Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Femtosecond Fluorescence Study of Vibrational Relaxation and Cooling dynamics of UV dyes

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Figure S1: Integrated spectral area ($M_0(t)$) of the fluorescence of PPO and pTP in cyclohexane, ethanol and dimethylformamide.

Figure S2: Transient fluorescence spectra of PPO and pTP in cyclohexane, ethanol and dimethylformamide upon 290 nm excitation and their F-C fits.

Figure S3: Fourier Transform spectra of the oscillations pattern of $M_1(t)$ from the fluorescence of PPO in CHex, EtOH and DMF.

Figure S4: Fluorescence spectra of PPO and pTP in cyclohexane as a function of temperature. Zero-phonon-line and width obtained from the F-C fit.

Figure S5: Eigenvectors and frequencies of the first 8 calculated low frequency normal modes of PPO molecule.

Table S1: Calculated vibration frequencies [cm^{-1}] of 2,5-diphenyloxazole and paraterphenyl.

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Figure S1: Integrated spectral area ($M_0(t)$) of the fluorescence of PPO (top) and pTP (bottom), in cyclohexane (blue), ethanol (green) and dimethylformamide (red).

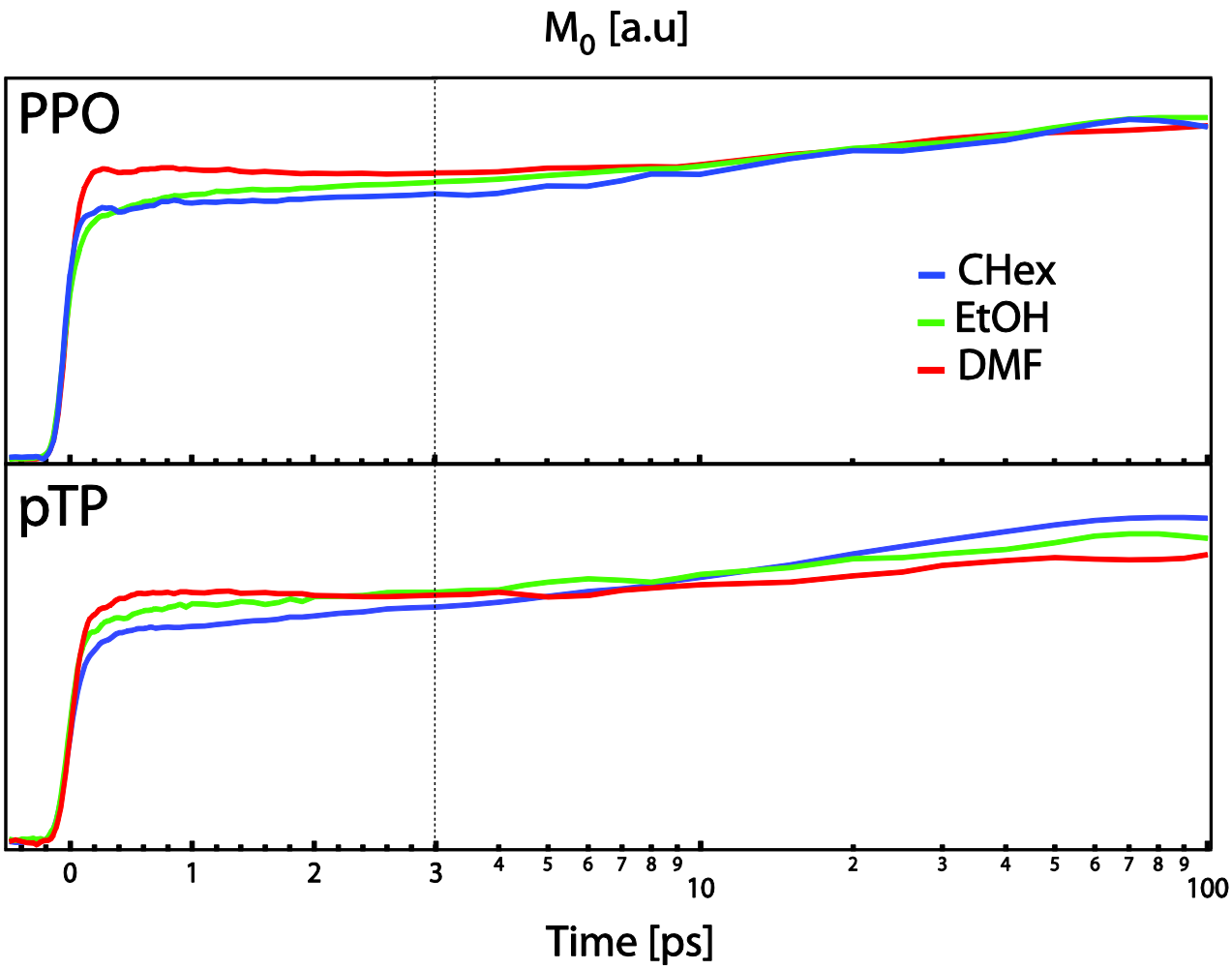

Figure S2: Representative selection of transient fluorescence spectra of PPO (top) and pTP (bottom) in cyclohexane (left), ethanol (middle) and dimethylformamide (right) upon 290 nm excitation (grey circles). The black traces are the F-C fits according to eq.(1). The spectra are vertically shifted for sake of clarity.

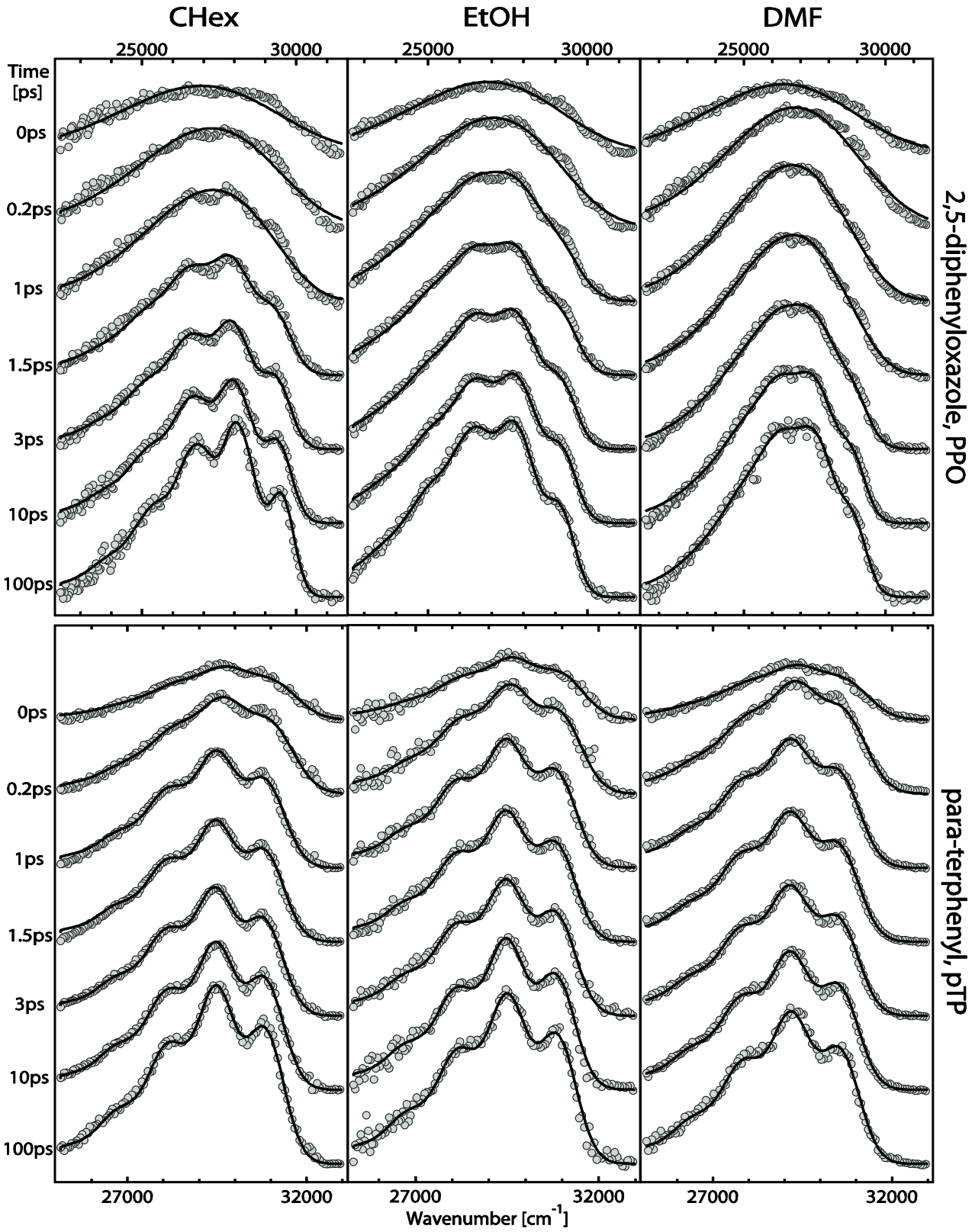

Figure S3: Fourier Transform spectra of the oscillations pattern (inset) of $M_1(t)$ from the fluorescence of PPO in CHex, EtOH and DMF.

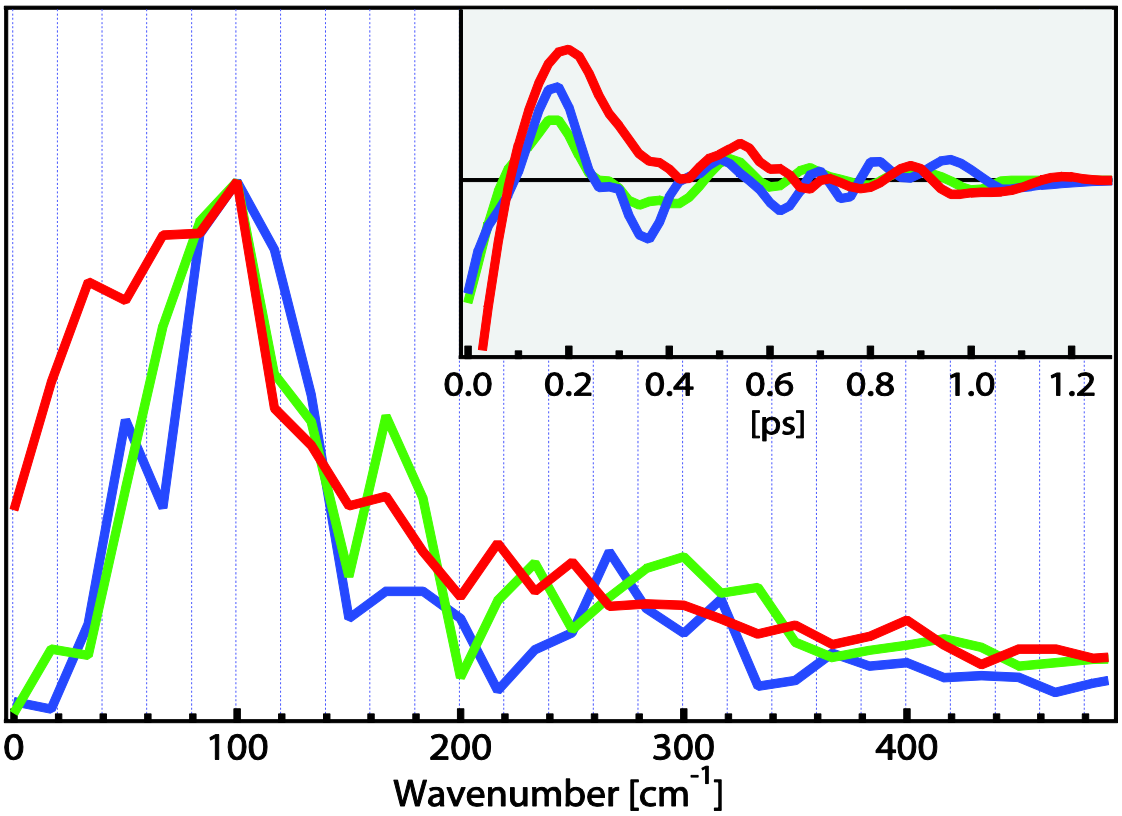

Figure S4: Fluorescence spectra of PPO and pTP in cyclohexane as a function of temperature (top). Zero-phonon-line and width obtained from the F-C fit of the spectra as a function of temperature (bottom).

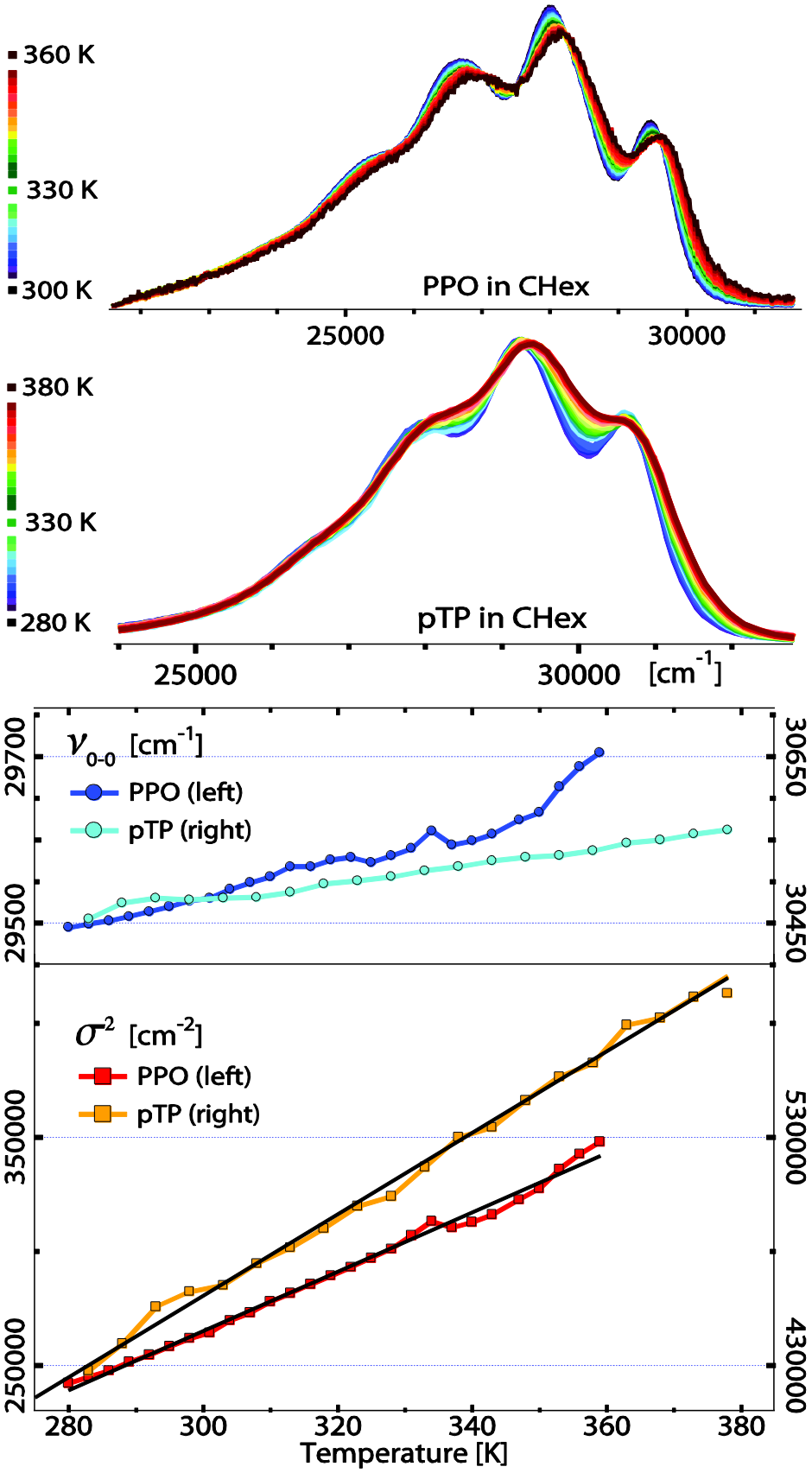

Figure S5: Eigenvectors and frequencies of the first 8 calculated low frequency normal modes of PPO molecule showing distinctive distortions: 1) torsion, 2) torsion plus out-of-plane bending, 3) and 6) in plane bending, 4) torsion plus waving, 5) waving, 6) cycles rotations, 7) torsion plus waving, 8) phenyl-oxazole-phenyl in-plane bending.

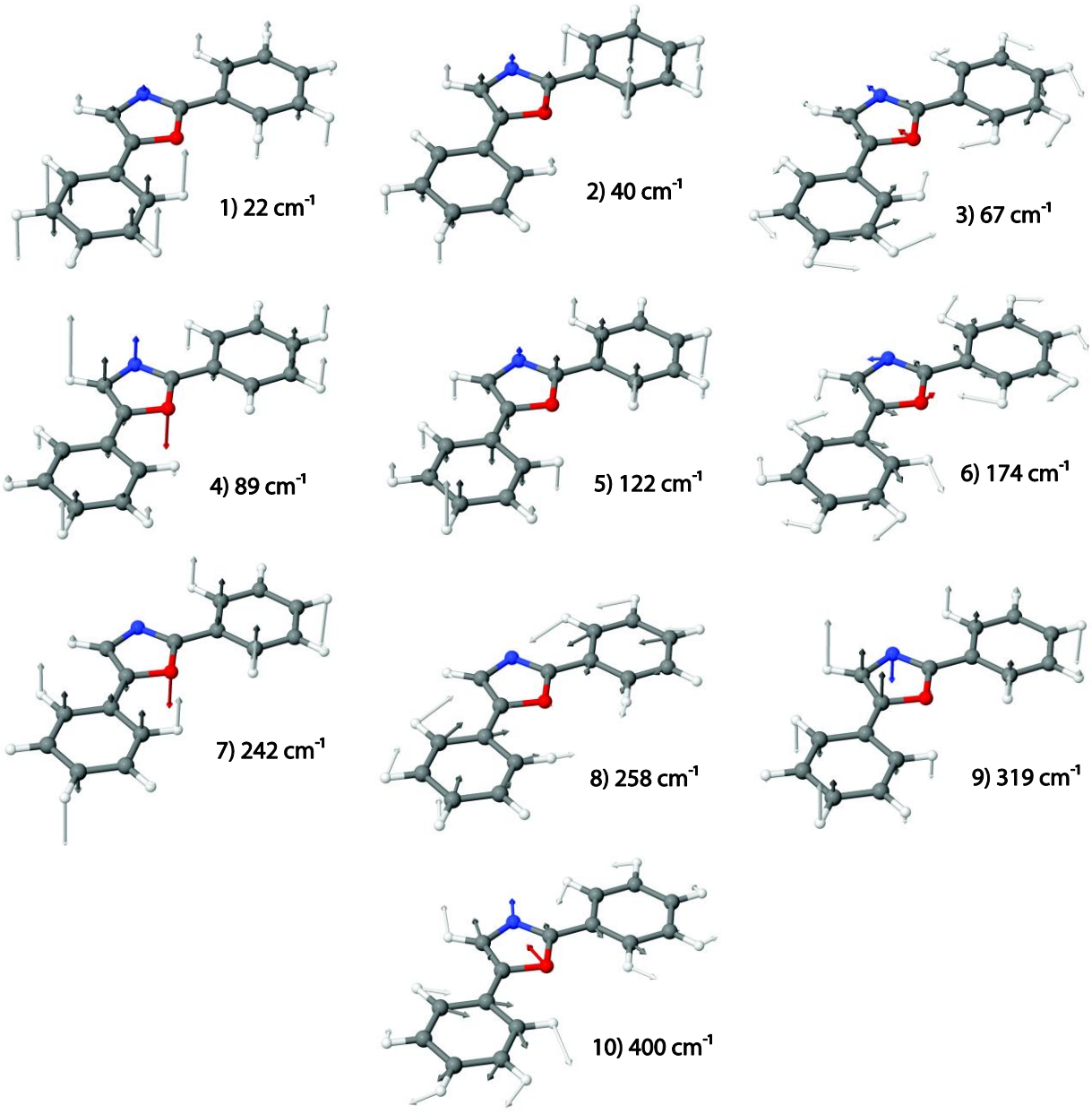

Table S1: Calculated vibration frequencies [cm^{-1}] of 2,5-diphenyloxazole and paraterphenyl using Gaussian 09.

2,5-diphenyloxazole (PPO)			*Paraterphenyl (pTP)*		
22.197	*938.7524*	*1539.4182*	*37.7187*	*860.5789*	*1345.4495*
40.2357	*954.2725*	*1582.3989*	*47.4843*	*861.0484*	*1355.5449*
67.6381	*965.8029*	*1619.732*	*69.4205*	*861.3511*	*1367.6649*
89.4556	*971.9922*	*1639.4616*	*87.9371*	*927.6518*	*1371.5828*
122.0644	*976.867*	*1643.289*	*122.7754*	*932.8443*	*1448.1141*
173.5672	*995.3387*	*1663.7843*	*139.0202*	*967.9381*	*1487.9403*
241.6276	*1001.6684*	*1666.3279*	*215.0135*	*969.658*	*1500.1635*
257.5644	*1016.0801*	*3185.0718*	*246.9088*	*971.4618*	*1535.0512*
319.2458	*1017.8459*	*3186.3794*	*297.1848*	*974.8939*	*1545.8631*
400.0564	*1052.3597*	*3192.6291*	*394.0119*	*994.9557*	*1570.6982*
406.9497	*1054.435*	*3196.4892*	*408.653*	*995.2094*	*1603.2985*
410.7374	*1088.8785*	*3202.698*	*416.1202*	*1016.3638*	*1635.7485*
413.9902	*1100.5253*	*3208.5221*	*420.6936*	*1016.8208*	*1639.8412*
496.3827	*1110.9995*	*3212.0968*	*422.1402*	*1022.3019*	*1660.7169*
514.5934	*1116.4951*	*3221.3173*	*424.9697*	*1027.6059*	*1662.3851*
529.8725	*1180.9504*	*3222.9266*	*526.6883*	*1054.0312*	*1669.5754*
632.3677	*1193.9611*	*3226.665*	*531.738*	*1068.2838*	*3180.4798*
633.1824	*1194.694*	*3276.598*	*584.7982*	*1076.2961*	*3180.6818*
670.5191	*1212.3933*		*625.1915*	*1113.1741*	*3185.6531*
690.0808	*1217.3336*		*631.7496*	*1113.6052*	*3187.3301*
703.6642	*1286.7216*		*634.3505*	*1151.9461*	*3187.6086*
705.137	*1324.5321*		*657.6552*	*1193.2208*	*3190.1498*
717.1158	*1329.3375*		*712.5691*	*1193.3584*	*3197.3372*
725.0532	*1347.6493*		*714.5254*	*1214.8069*	*3198.5421*
777.857	*1370.3619*		*715.091*	*1217.437*	*3201.6201*
791.5841	*1372.9701*		*739.8167*	*1229.9471*	*3203.9834*
841.9122	*1383.9495*		*772.1614*	*1306.4653*	*3206.1212*
855.2303	*1494.6534*		*787.7941*	*1314.256*	*3206.7577*
863.2776	*1495.7825*		*791.4184*	*1317.5643*	*3211.4557*
923.3448	*1529.9907*		*856.6086*	*1322.3169*	*3212.063*