Appendix A. Supplementary data

Theory of Raman scattering 1,2

The $\rho\sigma$ element of the polarizability tensor of an isolated molecule for a transition $gi \rightarrow gj$ is given by

$$\left(\alpha_{\rho\sigma}\right)_{gi,gj} = \frac{1}{h}\sum_{ev}\left(\frac{\left(M_{\rho}\right)_{ev,gj}\left(M_{\sigma}\right)_{gi,ev}}{v_{ev,gi} - v_0 + i\Gamma_e} + \frac{\left(M_{\rho}\right)_{gi,ev}\left(M_{\sigma}\right)_{ev,gj}}{v_{ev,gj} + v_0 + i\Gamma_e}\right)$$

(1)

$$\left(\alpha_{\rho\sigma}\right)_{e^f v^f : e^g v^i} = \frac{1}{h}\sum_{\substack{e^r v^r \neq e^g v^i, \\ e^f v^f}}\left(\frac{\left\langle v^f \middle| (p_\rho)_{e^f e^r} \middle| v^r \right\rangle \left\langle v^r \middle| (p_\sigma)_{e^r e^g} \middle| v^i \right\rangle}{\omega_{e^r v^r : e^g v^i} - \omega_1 - i\Gamma_{e^r v^r}} + \frac{\left\langle v^f \middle| (p_\sigma)_{e^f e^r} \middle| v^r \right\rangle \left\langle v^r \middle| (p_\rho)_{e^r e^g} \middle| v^i \right\rangle}{\omega_{e^r v^r : e^f v^f} + \omega_1 + i\Gamma_{e^r v^r}}\right)$$

Where h is Planck's constant and the sum goes over the excited vibronic states $e^r v^r$ (with damping factor $\Gamma_{e^r v^r}$ for electronic state e^r of the molecules), e^g is the ground electronic state, e^r is the excited electronic state, and v^i, v^r, v^f is the vibrational state. ω_1 is the frequency of plane-polarized incident light. ρ , $\sigma = x, y, z$ and they are independently refer to the molecular fixed coordinate system. Here $(p_\rho)_{e^f e^r}$, $(p_\sigma)_{e^r e^g}$ etc., refer to the amplitudes of the corresponding transition moments. $(p_\rho)_{e^f e^r} = \left\langle e^f \middle| \hat{p}_\rho \middle| e^r \right\rangle$, $\left\langle v^f \middle| (p_\rho)_{e^f e^r} \middle| v^r \right\rangle = \int \left(\theta_{e^r} \Phi_{v^r}^{e^r}\right)^* p_\rho \left(\theta_{e^f} \Phi_{v^f}^{e^f}\right) d\xi dQ$, where θ_{e^f} is the electronic wave function for state e^f and $\Phi_{v^f}^{e^f}$ is the v^f th vibrational state function of the electronic state e^f.

Let us assume that the only intermediate state i is an electronically excited state B, which in turn interacts through first order Herzberg-Teller coupling with just one other electronically excited state Q. Then the intermediate state becomes

$$i \equiv B\Phi_v^B = [B^0 + \sum_k h_{BQ}^k \left(\Delta E_{BQ}^0\right)^{-1} Q_k Q^0]\Phi_v^B \qquad (2)$$

Where B^0 and Q^0 are the electronic wave functions for the (ground-state) equilibrium nuclear configuration, h_{BQ}^k is the Herzberg-Teller coupling of the B^0 and Q^0 states through the normal coordinate Q_k ($h_{BQ}^k = \int \psi_B \left(\frac{\partial H}{\partial Q_k}\right)_{Q_k=0} \psi_Q d\xi$) and Φ_v^B is the vibrational wave function for the v mode in the B state.

When ω_1 approaches $\omega_{e^r v^r : e^g v^i}$, for the resonance or near-resonance conditions the second part of Eq.(1) may be ignored and only the lowest excited state e^r need be considered in the sum. After introducing the expressions for the transition moments and Eq. (2) as above, one obtains to first order in nuclear displacement

$$\left(\alpha_{\rho\sigma}\right)_{e^f v^f : e^g v^i} = A' + B'$$

(3)

Where

$$A' = \frac{1}{\hbar}(p_\rho)_{e^f e^r}^0 (p_\sigma)_{e^r e^g}^0 \sum_{v^r} \left(\frac{\left\langle v^{f(f)} \middle| v^{r(r)} \right\rangle \left\langle v^{r(r)} \middle| v^{i(g)} \right\rangle}{\omega_{e^r v^r : e^g v^i} - \omega_1 - i\Gamma_{e^r v^r}} \right)$$

$$B' = \frac{1}{\hbar^2}(p_\rho)_{e^f e^s}^0 \frac{h_{e^s e^r}^k}{\omega_{e^r} - \omega_{e^s}} (p_\sigma)_{e^r e^g}^0 \sum_{v^r} \left(\frac{\left\langle v^{f(f)} \middle| Q_k \middle| v^{r(r)} \right\rangle \left\langle v^{r(r)} \middle| v^{i(g)} \right\rangle}{\omega_{e^r v^r : e^g v^i} - \omega_1 - i\Gamma_{e^r v^r}} \right)$$

$$+ \frac{1}{\hbar^2}(p_\rho)_{e^f e^r}^0 \frac{h_{e^r e^s}^k}{\omega_{e^r} - \omega_{e^s}} (p_\sigma)_{e^s e^g}^0 \sum_{v^r} \left(\frac{\left\langle v^{f(f)} \middle| v^{r(r)} \right\rangle \left\langle v^{r(r)} \middle| Q_k \middle| v^{i(g)} \right\rangle}{\omega_{e^r v^r : e^g v^i} - \omega_1 - i\Gamma_{e^r v^r}} \right)$$

(4)

In these equations the exclusions $e^r \neq e^g, e^f; e^s \neq e^r$ apply, and the vibrational quantum numbers, v^i, v^r and v^f have been given additional superscripts as for example $v^{i(g)}$ to indicate the electronic state to which they refer.

Table S1 Experimental and RB3LYP /6-311G** **computed vibrational frequencies of** TCPP.

modes	Computed(cm^{-1})		Experimental(cm^{-1})		descriptions
	B3LYP/6-311G**	b	FT-Raman	FT-IR	
A1 ν_1	25.5497	95.24354			δ(phenyl- porph)
ν_2	28.6248	98.11723			γ(phenyl- porph)
ν_3	51.5395	119.53101			def(porph)
ν_4	78.7351	144.9453			def(porph)
ν_5	101.1972	165.93613			def(porph)
ν_6	116.9440	180.65152			def(porph)
ν_7	137.2996	199.67383			def(porph)+ γ(phenyl- COOH)
ν_8	145.6869	207.51176			breath (porph)
ν_9	163.4596	224.12035			δ(phenyl- COOH)
ν_{10}	172.1484	232.24003			def (porph)
ν_{11}	216.2756	273.4769			γ(pyr - porph)
ν_{12}	268.2958	322.08978			δ(phenyl- COOH)
ν_{13}	310.0895	361.14599			γ(phenyl- COOH)
ν_{14}	322.9855	373.1973			breath (porph+ phenyl)
ν_{15}	426.6560	470.07738	408.835		(phenyl twist)
ν_{16}	439.0170	481.62874			COO sci+ breath(porph+ phenyl)
ν_{17}	494.0149	533.02427			OCC sci+ phenyl def
ν_{18}	517.0371	554.53852			OCC sci+ phenyl def
ν_{19}	573.3178	607.13283			γ(phenyl+ porph)
ν_{20}	647.9832	676.90765			def (phenyl)
ν_{21}	656.1299	684.52074			γ(O-H)
ν_{22}	656.5787	684.94015			γ(O-H)
ν_{23}	667.3947	695.0477	638.3225		γ(porph)
ν_{24}	731.3698	754.83243			def (porph) +γ(phenyl)
ν_{25}	742.0102	764.77588		721.2466	γ(C-H,N-H,OH)
ν_{26}	767.2827	788.39303			γ(N-H)
ν_{27}	775.7722	796.32647			breath (porph+ phenyl)
ν_{28}	788.5149	808.23452	667.2495	767.5298	breath (pyr)+ γ(C-H,N-H,OH)
ν_{29}	815.3361	833.29894	788.7429		Pyr γ(C-H)
ν_{30}	836.3521	852.93839		798.3853	Porph γ(C-H,N-H)
ν_{31}	845.7882	861.75642			δ(C-N-C)

ν_{32}	875.1739	889.21736	848.5254		Phenyl γ(C-H)
ν_{33}	896.1705	908.83868			breath (porph+ phenyl)
ν_{34}	901.8914	914.18486		867.8101	δ(C-N-C) + Phenyl γ(C-H)
ν_{35}	979.9237	987.10605		964.2334	breath (pyr+ phenyl)
ν_{36}	999.9624	1005.83221			Phenyl γ(C-H)
ν_{37}	1009.9121	1015.13021			Phenyl γ(C-H)
ν_{38}	1019.6383	1024.21934			breath (porph+ pyr)
ν_{39}	1035.9183	1039.433	1002.803	1020.159	def (phenyl)
ν_{40}	1104.1074	1103.15572			breath (phenyl)+ ν(C-O)
ν_{41}	1110.0152	1108.67655	1078.013	1103.083	Pyr δ(C-H)
ν_{42}	1114.5010	1112.86853			Pyr δ(C-H)
ν_{43}	1133.6380	1130.75206	1130.082		phenyl (breath+ δ(C-H))
ν_{44}	1197.9218	1190.82527	1182.15	1176.365	phenyl δ(C-H)+δ(O-H)
ν_{45}	1226.7721	1217.78588		1222.648	phenyl (breath+ δ(C-H))+ δ(O-H)
ν_{46}	1249.5945	1239.11341	1236.149		ν(phenyl-C_m)+ breath (phenyl+ pyr)
ν_{47}	1298.2945	1284.62356	1288.216	1276.645	ν(C_α-C_β)+def(phenyl)
ν_{48}	1320.6398	1305.50524			ν(C_α-C_β)+def(phenyl)
ν_{49}	1335.5151	1319.40621	1359		phenyl δ(C-H)
ν_{50}	1380.2488	1361.20985	1384.639	1384.6	ν(C_α-C_β)
ν_{51}	1382.1701	1363.00531			breath (phenyl+ pyr) +δ(O-H)
ν_{52}	1427.8835	1405.72448		1401.995	phenyl δ(C-H)
ν_{53}	1468.9350	1444.08711			breath (porph+ pyr)
ν_{54}	1530.4286	1501.55288			ν(C_β-C_β)+ def(phenyl)
ν_{55}	1536.0691	1506.82392	1496.49		ν(C_β-C_β)+ def(phenyl)
ν_{56}	1567.9448	1536.61177			ν(C_α-C_m-C_α)$_{as}$
ν_{57}	1585.5561	1553.06953			ν(C_β-C_β)+ ν(C_α-C_m-C_α)$_s$
ν_{58}	1589.9711	1557.19534	1552.416		def(phenyl)+ breath (pyr)

ν_{59}	1639.4179	1603.40338	1608.341	1604.484	def(phenyl)
ν_{60}	1765.7730	1721.48222		1691.26	ν(C=O)
ν_{61}	3161.0890	3025.40502		2852.202	Phenyl ν(C-H) $_{as}$
ν_{62}	3163.1967	3027.37467			Phenyl ν(C-H) $_{as}$
ν_{63}	3183.6100	3046.45089			Phenyl ν(C-H)$_s$
ν_{64}	3189.2130	3051.6869			Phenyl ν(C-H)$_s$
ν_{65}	3240.6729	3099.77618		2923.556	Pyr ν(C-H)$_s$
ν_{66}	3250.3977	3108.864			Pyr ν(C-H)$_s$
ν_{67}	3568.6382	3406.25975			ν(N-H)$_s$
ν_{68}	3681.4816	3511.71191		3316	ν(O-H)$_s$
A2 ν_{69}	14.3805	84.80593			γ(phenyl- porph)
ν_{70}	48.6301	116.81218			δ(phenyl- porph)
ν_{71}	57.6409	125.23277			breath (porph)
ν_{72}	74.2056	140.71248			tors (phenyl-porph)
ν_{73}	86.4314	152.13749			γ(phenyl- porph)
ν_{74}	100.4565	165.24395			tors (phenyl-porph)
ν_{75}	165.7258	226.23811			γ(phenyl- COOH)
ν_{76}	211.1960	268.73001			δ(phenyl- COOH)
ν_{77}	290.2575	342.61298			breath (porph+ phenyl)
ν_{78}	301.6360	353.24619			γ (porph)
ν_{79}	334.4450	383.9062			γ(phenyl- COOH)
ν_{80}	348.7043	397.23152			δ(phenyl- COOH)
ν_{81}	424.9115	468.44715			γ (phenyl)
ν_{82}	444.4391	486.69569			sci(N-C_α-C_m)
ν_{83}	451.0906	492.91152			sci(N-C_α-C_m)
ν_{84}	481.8559	521.66169			sci(N-C_α-C_m+O-C-C)
ν_{85}	506.8482	545.01699			sci(N-C_α-C_m+O-C-C)
ν_{86}	551.1870	586.4516			sci(N-C_α-C_m)+ γ (phenyl)
ν_{87}	573.0430	606.87603			def(phenyl+ porph)
ν_{88}	648.1799	677.09147			def(phenyl)
ν_{89}	658.4613	686.69943			γ(O-H)
ν_{90}	669.6753	697.17892			breath (phenyl)+ sci(O-C-O)
ν_{91}	691.4018	717.48233	638.3225		γ(pyr)
ν_{92}	740.7701	763.61701			γ(O-H+phenyl)
ν_{93}	765.4978	786.72504			γ(C_α-C_m-C_α+O-H+C-H)

ν_{94}	784.0705	804.08123			breath (phenyl)
ν_{95}	798.1451	817.23395			γ(C-H+COO)
ν_{96}	836.5327	853.10716			def(pyr)
ν_{97}	873.4541	887.61021			Phenyl γ(C-H)
ν_{98}	885.8452	899.18969			def(pyr+porph)
ν_{99}	896.2864	908.94699			Phenyl γ(C-H)
ν_{100}	942.2874	951.93493			Pyr γ(C-H)
ν_{101}	946.0323	955.43453			Pyr γ(C-H)
ν_{102}	996.6330	1002.72089			Porph δ(C-H+N-H)+def(pyr)
ν_{103}	1000.9801	1006.78325			Pyr δ(C-H+N-H) + Phenyl γ(C-H)
ν_{104}	1010.3564	1015.54541			Phenyl γ(C-H)
ν_{105}	1021.9691	1026.39747			def (pyr+phenyl)
ν_{106}	1037.4145	1040.8312			def (pyr+phenyl)
ν_{107}	1103.3072	1102.40793			breath (phenyl)+ ν(C-O)
ν_{108}	1133.0918	1130.24164			Phenyl δ(C-H)
ν_{109}	1158.5848	1154.06485			Porph δ(C-H+N-H)+def(pyr)
ν_{110}	1197.5275	1190.4568			Phenyl δ(C-H,O-H)
ν_{111}	1225.3984	1216.50215			Phenyl δ(C-H,O-H)
ν_{112}	1237.2192	1227.54869			Porph δ(C-H+N-H)+def(pyr)
ν_{113}	1260.8592	1249.64027			$\nu(C_\alpha\text{-N-}C_\alpha)_{as}$
ν_{114}	1303.0344	1289.053			def (phenyl)
ν_{115}	1334.1269	1318.10894			Phenyl δ(C-H)
ν_{116}	1343.6117	1326.97248	1330.642		$\nu(C_m\text{-Phenyl})$+δ(N-H)
ν_{117}	1351.9851	1334.79743			def (pyr)+ pyr δ(C-H)
ν_{118}	1381.1368	1362.03969			$\nu(C\text{-}C\text{-}O)_{as}$
ν_{119}	1400.5850	1380.21403			def (pyr)+ pyr δ(C-H)
ν_{120}	1427.0812	1404.97473			def (Phenyl)+ Phenyl δ(C-H)
ν_{121}	1477.1699	1451.78262	1459.849		$\nu(C_\alpha\text{-}C_m\text{-}C_\alpha)_{as}$ +def (pyr)
ν_{122}	1533.5444	1504.46459	1496.49		def (Phenyl)+Phenyl δ(C-H)
ν_{123}	1574.0904	1542.35483			$\nu(C_\alpha\text{-}C_m\text{-}C_\alpha)_{as}$ +def (pyr)
ν_{124}	1589.0590	1556.34299			def (Phenyl+pyr)
ν_{125}	1637.8541	1601.94201			def (Phenyl)
ν_{126}	1764.5386	1720.32867			ν(C=O)
ν_{127}	3161.0575	3025.37558			Phenyl $\nu(C\text{-}H)_{as}$
ν_{128}	3163.1685	3027.34831			Phenyl $\nu(C\text{-}H)_{as}$
ν_{129}	3183.5961	3046.43791			Phenyl $\nu(C\text{-}H)_{as}$
ν_{130}	3189.1964	3051.67139			Phenyl $\nu(C\text{-}H)_{as}$
ν_{131}	3221.5976	3081.95031			Pyr $\nu(C\text{-}H)_{as}$
ν_{132}	3234.9128	3094.39336			Pyr $\nu(C\text{-}H)_{as}$
ν_{133}	3681.3686	3511.60631			ν(O-H)
B1 ν_{134}	29.8236	99.2375			δ(phenyl- porph)
ν_{135}	42.4992	111.08285			tilt (porph)
ν_{136}	66.4671	133.48085			tors (phenyl- porph)

ν_{137}	97.4701	162.45316			tors (phenyl- porph)
ν_{138}	126.0877	189.19631			γ(phenyl-COOH)
ν_{139}	130.4800	193.30091			γ(phenyl-COOH)
ν_{140}	178.0313	237.7376			γ(pyr-porph)+δ(phenyl-COOH)
ν_{141}	189.4619	248.4195			def(porph)
ν_{142}	238.3560	294.11103			δ(phenyl-COOH)
ν_{143}	292.4468	344.65888			def(porph) +γ(phenyl-COOH)
ν_{144}	335.5532	384.94182			γ(pyr-porph)
ν_{145}	363.4846	411.04371			δ(pyr-porph)
ν_{146}	393.8588	439.4284			δ(pyr-porph)
ν_{147}	426.8480	470.25681			δ(phenyl)
ν_{148}	470.1342	510.70776			δ(pyr-porph)
ν_{149}	500.6603	539.2344			Sci (O-C-C)
ν_{150}	538.0523	574.17722			γ(phenyl)
ν_{151}	581.0995	614.40483			γ(porph)+def(phenyl)
ν_{152}	648.8398	677.70814			def(phenyl)
ν_{153}	656.9887	685.32329			γ(O-H)
ν_{154}	664.8187	692.64043			δ(O-H)+ def(phenyl)
ν_{155}	688.0138	714.31625			γ(porph)
ν_{156}	735.6179	758.80228			γ(C-H)
ν_{157}	750.2934	772.51653			γ(C-H)
ν_{158}	780.1021	800.37276			def(phenyl)
ν_{159}	792.0155	811.50583			γ(C-H)+def(porph)
ν_{160}	819.0466	836.7664			Pyr γ(C-H)
ν_{161}	840.7795	857.07579			def(porph)
ν_{162}	873.9588	888.08185			Phenyl γ(C-H)
ν_{163}	888.8361	901.98469			Phenyl γ(C-H)+def(porph)
ν_{164}	901.1705	913.51118			Phenyl γ(C-H)+breath(pyr)
ν_{165}	946.0445	955.44594			Pyr γ(C-H)
ν_{166}	981.0061	988.11755			Breath (pyr+phenyl)
ν_{167}	1000.1652	1006.02173			Phenyl γ(C-H)
ν_{168}	1007.1368	1012.53669			Pyr δ(N-H+C-H)
ν_{169}	1010.8603	1016.0163			Phenyl γ(C-H)
ν_{170}	1036.0018	1039.51103			def(phenyl)
ν_{171}	1103.0848	1102.2001			δ(C-H)+breath(phenyl)
ν_{172}	1106.4308	1105.32693			Pyr δ(C-H)
ν_{173}	1133.1525	1130.29836			Phenylδ(C-H)
ν_{174}	1197.4929	1190.42447			Phenylδ(C-H)
ν_{175}	1216.3370	1208.03428			δ(N-H)+def(porph)
ν_{176}	1225.9590	1217.02604			δ(C-H+O-H+N-H)+def(porph)
ν_{177}	1247.0220	1236.70941			Pyr δ(C-H +N-H)+def(pyr)
ν_{178}	1272.1536	1260.19489			$\nu(C_\alpha\text{-}C_\beta)$+ ν(phenyl-C_m)
ν_{179}	1303.2701	1289.27326			def(phenyl)

ν_{180}	1334.7427	1318.6844			Phenylδ(C-H)
ν_{181}	1368.4888	1350.22013			ν(C_α-C_β)+def(porph)
ν_{182}	1381.2528	1362.14809			δ(O-H)
ν_{183}	1390.7615	1371.03397			δ(N-H) +def(pyr)
ν_{184}	1428.5086	1406.30864			def(phenyl)
ν_{185}	1506.9469	1479.60923			breath(pyr)
ν_{186}	1533.1405	1504.08715			def(phenyl)
ν_{187}	1557.5175	1526.86745			def(porph)
ν_{188}	1585.1987	1552.73554			def(porph+phenyl)
ν_{189}	1591.8478	1558.94912		1565.915	def(porph+phenyl)
ν_{190}	1638.1453	1602.21413			def(phenyl)
ν_{191}	1764.6578	1720.44006			ν(C=O)
ν_{192}	3161.0563	3025.37446			Phenyl ν(C-H) $_{as}$
ν_{193}	3163.1785	3027.35766			Phenyl ν(C-H) $_{as}$
ν_{194}	3183.5966	3046.43837			Phenyl ν(C-H) $_{as}$
ν_{195}	3189.2021	3051.67671			Phenyl ν(C-H) $_{s}$
ν_{196}	3234.8975	3094.37906			pyr ν(C-H) $_{as}$
ν_{197}	3240.6418	3099.74711			pyr ν(C-H) $_{s}$
ν_{198}	3681.3791	3511.61612			ν(O-H)
B2 ν_{199}	29.8279	99.24152			δ(phenyl- porph)
ν_{200}	41.3011	109.96323			γ((phenyl- porph)
ν_{201}	66.4929	133.50497			tors (phenyl- porph)
ν_{202}	95.8961	160.98226			tors (phenyl- porph)
ν_{203}	124.4816	187.69541			tors (phenyl- porph)+tilt (porph)
ν_{204}	126.3822	189.47152			γ(phenyl-COOH)
ν_{205}	159.4848	220.4059			δ(phenyl-COOH)+ γ(pyr- porph)
ν_{206}	190.4865	249.37698			Def(porph)
ν_{207}	229.5655	285.89631			γ((phenyl- porph)
ν_{208}	295.1186	347.15568			δ(phenyl- porph)
ν_{209}	332.5777	382.16121			γ((phenyl-porph)+ γ((pyr-porph)
ν_{210}	374.9498	421.75794			δ(pyr-porph)
ν_{211}	393.2798	438.88732			δ(pyr-porph)
ν_{212}	426.8981	470.30362			γ(phenyl)
ν_{213}	477.6651	517.74539			δ(pyr-porph)+sci(O-C-C)
ν_{214}	502.5896	541.03733			sci(O-C-C) +δ(pyr-porph)
ν_{215}	531.8394	568.37127			γ(phenyl)
ν_{216}	565.4317	599.76327			Tilt(porph)+ γ(C-H)
ν_{217}	620.0311	650.78641			γ(N-H)
ν_{218}	647.8638	676.79607			def(phenyl)
ν_{219}	656.4529	684.82259			γ(O-H)
ν_{220}	665.7884	693.54661			def(phenyl)

ν_{221}	678.0467	705.00199			γ(N-H+pyr)
ν_{222}	733.1975	756.54041			γ(phenyl+O-H)
ν_{223}	758.2657	779.96665			Tilt(porph)+γ(C-H)
ν_{224}	780.0987	800.36959			def(phenyl)
ν_{225}	787.8928	807.65317			def(porph)
ν_{226}	827.4111	844.58302			def(porph)+ pyr γ(C-H)
ν_{227}	829.9787	846.98245			def(porph)+ pyr γ(C-H)
ν_{228}	874.5205	888.60676			phenyl γ(C-H)
ν_{229}	886.2978	899.61264			def(porph)+ phenyl γ(C-H)
ν_{230}	900.7865	913.15233			def(pyr)+ phenyl γ(C-H)
ν_{231}	942.7878	952.40255			pyr γ(C-H)
ν_{232}	997.4069	1003.4441			$\nu(C_\alpha\text{-}C_\beta)$+def(porph)
ν_{233}	1002.0031	1007.73925			$\nu(C_\alpha\text{-}C_\beta)$+def(porph)
ν_{234}	1010.6890	1015.85622			phenyl γ(C-H)
ν_{235}	1015.0353	1019.91784			Def(pyr+phenyl)
ν_{236}	1036.8413	1040.29554			Def(phenyl)
ν_{237}	1088.9618	1089.00215			Pyr δ(C-H)
ν_{238}	1103.6011	1102.68258			Breath (phenyl)+ ν(C-O)
ν_{239}	1133.3345	1130.46844			Phenyl δ(C-H)
ν_{240}	1181.5347	1175.51153			Def(pyr)
ν_{241}	1197.5426	1190.47091			Phenyl δ(C-H)
ν_{242}	1224.7019	1215.85128			Breath (phenyl)
ν_{243}	1233.5443	1224.1145			Breath (pyr) + $\nu(C_m\text{-Ph})$
ν_{244}	1297.1700	1283.57272			Def(porph+phenyl)
ν_{245}	1308.8502	1294.48786			Def(porph+phenyl)
ν_{246}	1334.9541	1318.88196			Phenyl δ(C-H)
ν_{247}	1367.3438	1349.15013			$\nu(C_\alpha\text{-}C_\beta)$+def(porph)
ν_{248}	1381.2023	1362.1009			Sci (H-O-C)
ν_{249}	1424.9503	1402.98341			Def(pyr)
ν_{250}	1428.7368	1406.52189			Phenyl δ(C-H)+ Def(phenyl)
ν_{251}	1496.5166	1469.86211			$\nu(C_\beta\text{-}C_\beta)+\nu(C_\alpha\text{-}C_m)$
ν_{252}	1532.1697	1503.17993			Phenyl δ(C-H)+ Def(phenyl)
ν_{253}	1543.7643	1514.01509			$\nu(C_\beta\text{-}C_\beta+C_\alpha\text{-}C_m)+\nu(C_\alpha\text{-}C_m)$
ν_{254}	1587.4837	1554.87087			Phenyl δ(C-H)+ Def(phenyl)
ν_{255}	1637.9556	1602.03686			Phenyl δ(C-H)+ Def(phenyl)
ν_{256}	1764.8031	1720.57585			ν(C=O)
ν_{257}	3161.0758	3025.39269			Phenyl $\nu(C\text{-}H)_{as}$
ν_{258}	3163.1648	3027.34486			Phenyl $\nu(C\text{-}H)_{as}$
ν_{259}	3183.6046	3046.44585			Phenyl $\nu(C\text{-}H)_{as}$
ν_{260}	3189.1967	3051.67167			Phenyl $\nu(C\text{-}H)_{as}$
ν_{261}	3221.6041	3081.95638			Pyr $\nu(C\text{-}H)_{as}$
ν_{262}	3250.3883	3108.85522			Pyr $\nu(C\text{-}H)_{s}$
ν_{263}	3524.9453	3365.42873			Pyr $\nu(N\text{-}H)_{as}$

ν_{264}	3681.3771	3511.61425			ν(O-H) $_{as}$

Note: [a]B3LYP/6-311G** (d,p), b=0.9345*a+71.3674; [b]The ν,δ,γ denote stretching, in-plane bending and out-of-plane bending modes, respectively; pyr denotes pyrrole, porph denotes porphine ring. The subscripts s and as represent the symmetric and asymmetric modes, respectively. Symbols def, tors, sci and breath denote deformation (ip), torsion, scissor and breathing motion, respectively.

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