

Supporting Information

Structure characterization of [*N*-phenylamino(2-boronphenyl)-*R*-methyl]phosphonic acid by vibrational spectroscopy and density functional theory calculations

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Table 2 The calculated wavenumbers and potential energy distribution (PED, %) for the FT-Raman and FT-IR spectra of [PhN-(2-PhB(OH)₂)-R-Me]PO₃H₂^a

wavenumbers / cm ⁻¹			
Calc.	Exp.		Assignment
	FT – Raman	FT – IR	
412			$\delta_p(\text{bridge})(35)$, $\gamma_s(\text{bridge})$, $\gamma_{as}(\text{bridge})$
412			$\delta_{as}(\text{PO}_3)(37)$, $\gamma_{as}(\text{bridge})$, $\gamma_s(\text{bridge})$, $\delta_p(\text{bridge})$
415			$\gamma_{as}(\phi)(58)$, $\gamma_{as}(\text{bridge})$, $\gamma_s(\text{bridge})$
415			$\gamma_{as}(\phi)(68)$, $\delta_{as}(\text{PO}_3)$
417			$\delta_{as}(\text{PO}_3)(26)$, $\gamma_{as}(\text{bridge})$, $\gamma_{as}(\phi)$, $\gamma_s(\text{bridge})$, $\delta_p(\text{bridge})$
420			$\delta_p(\text{bridge})(38)$, $\gamma_s(\text{bridge})$, $\gamma_{as}(\text{bridge})$
449	432	430	$\gamma_{as}(\phi)_B(31)$, $\delta_{oop}(\text{CC}_L(\text{C}_a)\text{C})_{\phi B}$, $\delta_s(\text{C}_a\text{PO}_3)$, $\delta_p(\text{bridge})$
451	474		$\gamma_{as}(\phi)_B(29)$, $\delta_{oop}(\text{CC}_L(\text{C}_a)\text{C})_{\phi B}$, $\delta_s(\text{C}_a\text{PO}_3)$, $\gamma_{as}(\text{bridge})$
498			$\gamma_{as}(\text{bridge})(39)$, $\gamma_s(\text{bridge})$, $\delta_p(\text{bridge})$
499	490	491	$\delta_p(\text{bridge})$, $\gamma_s(\text{bridge})$, $\gamma_{as}(\text{bridge})$, $\delta_{oop}(\text{CC}_L(\text{C}_a)\text{C})_{\phi B}$
516			$\delta_{oop}(\text{CC}_L(\text{N})\text{C})_{\phi}(22)$, $\gamma_{as}(\phi)$, $\gamma_{as}(\text{bridge})$, $\gamma_s(\text{bridge})$
517			$\delta_{oop}(\text{CC}_L(\text{N})\text{C})_{\phi}(22)$, $\gamma_{as}(\phi)$, $\delta_p(\text{bridge})$, $\gamma_s(\text{bridge})$, $\gamma_{as}(\text{bridge})$
522			$\gamma_{as}(\text{bridge})(45)$, $\gamma_s(\text{bridge})$, $\delta_p(\text{bridge})$
531		533	$\delta_p(\text{bridge})$, $\gamma_s(\text{bridge})$, $\gamma_{as}(\text{bridge})$

539			$\delta_{\text{oop}}(\text{CLC}_{\text{B}(\text{OH})_2(\text{B})\text{C}})_{\phi\text{B}}(30), \gamma_{\text{as}}(\phi)_{\text{B}}, \delta_{\text{p}}(\text{bridge})$
541			$\gamma_{\text{as}}(\phi)_{\text{B}}(31), \delta_{\text{oop}}(\text{C}_{\text{L}}\text{C}_{\text{B}(\text{OH})_2(\text{B})\text{C}})_{\phi\text{B}}$
553	543		$\delta_{\text{p}}(\text{bridge})(48), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
563			$\gamma_{\text{as}}(\text{bridge})(27), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge}), \gamma_{\text{as}}(\phi)_{\text{B}}$
574			$\delta_{\text{p}}(\text{bridge})(49), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
579			$\delta_{\text{as}}(\phi)(26), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge})$
581	591	591	$\delta_{\text{p}}(\text{bridge})(36), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
599			$\gamma_{\text{as}}(\text{bridge})(50), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
616			$\delta_{\text{oop}}(\text{CBO}_2)(36), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
618			$\delta_{\text{oop}}(\text{CBO}_2)(44), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge})$
627	617	617	$\delta_{\text{as}}(\phi)(34), \delta_{\text{oop}}(\text{CBO}_2), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge})$
628			$\delta_{\text{oop}}(\text{CBO}_2)(38), \delta_{\text{as}}(\phi), \gamma_{\text{as}}(\text{bridge})$
659	635	636	$\delta_{\text{p}}(\text{bridge})(25), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge})$
660			$\delta_{\text{oop}}(\text{CBO}_2)(18), \gamma_{\text{as}}(\text{bridge}), \delta_{\text{as}}(\phi)_{\text{B}}, \delta(\text{C}_{\text{L}}\text{C}_{\alpha}(\text{P})\text{N}), \gamma_{\text{s}}(\text{bridge})$
696		688	$\delta_{\text{p}}(\text{bridge})(46), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
697			$\gamma_{\text{as}}(\text{bridge})(34), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
699			$\delta_{\text{p}}(\phi)(54), \delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}, \delta_{\text{p}}(\text{bridge})$
699			$\delta_{\text{p}}(\phi)(25), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
717		710	$\gamma_{\text{as}}(\text{bridge})(32), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
720	722		$\delta_{\text{p}}(\text{bridge})(49), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$

728			$\gamma(\text{C}_\alpha\text{PO}_3\text{H})(23), \gamma_{\text{as}}(\text{bridge}), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge}), \delta_{\text{p}}(\phi)_{\text{B}}$
732			$\delta_{\text{p}}(\text{bridge})(52), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
742			$\gamma_{\text{as}}(\text{bridge})(19), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\phi)_{\text{B}}$
746	745	742	$\delta_{\text{p}}(\text{bridge})(18), \delta_{\text{p}}(\phi)_{\text{B}}, \gamma_{\text{s}}(\text{bridge})$
760			$\delta_{\text{p}}(\phi)_{\text{B}}(30), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}_\text{B}(\text{OH})_2(\text{B})\text{C})_{\phi\text{B}}$
760			$\delta_{\text{p}}(\phi)_{\text{B}}(32), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}_\text{B}(\text{OH})_2(\text{B})\text{C})_{\phi\text{B}}, \delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}$
765			$\delta_{\text{p}}(\phi)_{\text{B}}(26), \delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}, \delta_{\text{oop}}(\text{C}_\text{L}\text{C}_\text{B}(\text{OH})_2(\text{B})\text{C})_{\phi\text{B}}$
768			$\delta_{\text{p}}(\text{bridge})(30), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
791			$\gamma_{\text{s}}(\text{bridge})(43), \gamma_{\text{as}}(\text{bridge}), \delta_{\text{s}}(\text{bridge}), \delta_{\text{as}}(\text{bridge})$
793	775	777	$\delta_{\text{oop}}(\text{CC}_\text{L}(\text{C}_\alpha)\text{C})_{\phi\text{B}}(36), \delta_{\text{p}}(\phi)_{\text{B}}, \delta_{\text{oop}}(\text{C}_\text{L}\text{C}_\text{B}(\text{OH})_2(\text{B})\text{C})_{\phi\text{B}}$
794			$\delta_{\text{oop}}(\text{CC}_\text{L}(\text{C}_\alpha)\text{C})_{\phi\text{B}}(36), \delta_{\text{p}}(\phi)_{\text{B}}, \delta_{\text{oop}}(\text{C}_\text{L}\text{C}_\text{B}(\text{OH})_2(\text{B})\text{C})_{\phi\text{B}}$
822	808	809	$\delta_{\text{p}}(\text{bridge})(43), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
823	826	827	$\nu(\text{PO})(12), \gamma_{\text{as}}(\text{bridge})$
830			$\delta_{\text{p}}(\text{bridge})(56), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
831			$\delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}(39), \delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}$
838			$\delta_{\text{p}}(\text{bridge})(62), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
843			$\nu(\text{PO})(38)$
852			$\delta_{\text{p}}(\text{bridge})(62), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
878			$\delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}}(12)$
880			$\delta_{\text{p}}(\text{bridge})(16), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}}, \delta_{\text{oop}}(\text{C}_\text{B}(\text{OH})_2\text{C}(\text{H})\text{C})_{\phi\text{B}},$

			$\gamma_s(\text{bridge})$
883			$\delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}}(14), \delta_{\text{oop}}(\text{CC}_\text{L}(\text{C}_\alpha)\text{C})_{\phi\text{B}},$ $\delta_{\text{oop}}(\text{C}_{\text{B}(\text{OH})_2}\text{C}(\text{H})\text{C})_{\phi\text{B}}, \delta_{\text{p}}(\phi)_\text{B}$
886	884	882	$\delta_{\text{p}}(\text{bridge})(35), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
893			$\delta_{\text{p}}(\text{bridge})(33), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
893			$\delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}(40), \delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}$
919	899	903	$\mathbf{v}(\text{PO})(30), \delta_{\text{oop}}(\text{CC}_\text{L}(\text{C}_\alpha)\text{C})_{\phi\text{B}}$
924		924	$\mathbf{v}(\text{PO})(22), \delta_{\text{p}}(\text{bridge})$
952	934		$\delta_{\text{oop}}(\text{C}_{\text{B}(\text{OH})_2}\text{C}(\text{H})\text{C})_{\phi\text{B}}(27), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}},$ $\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}, \gamma_{\text{as}}(\phi)_\text{B}$
952			$\delta_{\text{oop}}(\text{C}_{\text{B}(\text{OH})_2}\text{C}(\text{H})\text{C})_{\phi\text{B}}(27), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}},$ $\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}, \gamma_{\text{as}}(\phi)_\text{B}$
960			$\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}(54), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}$
960			$\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}(51), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}$
976			$\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}(69), \delta_{\text{p}}(\phi), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}$
976			$\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi}(65), \delta_{\text{oop}}(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}, \delta_{\text{p}}(\phi)$
987			$\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}(48), \delta_{\text{p}}(\phi)_\text{B}$
987	999	983	$\delta_{\text{oop}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}(48), \delta_{\text{p}}(\phi)_\text{B}$
998			$\delta_{\text{trig}}(\phi)(36), \rho_{\text{b}}(\text{POH}), \gamma_{\text{as}}(\text{bridge})$
998			$\delta_{\text{p}}(\text{bridge})(46), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
999	1008	998	$\delta_{\text{trig}}(\phi)(40), \delta_{\text{p}}(\text{bridge}), \rho_{\text{b}}(\text{POH}), \gamma_s(\text{bridge})$

1000			$\rho_b(\text{POH})(36), \delta_{\text{trig}}(\phi), \gamma_{\text{as}}(\text{bridge}), \gamma_s(\text{bridge})$
1003			$\delta_p(\text{bridge})(51), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1008			$\gamma_{\text{as}}(\text{bridge})(29), \gamma_s(\text{bridge}), \rho_r(\text{BO}(\text{H})\text{H})_{\text{bridge}}, \delta_p(\text{bridge})$
1036			$v(\text{CC})_{\phi}(44), \gamma_{\text{as}}(\text{bridge})$
1036	1031	1021	$v(\text{CC})_{\phi}(51)$
1045			$\gamma_{\text{as}}(\text{bridge})(41), \gamma_s(\text{bridge}), \delta_p(\text{bridge})$
1045		1042	$\delta_p(\text{bridge})(31), v(\text{CC})_{\phi\text{B}}, \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1064			$\gamma_{\text{as}}(\text{bridge})(53), \gamma_s(\text{bridge}), \delta_p(\text{bridge})$
1077			$\delta_p(\text{bridge})(35), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge}), \delta_{\text{trig}}(\phi)_{\text{B}}$
1082			$\gamma_{\text{as}}(\text{bridge})(29), v(\text{C}_{\alpha}\text{N}), \gamma_s(\text{bridge}), \delta_p(\text{bridge})$
1084	1074	1073	$v(\text{C}_{\alpha}\text{N})(14), \delta_p(\text{bridge})$
1106		1090	$\gamma_{\text{as}}(\text{bridge})(48), \gamma_s(\text{bridge}), \delta_p(\text{bridge})$
1108			$v(\text{C}_{\alpha}\text{N})(24)$
1112			$\gamma_{\text{as}}(\text{bridge})(51), \gamma_s(\text{bridge}), \delta_p(\text{bridge})$
1126			$\delta_p(\text{bridge})(36), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1142			$\rho_b(\text{POH})(31), \gamma_{\text{as}}(\text{bridge}), \delta_p(\text{bridge}), \gamma_s(\text{bridge})$
1143			$\delta_p(\text{bridge})(45), \gamma_s(\text{bridge}), \gamma_{\text{as}}(\text{bridge}), \rho_b(\text{POH})$
1165	1161	1162	$\rho_r(\text{CC}(\text{H})\text{C})_{\phi}(58), \delta_p(\text{bridge}), \gamma_s(\text{bridge})$
1165			$\rho_r(\text{CC}(\text{H})\text{C})_{\phi}(45), \gamma_{\text{as}}(\text{bridge}), \gamma_s(\text{bridge}), \delta_p(\text{bridge})$
1171			$\rho_r(\text{CC}(\text{H})\text{C})_{\phi\text{B}}(59), \rho_r(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}}$

1171	1181	1177	$\rho_r(\text{CC}(\text{H})\text{C})_{\phi\text{B}}(60), \rho_r(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi\text{B}}$
1180			$\gamma_{\text{as}}(\text{bridge})(55), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
1189			$\delta_{\text{p}}(\text{bridge})(28), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge}), \nu(\text{C}_\text{L}\text{C}_\alpha)$
1193			$\gamma_{\text{as}}(\text{bridge})(53), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
1193			$\rho_r(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}(26), \rho_r(\text{CC}(\text{H})\text{C})_{\phi}, \delta_{\text{p}}(\text{bridge})$
1194	1188	1189	$\rho_r(\text{C}_\text{L}\text{C}(\text{H})\text{C})_{\phi}(34), \rho_r(\text{CC}(\text{H})\text{C})_{\phi}$
1216		1206	$\nu(\text{P}=\text{O})(16), \rho_r(\text{C}_\text{L}\text{C}_\alpha(\text{H})\text{P}), \rho_r(\text{C}_\alpha(\text{H},\text{P})\text{N}),$ $\rho_r(\text{C}_\text{L}\text{C}_\alpha(\text{H},\text{P})\text{N})$
1220			$\delta_{\text{p}}(\text{bridge})(44), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1225			$\delta_{\text{p}}(\text{bridge})(51), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1234		1227	$\nu(\text{P}=\text{O})(46), \rho_r(\text{C}_\text{L}\text{C}_\alpha(\text{H})\text{P}), \rho_r(\text{C}_\alpha(\text{H},\text{P})\text{N}),$ $\rho_r(\text{C}_\text{L}\text{C}_\alpha(\text{H},\text{P})\text{N})$
1244	1242		$\delta_{\text{p}}(\text{bridge})(36), \gamma_{\text{s}}(\text{bridge}), \nu(\text{P}=\text{O}), \gamma_{\text{as}}(\text{bridge})$
1253			$\gamma_{\text{as}}(\text{bridge})(31), \gamma_{\text{s}}(\text{bridge}), \delta_{\text{p}}(\text{bridge})$
1255			$\delta_{\text{p}}(\text{bridge})(48), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1271		1264	$\delta_{\text{p}}(\text{bridge})(42), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1271			$\gamma_{\text{as}}(\text{bridge})(19), \gamma_{\text{s}}(\text{bridge}), \rho_r(\text{C}_\alpha(\text{H},\text{P})\text{N}), \rho_r(\text{C}_\text{L}\text{C}_\alpha(\text{H},\text{P})\text{N})$
1286		1285	$\delta_{\text{p}}(\text{bridge})(39), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1286			$\gamma_{\text{as}}(\text{bridge})(14), \nu(\text{C}_\text{L}\text{C}_{\text{B}(\text{OH})_2})_{\phi\text{B}}, \gamma_{\text{s}}(\text{bridge}), \rho_r(\text{C}_\text{L}\text{C}_\alpha(\text{H},\text{P})\text{N}),$ $\rho_r(\text{C}_\alpha(\text{H},\text{P})\text{N})$
1317			$\delta_{\text{p}}(\text{bridge})(49), \gamma_{\text{s}}(\text{bridge}), \gamma_{\text{as}}(\text{bridge})$
1321			$\gamma_{\text{as}}(\text{bridge})(14), \nu(\text{C}_\text{L}\text{C})_{\phi}, \gamma_{\text{s}}(\text{bridge})$

1321			$\delta_{\text{p(bridge)}}(\mathbf{35}), \gamma_{\text{s(bridge)}}, \gamma_{\text{as(bridge)}}$
1338			$\rho_{\text{r}}(\text{C}_{\text{L}}\text{C}_{\alpha}(\text{H},\text{P})\text{N})(20), \gamma_{\text{as(bridge)}}, \gamma_{\text{s(bridge)}}$
1339			$\rho_{\text{r}}(\text{C}_{\text{L}}\text{C}_{\alpha}(\mathbf{H},\mathbf{P})\mathbf{N})(\mathbf{30}), \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}_{\alpha}(\mathbf{H})\mathbf{P})$
1346			$\gamma_{\text{as(bridge)}}(32), \gamma_{\text{s(bridge)}}, \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}(\text{H})\text{C})_{\phi}, \delta_{\text{p(bridge)}}$
1346	1330	1330	$\delta_{\text{p(bridge)}}(\mathbf{26}), \gamma_{\text{s(bridge)}}, \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}(\mathbf{H})\mathbf{C})_{\phi}, \gamma_{\text{as(bridge)}}$
1349		1363	$\gamma_{\text{as(bridge)}}(38), \gamma_{\text{s(bridge)}}, \nu(\text{BO}), \delta_{\text{p(bridge)}}$
1363			$\delta_{\text{p(bridge)}}(\mathbf{50}), \gamma_{\text{as(bridge)}}, \gamma_{\text{s(bridge)}}$
1364			$\gamma_{\text{as(bridge)}}(53), \gamma_{\text{s(bridge)}}, \delta_{\text{p(bridge)}}$
1446	1428	1428	$\rho_{\text{r}}(\text{CC}(\mathbf{H})\mathbf{C})_{\phi}(\mathbf{36}), \nu(\text{CC})_{\phi}, \rho_{\text{r}}(\text{C}_{\alpha}\mathbf{N}(\mathbf{H})\mathbf{C}_{\text{L}})$
1449			$\rho_{\text{r}}(\text{CC}(\text{H})\text{C})_{\phi}(40), \nu(\text{CC})_{\phi}, \rho_{\text{r}}(\text{C}_{\alpha}\text{N}(\text{H})\text{C}_{\text{L}})$
1450			$\rho_{\text{r}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}(47), \nu(\text{C}_{\text{L}}\text{C})_{\phi\text{B}}, \nu(\text{CC})_{\phi\text{B}}$
1450		1450	$\rho_{\text{r}}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}(43), \nu(\text{CC})_{\phi\text{B}}, \nu(\text{C}_{\text{L}}\text{C})_{\phi\text{B}}$
1495			$\rho_{\text{r}}(\text{C}_{\text{B}}(\text{OH})_2\text{C}(\text{H})\text{C})_{\phi\text{B}}(16), \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}(\text{H})\text{C})_{\phi\text{B}}, \nu(\text{C}_{\text{L}}\text{C}_{\text{B}}(\text{OH})_2)_{\phi\text{B}},$ $\gamma_{\text{as(bridge)}}$
1496			$\delta_{\text{p(bridge)}}(21), \rho_{\text{r}}(\text{C}_{\text{B}}(\text{OH})_2\text{C}(\text{H})\text{C})_{\phi\text{B}}, \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}(\text{H})\text{C})_{\phi\text{B}}, \gamma_{\text{s(bridge)}},$ $\gamma_{\text{as(bridge)}}$
1510		1495	$\rho_{\text{r}}(\text{CC}(\mathbf{H})\mathbf{C})_{\phi}(\mathbf{28}), \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}(\mathbf{H})\mathbf{C})_{\phi}, \nu(\text{CC})_{\phi}$
1510			$\rho_{\text{r}}(\text{CC}(\text{H})\text{C})_{\phi}(29), \rho_{\text{r}}(\text{C}_{\text{L}}\text{C}(\text{H})\text{C})_{\phi}, \nu(\text{CC})_{\phi}$
1519	1509		$\rho_{\text{r}}(\text{C}_{\alpha}\mathbf{N}(\mathbf{H})\mathbf{C}_{\text{L}})(\mathbf{50})$
1526			$\rho_{\text{r}}(\text{C}_{\alpha}\text{N}(\text{H})\text{C}_{\text{L}})(56)$
1587	1588	1590	$\nu(\text{CC})_{\phi\text{B}}(\mathbf{40}), \nu(\text{C}_{\text{L}}\text{C}_{\text{B}}(\text{OH})_2)_{\phi\text{B}}, \rho_{\text{r}}(\text{CC}(\mathbf{H})\mathbf{C})_{\phi\text{B}}$

1587			$\nu(\text{CC})_{\phi\text{B}}(\mathbf{40}), \nu(\text{C}_\text{L}\text{C}_\text{B}(\text{OH})_2)_{\phi\text{B}}, \rho_\text{r}(\text{CC}(\text{H})\text{C})_{\phi\text{B}}$
1607			$\nu(\text{CC})_{\phi}(\mathbf{33}), \nu(\text{C}_\text{L}\text{C})_{\phi}$
1607			$\nu(\text{CC})_{\phi}(\mathbf{33}), \nu(\text{C}_\text{L}\text{C})_{\phi}$
1620	1606	1604	$\nu(\text{CC})_{\phi\text{B}}(\mathbf{30}), \nu(\text{C}_\text{L}\text{C})_{\phi\text{B}}$
1620			$\nu(\text{CC})_{\phi\text{B}}(\mathbf{18}), \nu(\text{C}_\text{L}\text{C})_{\phi\text{B}}$
1625		1635	$\nu(\text{CC})_{\phi}(\mathbf{42}), \delta_\text{as}(\phi)$
1625			$\nu(\text{CC})_{\phi}(\mathbf{42}), \delta_\text{as}(\phi)$
2938	2922	2924	$\nu(\text{C}_\alpha\text{H})(\mathbf{99})$
2938		2957	$\nu(\text{C}_\alpha\text{H})(\mathbf{99})$
3107	3056	3058	$\nu(\text{CH})_{\phi\text{B}}(\mathbf{91})$
3107			$\nu(\text{CH})_{\phi\text{B}}(\mathbf{91})$
3116			$\nu(\text{CH})_{\phi\text{B}}(\mathbf{89})$
3116			$\nu(\text{CH})_{\phi\text{B}}(\mathbf{89})$
3118			$\nu(\text{CH})_{\phi}(\mathbf{97})$
3118			$\nu(\text{CH})_{\phi}(\mathbf{97})$
3126			$\nu(\text{CH})_{\phi}(\mathbf{98})$
3126			$\nu(\text{CH})_{\phi}(\mathbf{98})$
3130			$\nu(\text{CH})_{\phi\text{B}}(\mathbf{92})$
3130			$\nu(\text{CH})_{\phi\text{B}}(\mathbf{92})$
3145	3069		$\nu(\text{CH})_{\phi}(\mathbf{67}), \nu(\text{CH})_{\phi\text{B}}$

3145		v(CH)_φ(74), v(CH)_{φB}
3145		v(CH)_{φB}(75), v(CH)_φ
3145		v(CH)_{φB}(66), v(CH)_φ
3177		v(CH)_φ(97)
3177		v(CH)_φ(97)
3180		v(CH)_φ(97)
3180		v(CH)_φ(97)
3398		v(NH)(96)
3405	3482	v(NH)(96)
3424		v(OH)_{POH}(83), v(OH)_{BOHbridge}
3430		v(OH)_{POH}(67), v(OH)_{BOHbridge}
3467		v(OH)_{BOHbridge}(73), v(OH)_{POH}
3500	3503	v(OH)_{BOHbridge}(83), v(OH)_{POH}
3778		v(OH)_{POH}(100)
3778		v(OH)_{POH}(100)
3791		v(OH)_{BOH}(99)
3791		v(OH)_{BOH}(98)

^aAbbreviations: v, stretching; ρ_r, rocking; δ, deformation; γ, torsion; p, puckering; δ_{trig}, trigonal deformation; s, symmetric; as, antisymmetric; oop, out-of-plane vibrations; φ, aromatic ring; B, phenylboronic acid ring; bridge, hydrogen bonds [(HOBO)₂]; C_L, carbon atom of the aromatic ring connected to the aliphatic chain; C_α, tetrahedral carbon atom; bold, vibrations related to band with Raman Intensity > 0.4 [%]

