symmetry

MDPI

Article

Vibrational Circular Dichroism Detects Symmetry Breaking due to Conformational Mobility in C_2-Symmetry Chiral Molecules and Provides Further Insight into Inter-Chromophoric Interactions

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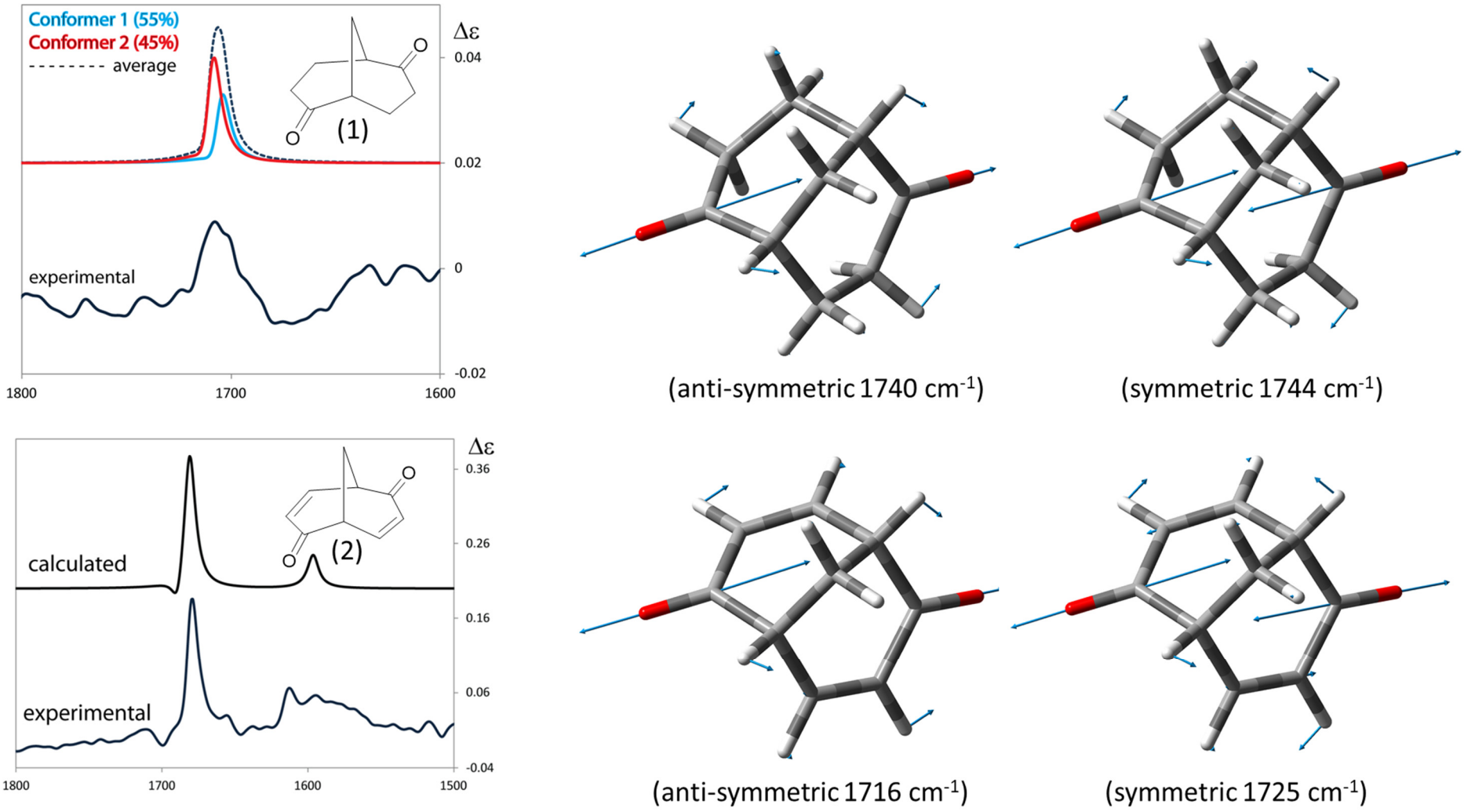


Figure SI-1. Calculated spectra and carbonyl stretching normal modes description for compounds 1-cc conformer (top) and 2 (bottom).

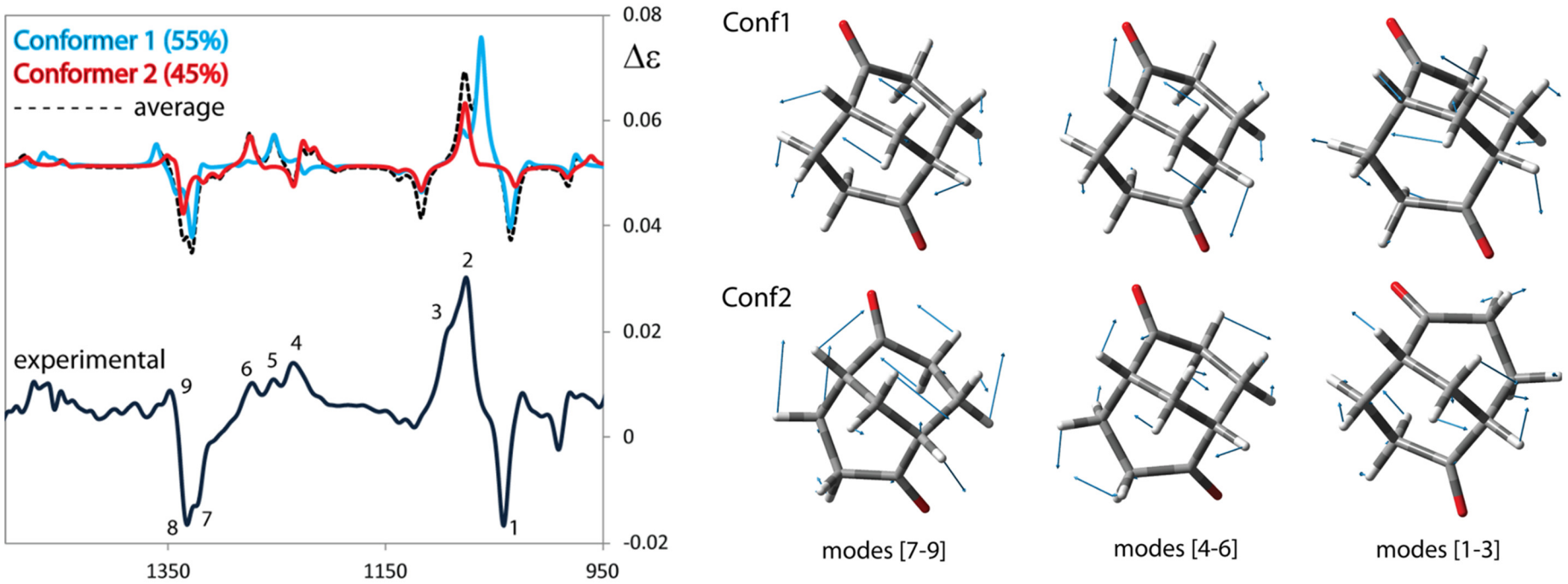


Figure SI-2. Calculated spectra and description of vibrational modes in the MID-IR region of compound 1-cc conformer. Modes are grouped and displayed for vibration transition type (only relative phases change within each group).

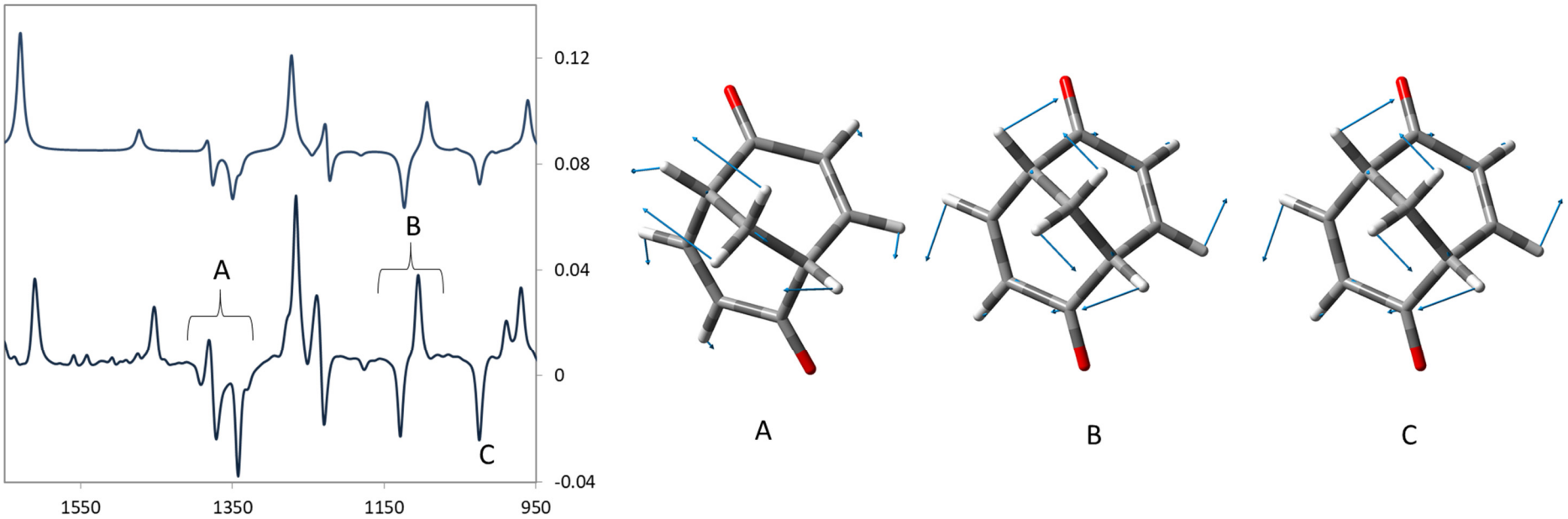


Figure SI-3. Calculated spectra and description of vibrational modes in the MID-IR region of compound 2.

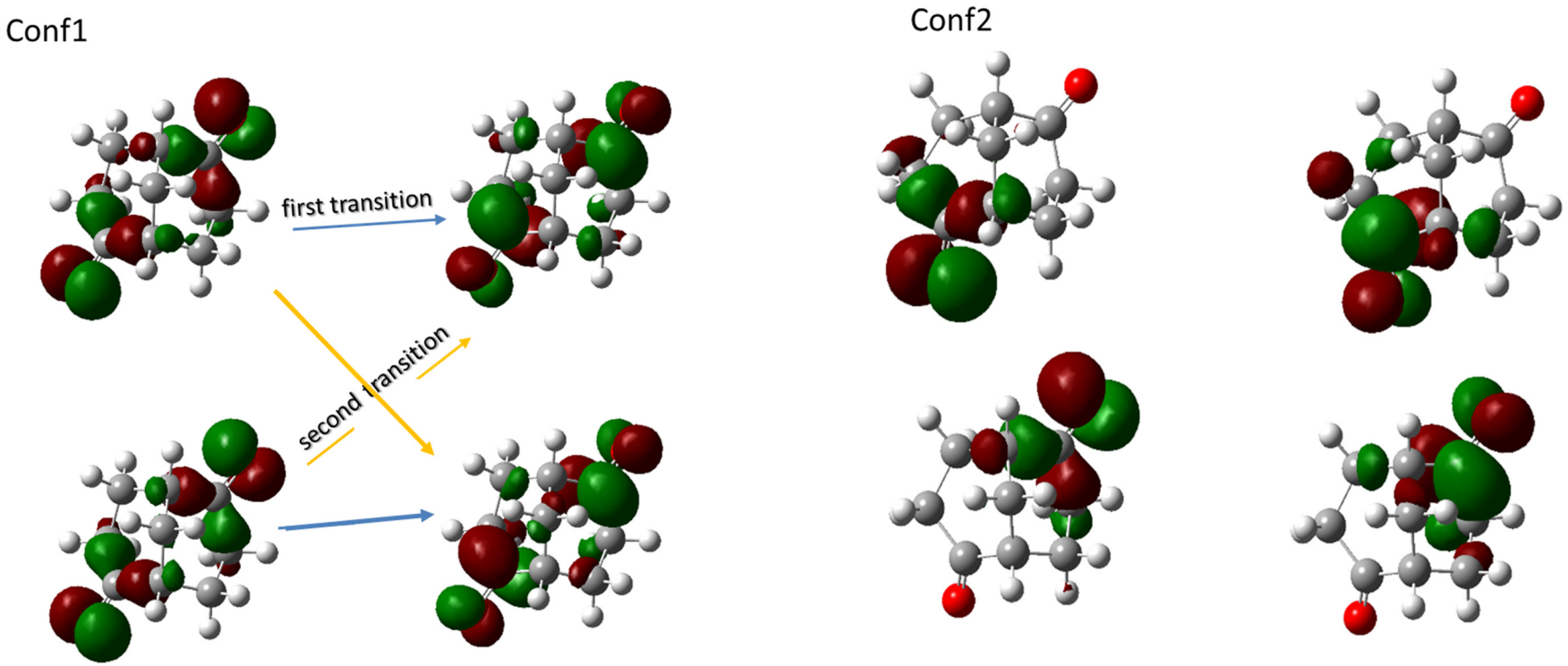


Figure SI-4. Natural Transition Orbital investigation of first and second electronic transitions of compound 1 for both the cc and cb conformers. Level of theory CAM-B3LYP/aug-cc-pVDZ.

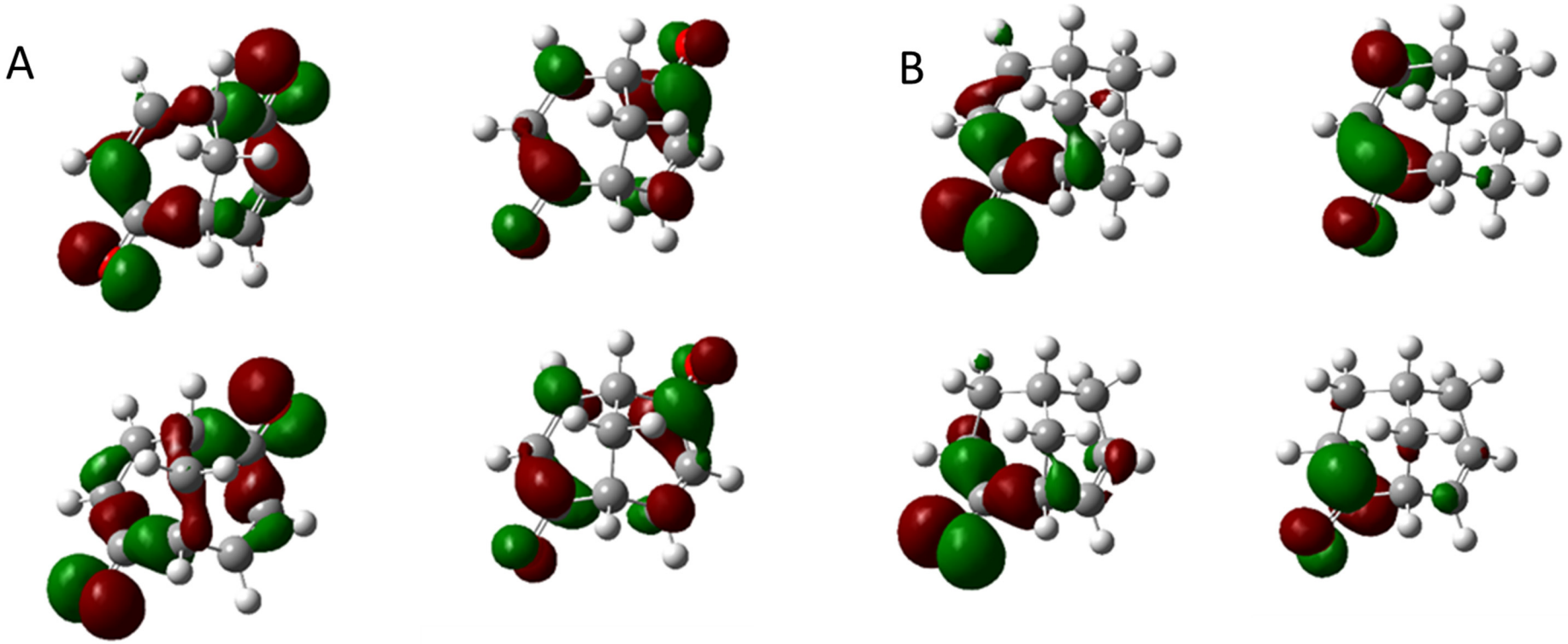
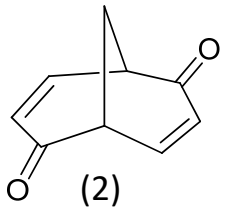


Figure SI-5. Molecular orbitals involved in the first and second electronic transitions of compound 2. Level of theory CAM-B3LYP/aug-cc-pVDZ.

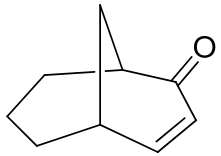
Table SI-1. Compound **1** in **cc** and **cb** conformation, and mono-ketone model. APT and AAT (a.u) of C and O atoms are reported in the reference cartesian system of each carbonyl group, z axis pointing towards the O atom, y-axis pointing towards the nearby asymmetric carbon C*.

A	**1-cc**	**APT**			**AAT**				**cm-1**	**Dip. str.**	**Rot. str.**	**E-M**
	C							antis.	1775	1015	59	24
		0.031	-0.013	-0.106	0.055	0.574	0.080	symm.	1779	10	-20	180
		0.055	0.890	-0.052	-1.206	0.046	-0.126					
		-0.105	**-0.006**	**1.313**	**-0.154**	**0.118**	**0.041**					
	O											
		-0.299	0.003	0.037	-0.009	-1.555	-0.063					
		-0.023	-0.533	0.015	1.279	-0.013	0.030					
		0.040	**0.021**	**-1.224**	**0.173**	**-0.150**	**-0.061**					
B	**1-cb**	**APT**			**AAT**				**cm-1**	**Dip. str.**	**Rot. str.**	**E-M**
	C							antis.	1779	864	112	59
		0.096	-0.009	0.015	-0.129	0.675	0.107	symm.	1783	116	-39	104
		0.083	0.929	-0.001	-1.016	0.049	-0.740					
		-0.150	**-0.040**	**1.193**	**-0.409**	**0.634**	**0.106**					
	O							Average		1005	54	
		-0.337	-0.001	0.023	0.051	-1.576	-0.063					
		-0.024	-0.544	0.032	1.168	-0.011	0.405					
		0.130	**0.052**	**-1.168**	**0.321**	**-0.651**	**-0.042**					
	C											
		0.017	0.011	-0.064	0.035	0.558	0.025					
		0.069	0.848	-0.081	-1.206	0.099	0.073					
		-0.033	**-0.024**	**1.360**	**-0.142**	**0.048**	**0.031**					
	O											
		-0.286	0.000	0.022	-0.016	-1.529	-0.051					
		-0.028	-0.520	0.025	1.287	-0.029	-0.040					
		-0.009	**0.023**	**-1.234**	**0.133**	**-0.043**	**-0.063**					
C	**Mono-ketone**	**APT**			**AAT**				**cm-1**	**Dip. str.**	**Rot. str.**	**E-M**
	C											
		0.032	-0.013	-0.101	0.060	0.574	0.087					
		0.061	0.888	-0.048	-1.128	0.018	-0.134					
		-0.101	**-0.004**	**1.307**	**-0.162**	**0.091**	**0.026**					
	O											
		-0.304	0.003	0.037	-0.016	-1.532	-0.069					
		-0.025	-0.537	0.013	1.241	-0.003	0.028					
		0.040	**0.017**	**-1.243**	**0.192**	**-0.126**	**-0.050**					

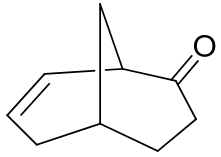
Table SI-2. Compound **2** and mono-ketone diene models. APT and AAT (a.u.) of C and O atoms are reported in the reference cartesian system of each carbonyl group, z axis pointing towards the O atom, y-axis pointing towards the nearby asymmetric carbon C*.



(2)



(α,β)



(β,γ)

A	**2**	**APT**			**AAT**				**cm-1**	**Dip. str.**	**Rot. str.**	**E-M**
	C							antis.	1750	1334	388	15
		0.110	0.025	0.014	0.006	0.535	0.433	symm.	1759	44	-95	180
		0.144	0.871	0.094	-2.093	0.482	-0.406	.				
		-0.195	**-0.053**	**1.542**	**-0.309**	**0.260**	**0.318**	sum		1378	293	
	O											
		-0.313	0.002	-0.004	0.013	-1.474	-0.130					
		-0.026	-0.500	-0.017	1.427	-0.104	0.154					
		0.128	**0.056**	**-1.358**	**0.305**	**-0.311**	**-0.225**					
B	**α,β**	**APT**			**AAT**				**cm-1**	**Dip. str.**	**Rot. str.**	**E-M**
	C								1742	603	51	80
		0.137	-0.012	-0.060	-0.028	0.475	0.359					
		0.035	0.865	0.267	-1.498	0.176	-0.342					
		-0.152	**0.018**	**1.369**	**-0.421**	**0.353**	**0.040**					
	O											
		-0.343	0.005	0.022	0.037	-1.473	-0.091					
		-0.006	-0.528	-0.046	1.288	-0.051	0.181					
		0.100	**0.027**	**-1.283**	**0.357**	**-0.375**	**-0.038**					
C	**β,γ**	**APT**			**AAT**				**cm-1**	**Dip. str.**	**Rot. str.**	**E-M**
	C								1781	612	67	39
		0.009	0.020	-0.026	0.103	0.544	0.159					
		0.098	0.865	-0.209	-1.245	0.161	-0.046					
		-0.052	**-0.050**	**1.458**	**-0.060**	**-0.115**	**0.174**					
	O											
		-0.280	0.000	0.009	-0.041	-1.484	-0.096					
		-0.037	-0.519	0.057	1.256	-0.041	-0.034					
		0.010	**0.030**	**-1.318**	**0.082**	**0.061**	**-0.158**					