclohexylacetate) ₆	1595	1636	1605
	1443	1455	1433
	530	493	516
Zn ₄ O(2-phenylbutirate) ₆	1601	1637	1606
	1418	1436	1415
	522	490	513
	441	430	456
parameter	0.9542	44.3685	
error	0.006508	7.8488	
R ²	0.9994		

