Electronic Supplementary Information

Vibronic Bandshape of Absorption Spectra of Dibenzoylmethanatoboron Difluoride Derivatives: Analysis Based on Ab Initio Calculations

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Table S1. Estimated characteristic hard mode frequency $\langle\Omega_{\text{hard}}\rangle$, full width at half maximum of the soft mode spectrum Γ_{soft}, and γ parameter (see text) for $DBMBF_2$ and its derivatives

Derivative	$\langle\Omega_{\text{hard}}\rangle$, cm^{-1}	Γ_{soft}, cm^{-1}	$\gamma = \Gamma_{\text{soft}} / \langle\Omega_{\text{hard}}\rangle$
3m-a peak 2	1203	821	0.68
4m-a peak 2	1203	848	0.70
4o-b peak 1	1278	962	0.75
3o-b peak 2	1211	1065	0.88
3m-b peak 1	1334	1214	0.91
3o-b peak 1	1249	1148	0.92
4p peak 1	1300	1293	0.99
3p peak 1	1295	1310	1.01
4o-b peak 2	1183	1217	1.03
4m-b peak 1	1362	1417	1.04
2p peak 1	1332	1472	1.10
4m-b peak 2	1206	1341	1.11
1	1370	1524	1.11
2m-b peak 1	1381	1538	1.11
2m-a peak 1	1376	1648	1.20
3m-a peak 1	1317	1638	1.24
3m-b peak 2	1204	1500	1.25
4m-a peak 1	1281	1634	1.28
2o-b peak 1	1278	1817	1.42

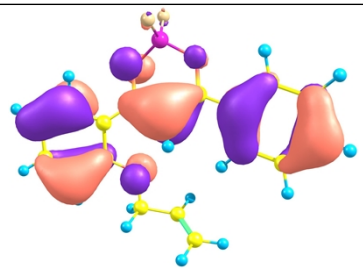
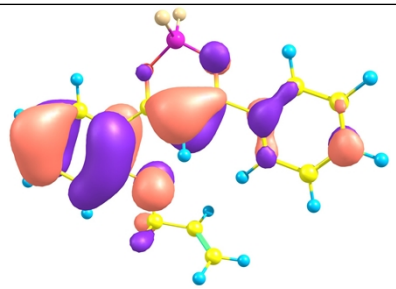
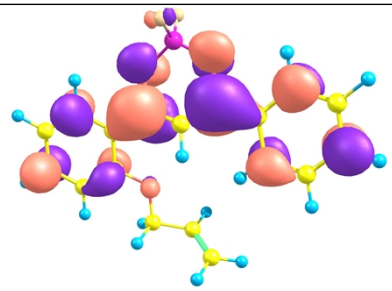
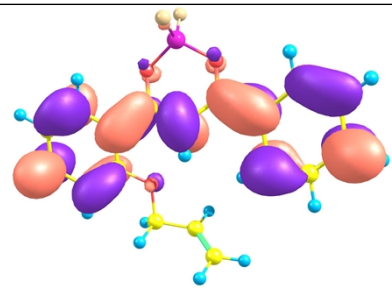
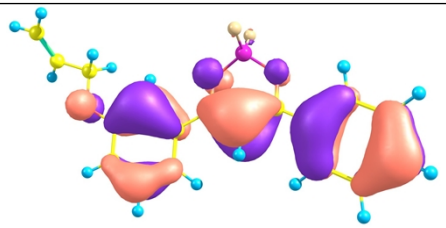
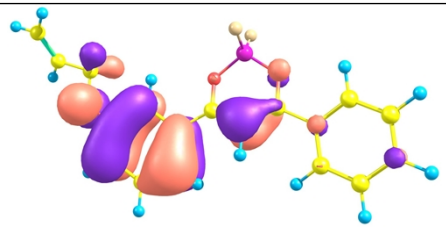
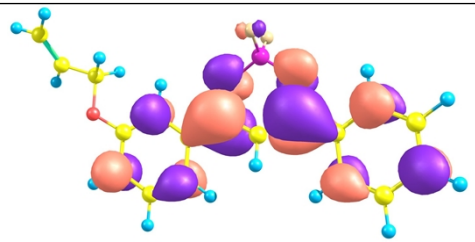
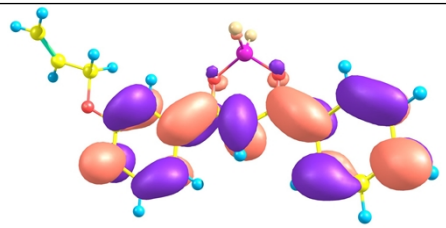
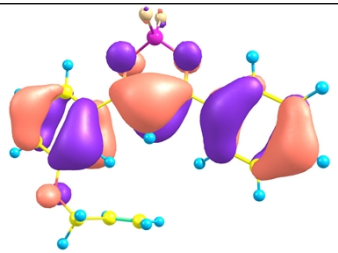
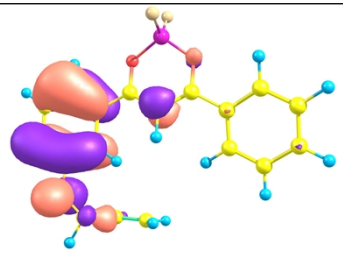
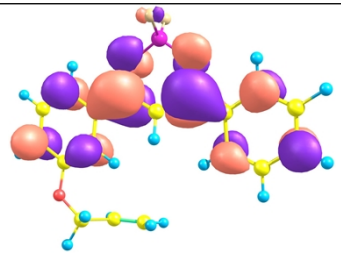
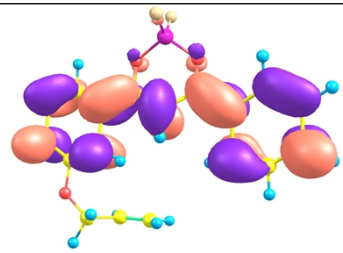
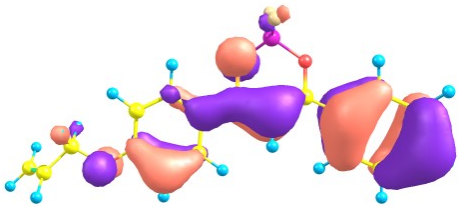
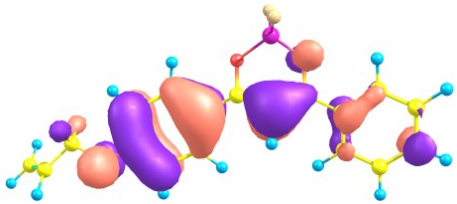
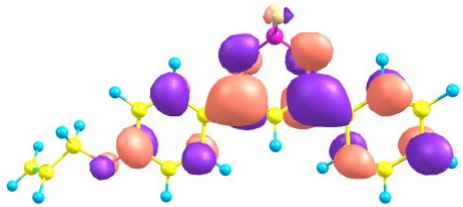
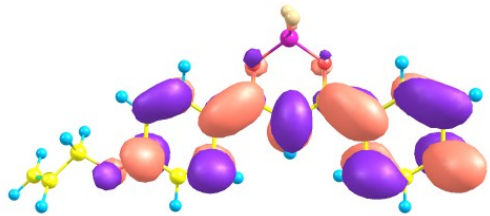
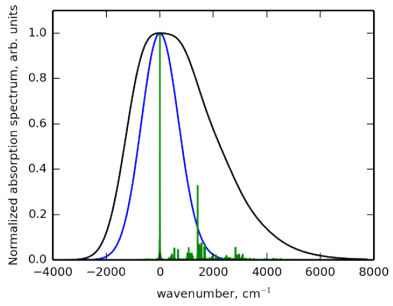
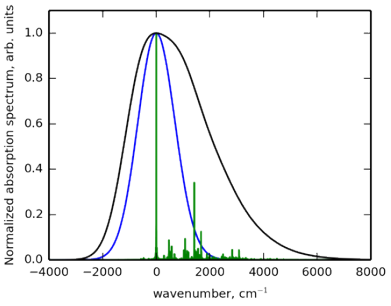
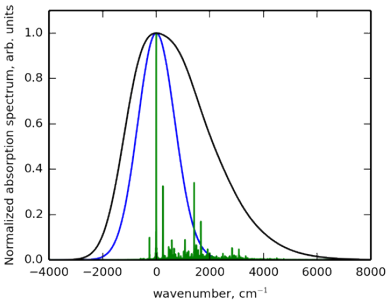
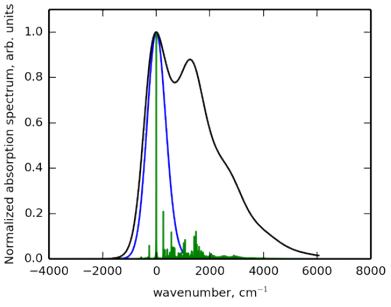
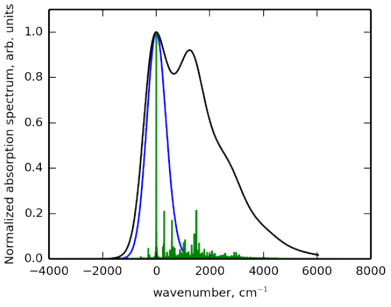
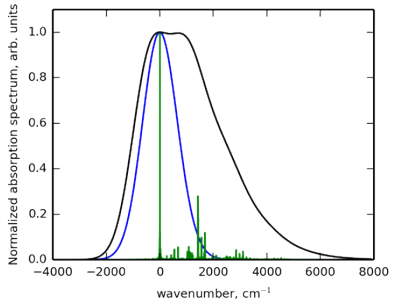
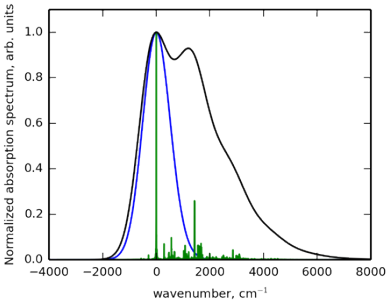
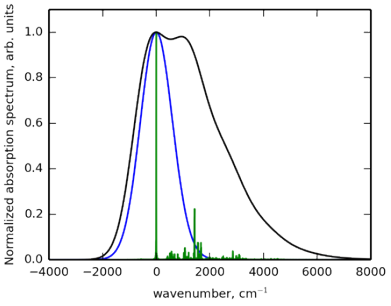
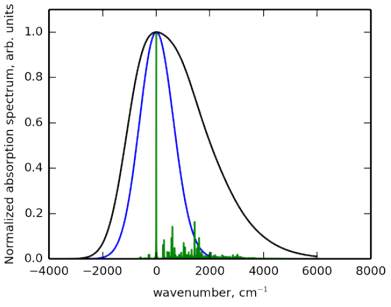
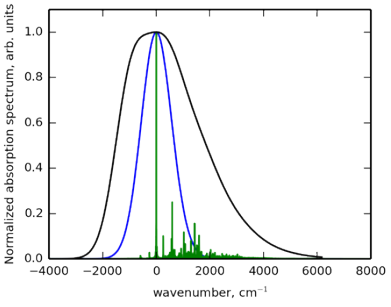
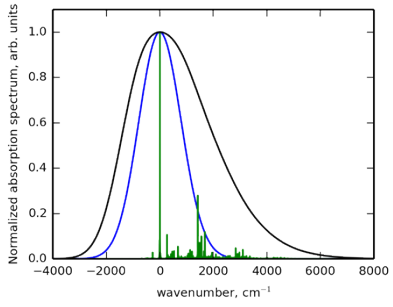
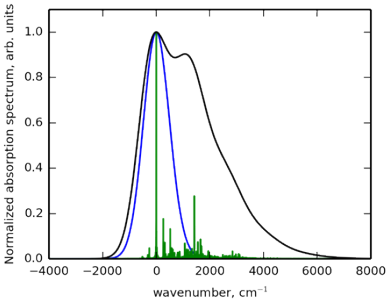
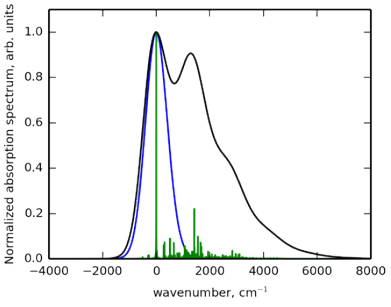
	HOMO–1	HOMO	LUMO	LUMO+1
4o-b				
4m-a				
4m-b				
4p				

Figure S1. Frontier orbitals (HOMO–1, HOMO, LUMO, and LUMO+1) of O-allyl DBMBF$_2$ isomers.

	2 (–CH_3)	***3*** (–O–CH_3)	***4*** (–O–CH_2–CH=CH_2)
m-a peak 1			
m-a peak 2			
m-b peak 1			
m-b peak 2			
o-b peak 1			

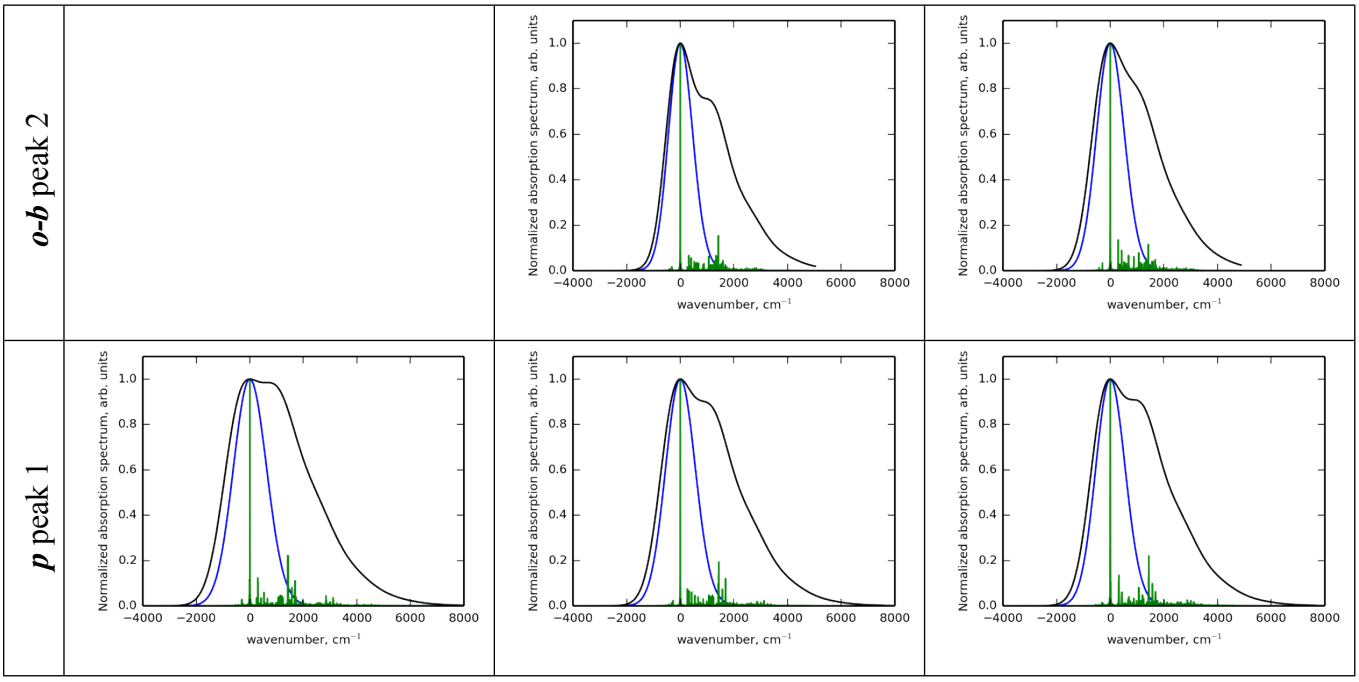
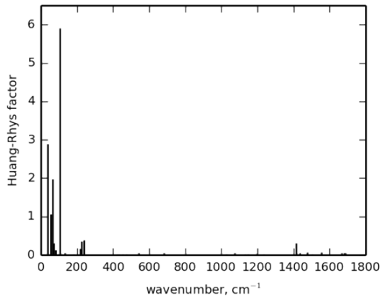
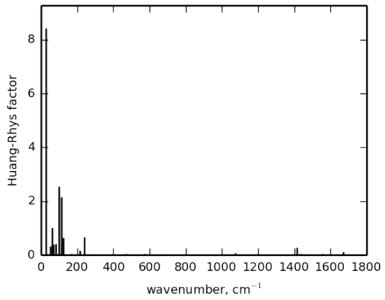
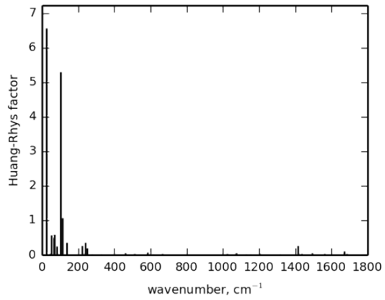
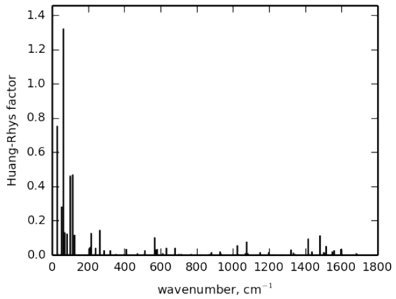
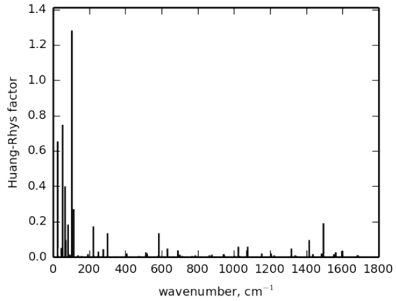
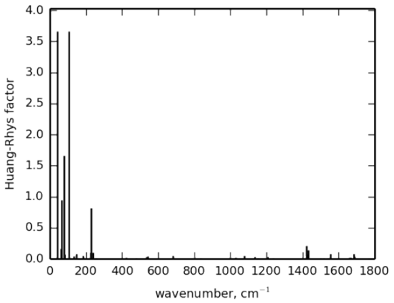
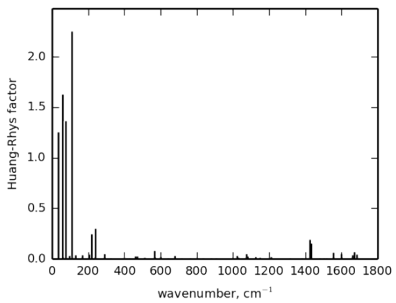
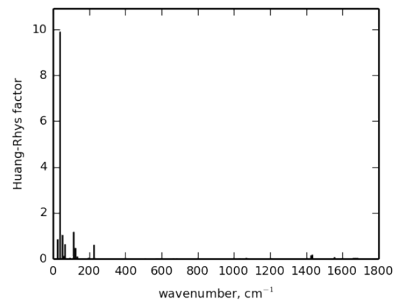
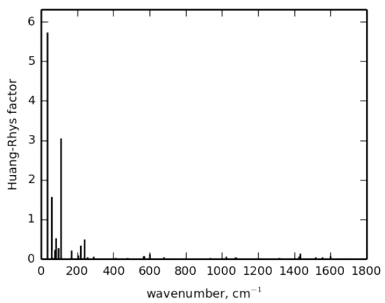
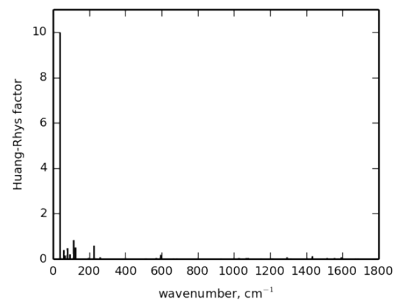
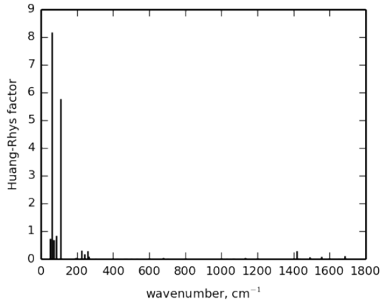
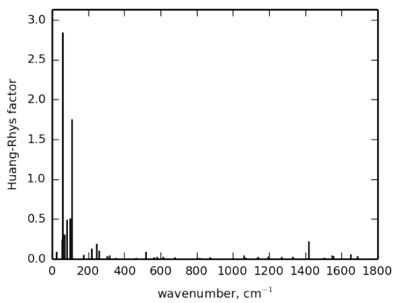
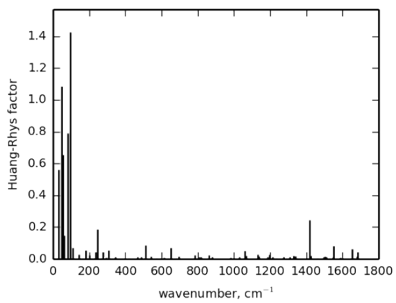


Figure S2. Total absorption spectra of $DBMBF_2$ derivatives (black) and its deconvolution into the soft (blue) and the hard (green) mode contributions.

	2 ($–CH_3$)	***3*** ($–O–CH_3$)	***4*** ($–O–CH_2–CH=CH_2$)
m-a peak 1			
m-a peak 2			
m-b peak 1			
m-b peak 2			
o-b peak 1			

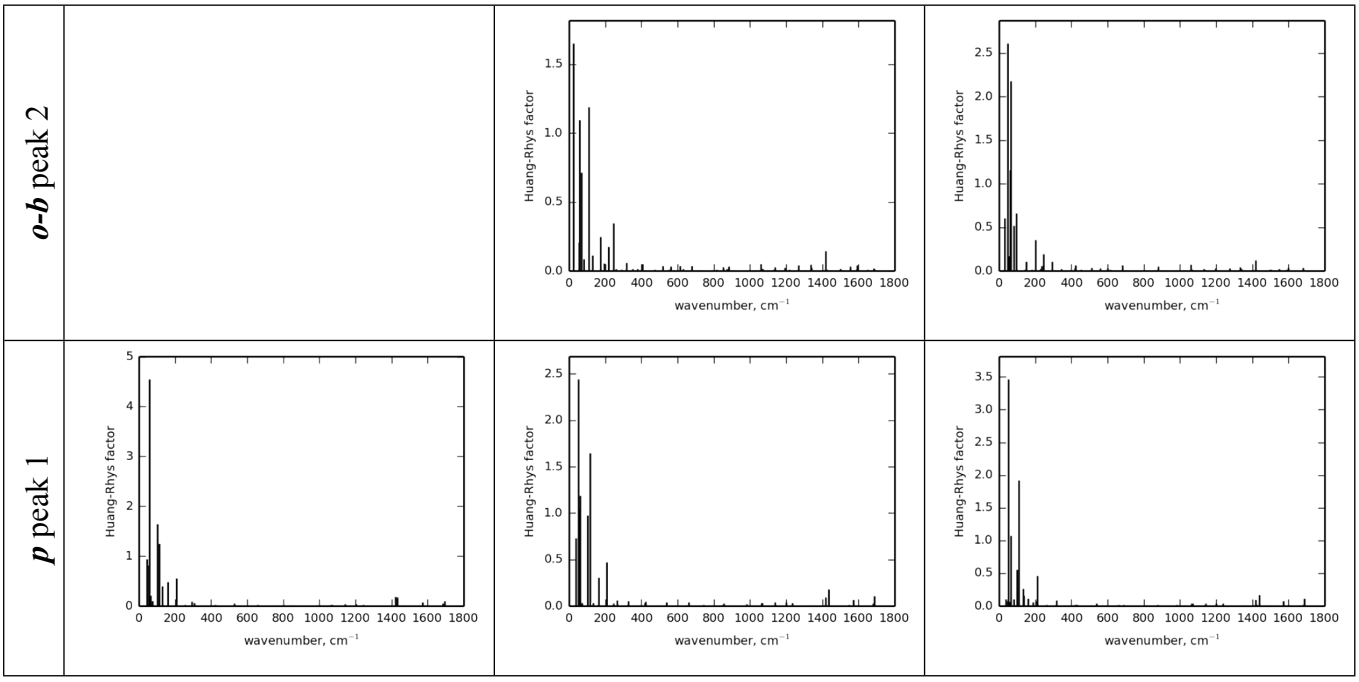
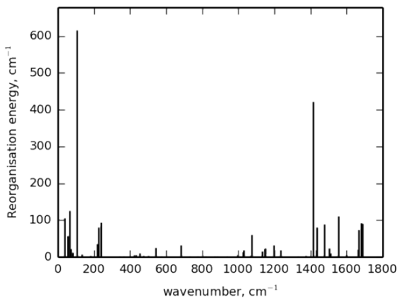
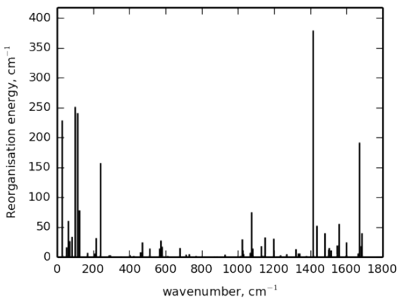
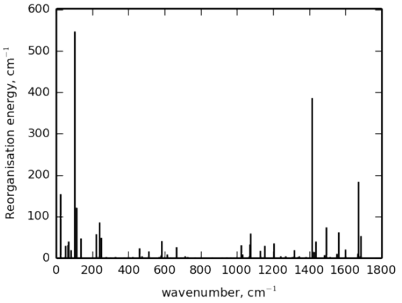
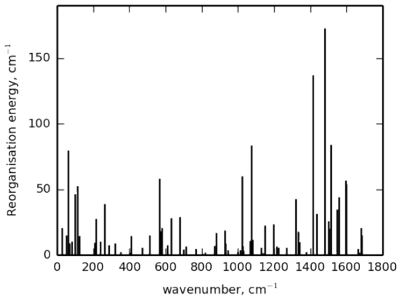
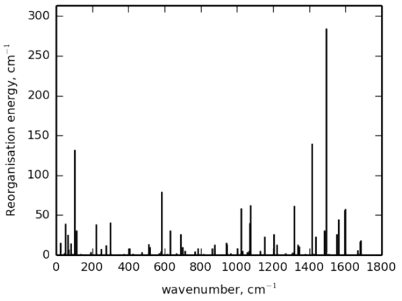
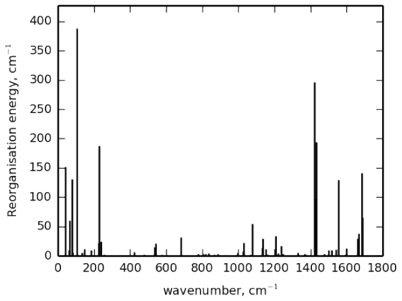
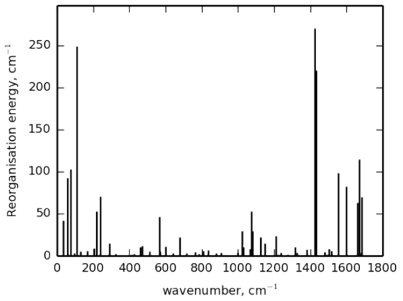
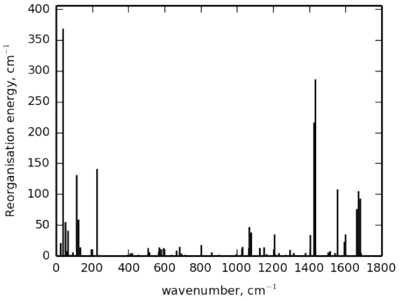
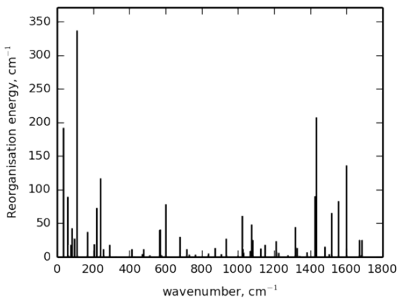
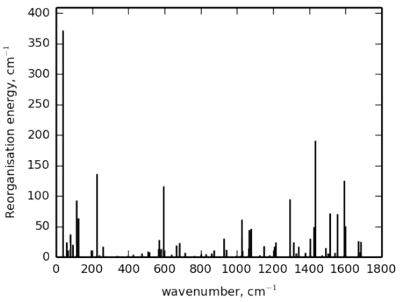
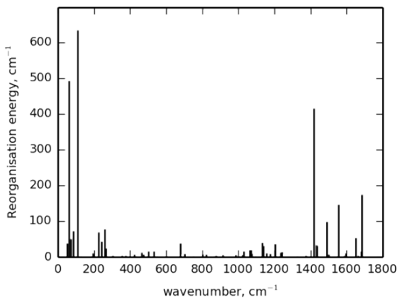
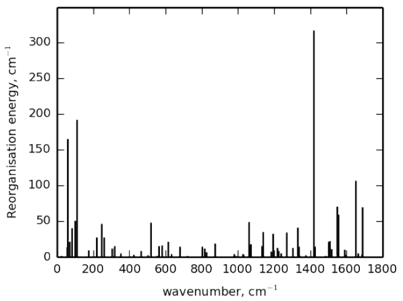
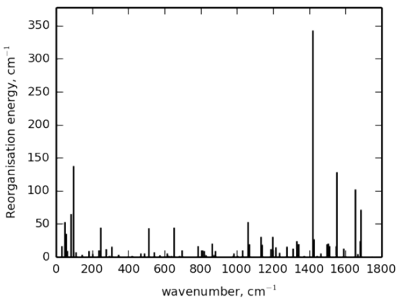


Figure S3. Per-mode Huang-Rhys factor distribution for various $DBMBF_2$ derivatives at 0–1800 cm^{-1}.

	2 (–CH_3)	***3*** (–O–CH_3)	***4*** (–O–CH_2–CH=CH_2)
m-a peak 1			
m-a peak 2			
m-b peak 1			
m-b peak 2			
o-b peak 1			

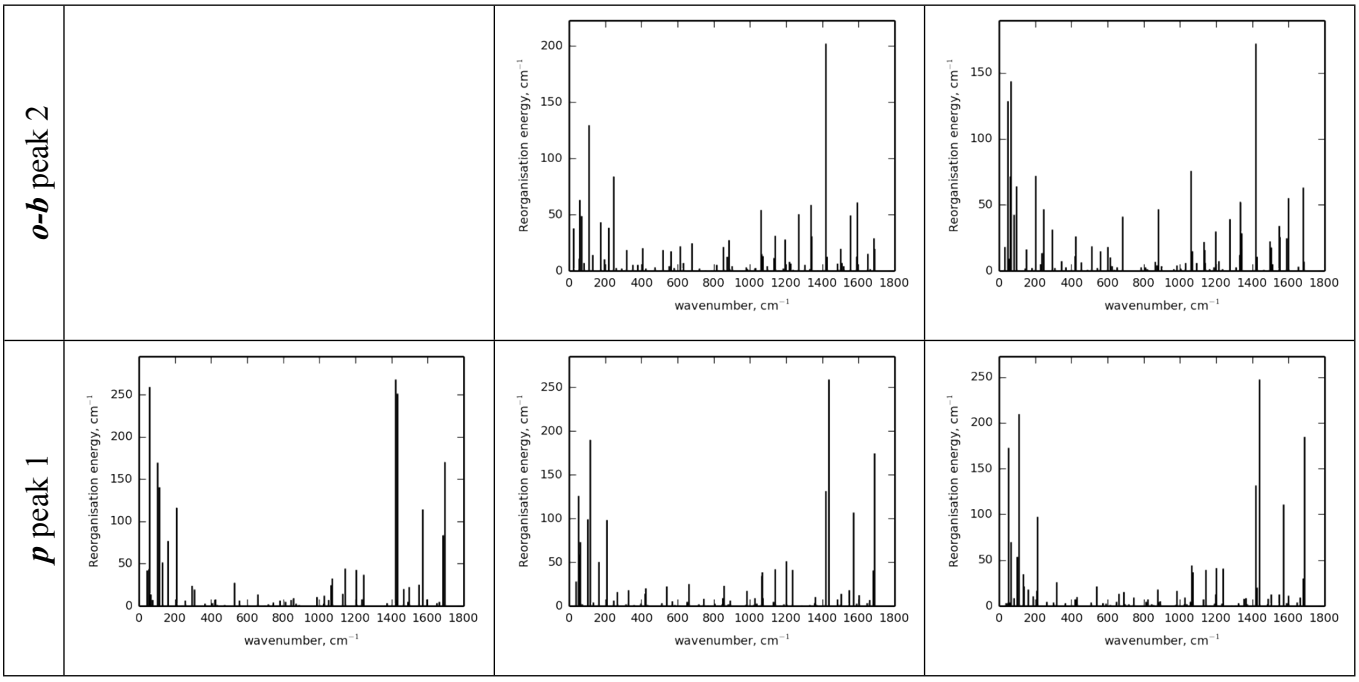
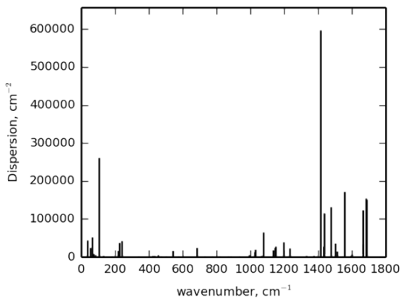
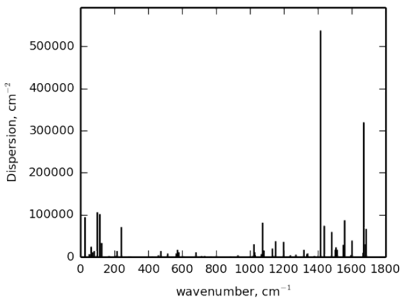
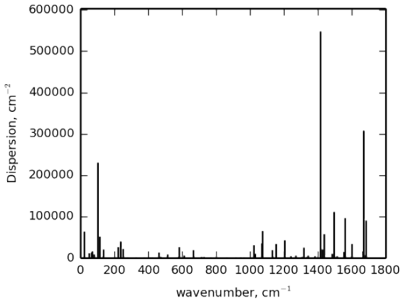
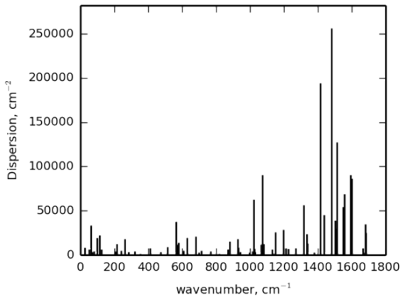
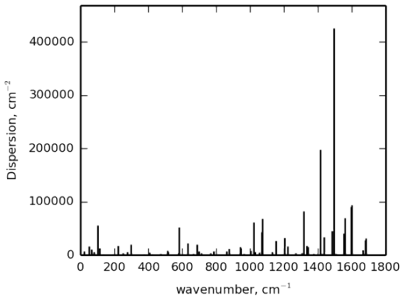
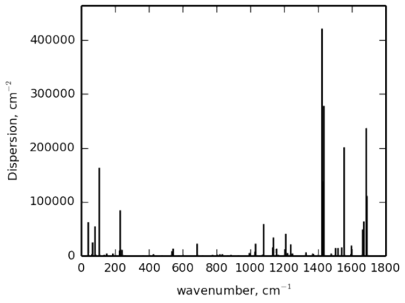
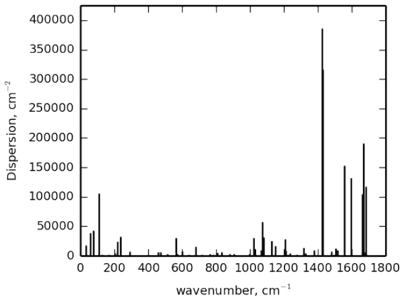
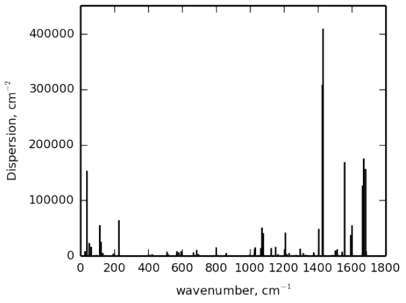
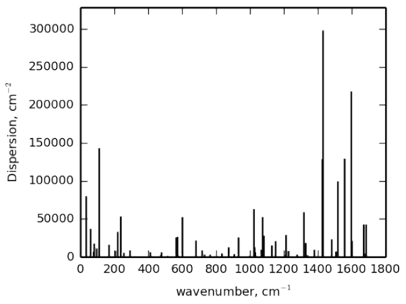
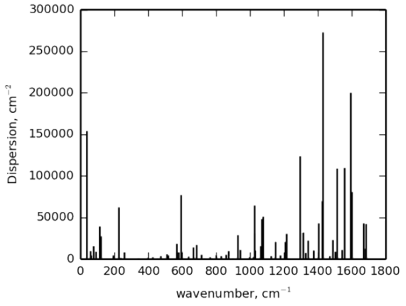
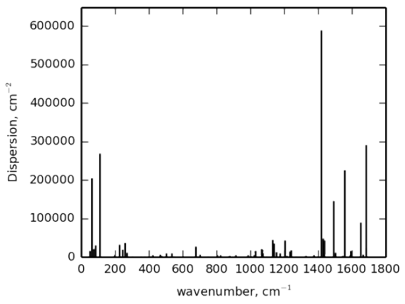
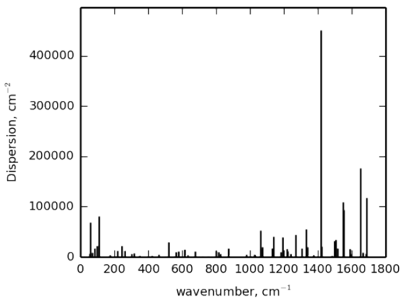
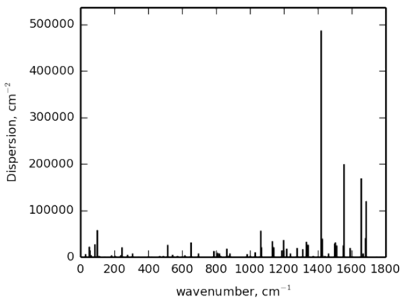


Figure S4. Per-mode reorganization energy contributions for various $DBMBF_2$ derivatives at 0–1800 cm^{-1}.

	2 ($–CH_3$)	***3*** ($–O–CH_3$)	***4*** ($–O–CH_2–CH=CH_2$)
m-a peak 1			
m-a peak 2			
m-b peak 1			
m-b peak 2			
o-b peak 1			

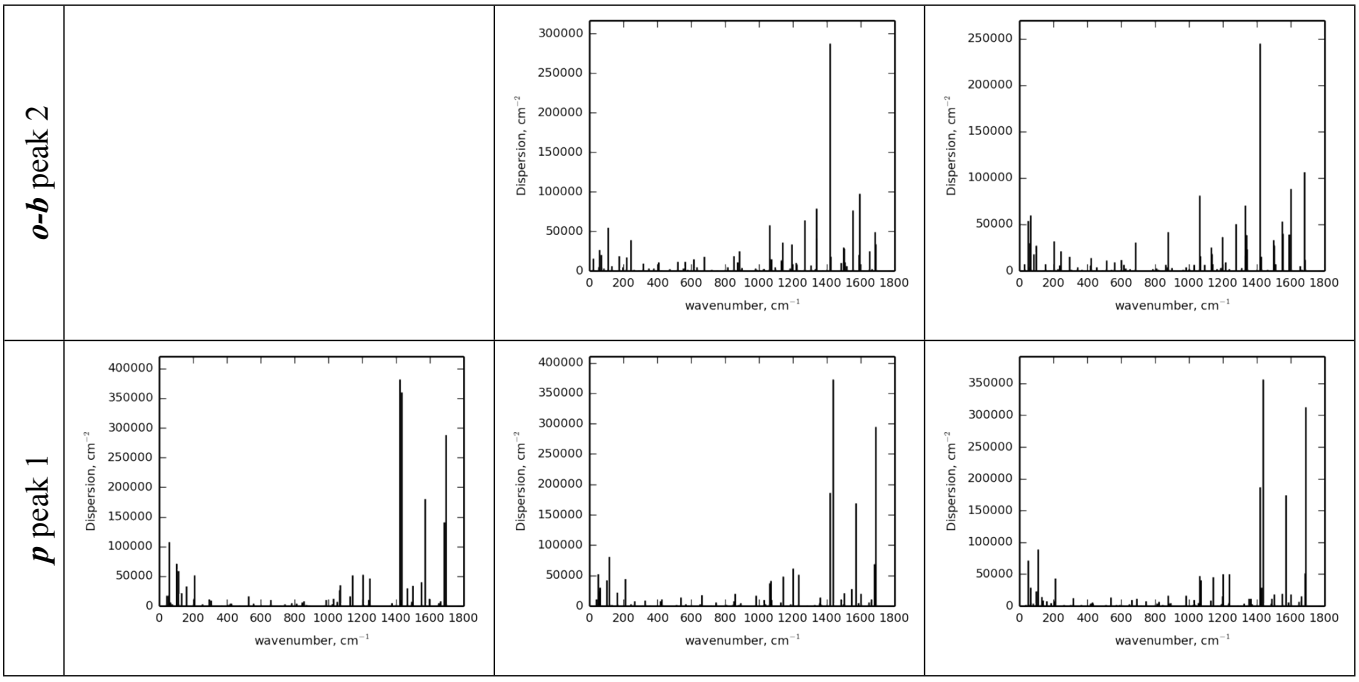
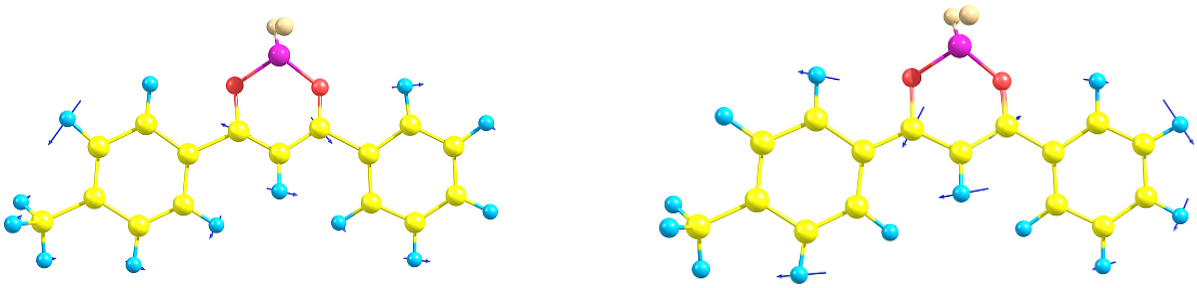


Figure S5. Per-mode contributions to the band dispersion for various $DBMBF_2$ derivatives at 0–1800 cm^{-1}.



(a) (b)

Figure S6. Atomic displacements of ***2p*** corresponding to the modes at (a) 1420 cm^{-1} and (b) 1432 cm^{-1}.

(a) (b)

Figure S7. Atomic displacements of ***4p*** corresponding to the modes at (a) 1415 cm^{-1} and (b) 1435 cm^{-1}.

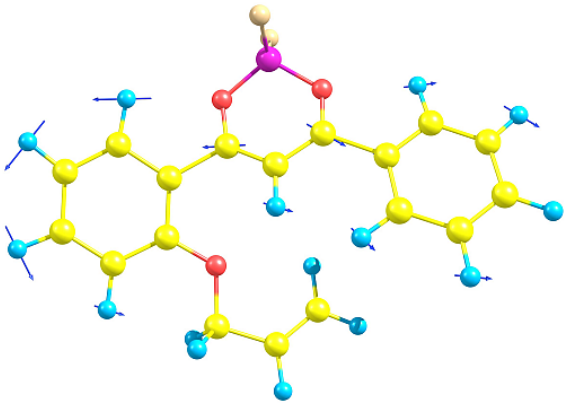
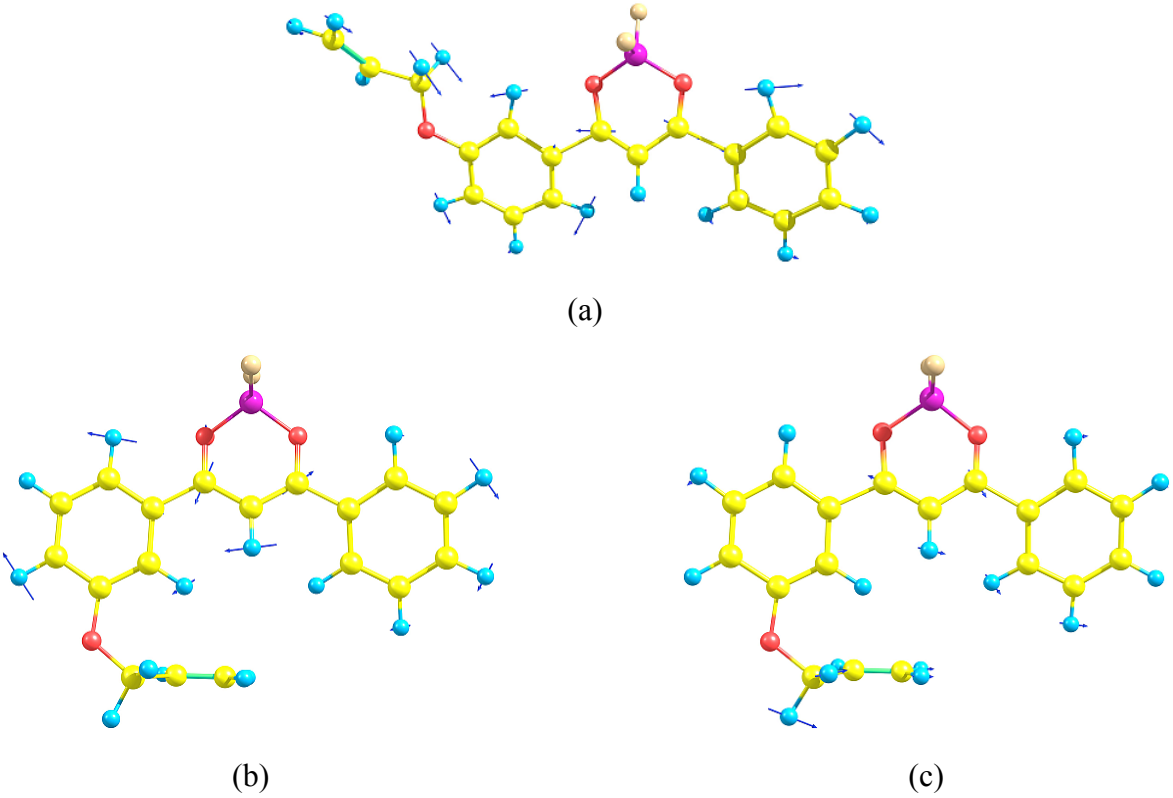


Figure S8. Atomic displacements of ***4o-b*** corresponding to the mode at 1414 cm^{-1}.



(a)

(b)

(c)

Figure S9. Atomic displacements corresponding to the modes (a) at 1412 cm^{-1} for ***4m-a*** and (b) at 1421 cm^{-1} and (c) 1427 cm^{-1} for ***4m-b***.

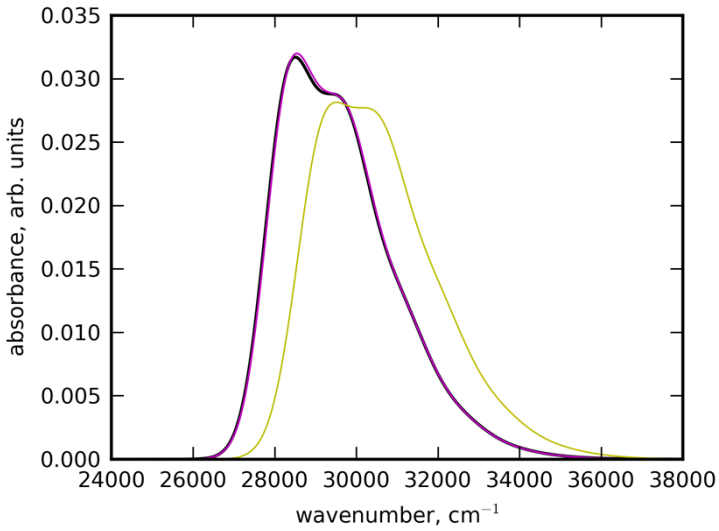


Figure S10. Calculated absorption spectra for ***2p*** (yellow), ***3p*** (magenta), and ***4p*** (black).

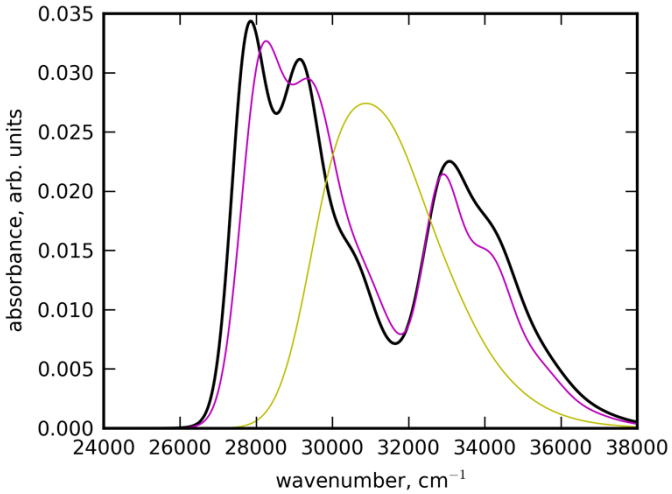


Figure S11. Calculated absorption spectra for ***2o*** (yellow), ***3o*** (magenta), and ***4o*** (black).

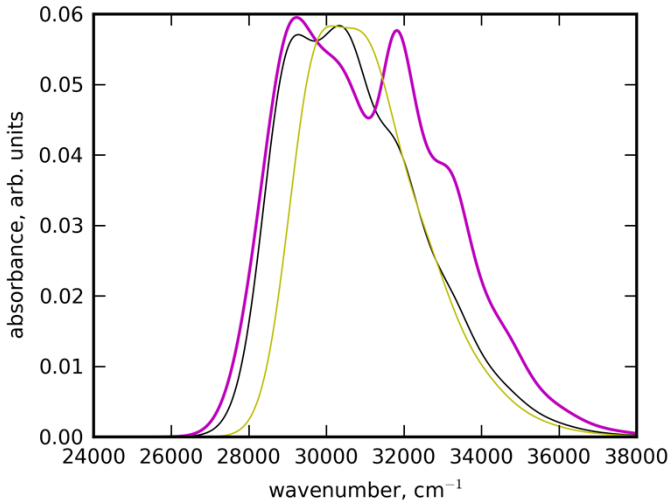


Figure S12. Calculated absorption spectra for ***2m*** (yellow), ***3m*** (magenta), and ***4m*** (black).