On the low volatility of cyclic esters: An infrared spectroscopy comparison between dimers of γ-butyrolactone and methyl propionate

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Supplementary Information

	$\tilde{\nu}_{\mathrm{C=O}}$	(@Ar)	$\tilde{\nu}_{\mathrm{C-O}}$	(@Ar)
A	1825	(1814)	1155	–
B	1817	(1807)	–	–
C	1846	–	–	–
D	1809	(1807)	1172	(1188)
D’	1804	(1800)	1179	–
E	1790	(1785)	1190	(1177)

Table S1: Experimental C−O and C=O stretching wavenumbers $\tilde{\nu}_{\mathrm{C-O}}$ and $\tilde{\nu}_{\mathrm{C=O}}$ for 3L in cm^{-1}, without and with (@Ar) Ar embedding.

	B3LYP/ 6-311++G(d,p)	MP2/ 6-311+G(d)
$\tilde{\nu}_{\mathrm{C=O}}(\mathrm{M})$	1850(457)	1842(380)
$\tilde{\nu}_{\mathrm{C=O}}(\mathrm{Z_{het}})$	1819(0)	1823(0)
	1836(789)	1839(640)
$\tilde{\nu}_{\mathrm{C=O}}(\mathrm{T_B})$	1814(14)	1816(45)
	1823(354)	1823(127)
	1828(861)	1833(735)
$\tilde{\nu}_{\mathrm{C-O}}(\mathrm{M})$	1157(228)	1185(228)
$\tilde{\nu}_{\mathrm{C-O}}(\mathrm{Z_{het}})$	1165(0)	1186(0)
	1177(380)	1201(373)
$\tilde{\nu}_{\mathrm{C-O}}(\mathrm{T_B})$	1170(26)	1192(58)
	1173(58)	1196(55)
	1184(448)	1211(358)

Table S2: Comparison of the calculated peak positions $\tilde{\nu}_{\mathrm{C=O}}$ and $\tilde{\nu}_{\mathrm{C-O}}$ in cm^{-1} and IR intensities in $\mathrm{km\,mol}^{-1}$ (in parentheses) of the most stable cluster structures of 3L.

	$\tilde{\nu}_{\mathrm{C=O}}$	$\tilde{\nu}_{\mathrm{C-O}}$
A	1767	1207
A’	–	1184
D	1762	1216
D’	–	1190
E	1756	1216
E’	1754	1190

Table S3: Experimental stretching wavenumbers $\tilde{\nu}_{\mathrm{C=O}}$ and $\tilde{\nu}_{\mathrm{C-O}}$ in cm^{-1} for methyl propionate (2E1) expanded in helium.

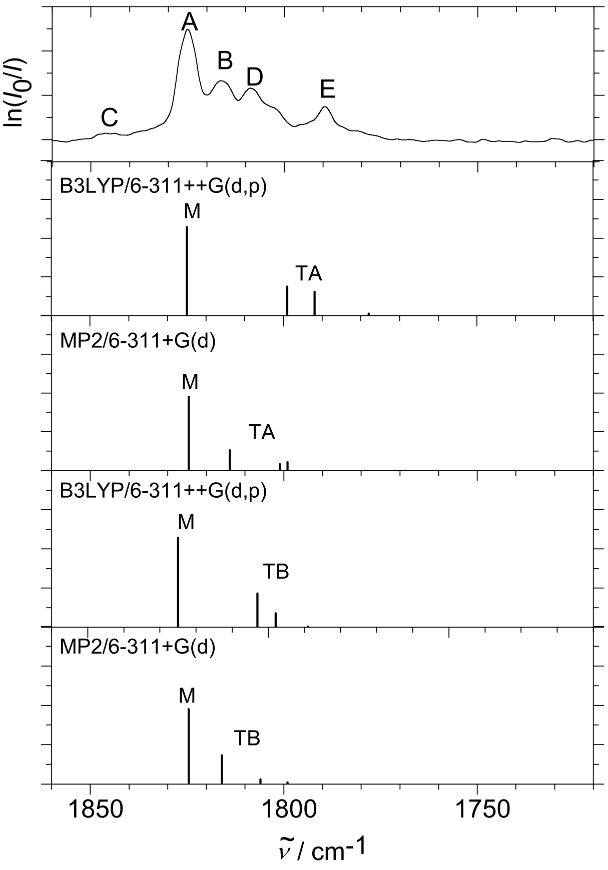

Figure S1: Spectral simulations of γ-butyrolactone expansions, matching the C=O stretching transitions of the monomer to experiment and including the two most stable trimer structures.

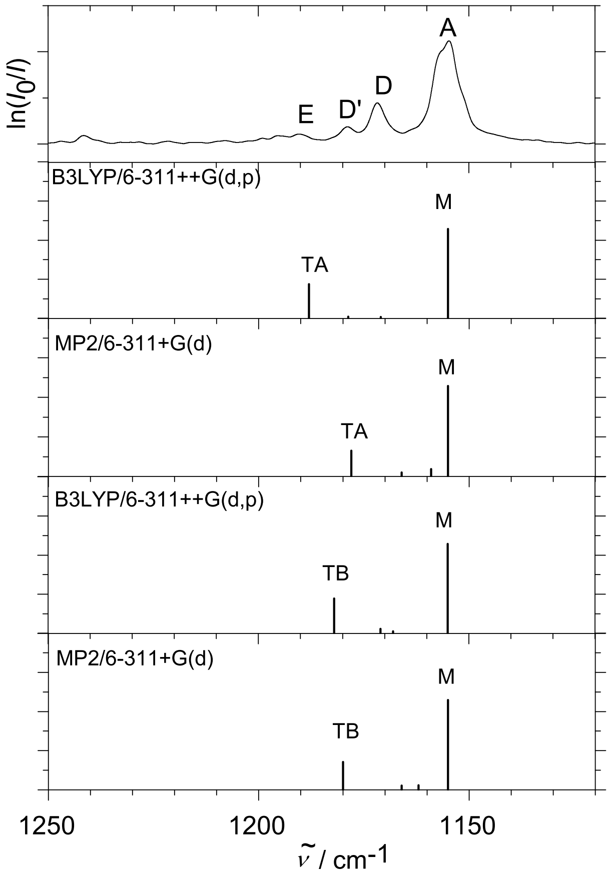

Figure S2: Spectral simulations of γ-butyrolactone expansions, matching the C$-$O stretching transitions of the monomer to experiment and including the two most stable trimer structures.

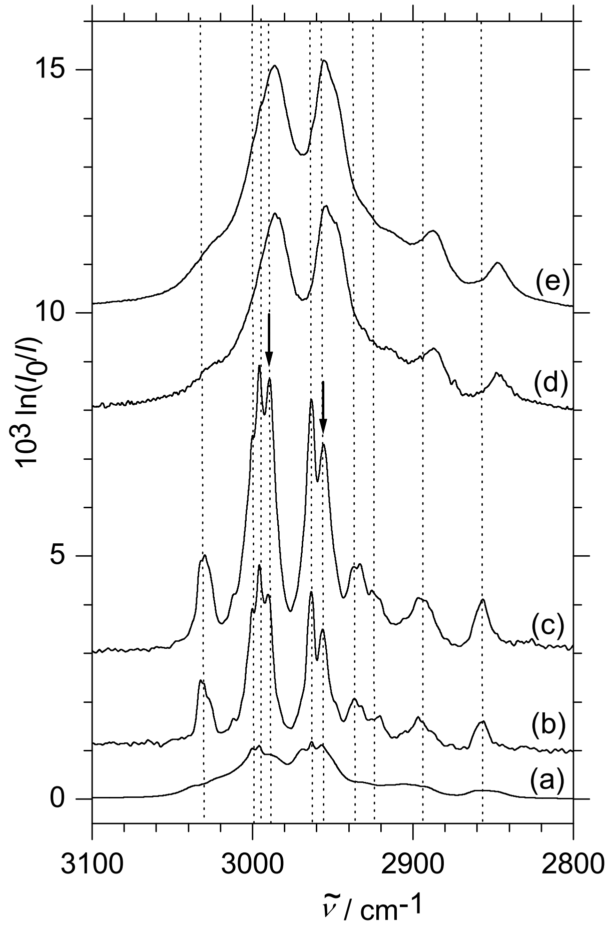

Figure S3: C–H stretching region of the IR spectrum of 2E1 (a) Gas phase measured at 80 mbar at a concentration of 0.7 % 2E1 in helium, scaled by $\frac{1}{400}$. (b) Jet spectrum at a stagnation pressure of 0.4 bar, 0.4 % 2E1 in helium. (c) Increased concentration (0.7 %). (d) ATR spectrum, scaled by $\frac{1}{100}$. (e) Transmission spectrum of liquid 2E1, scaled by $\frac{1}{100}$.