Supporting Information

Influence of Substituent Type and Position on the Adsorption Mechanism of Phenylboronic Acids: Infrared, Raman, and Surface-Enhanced Raman Spectroscopy Studies

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FT-IR measurements

FT- IR spectra were collected for thin pellets which contain 200 mg KBr and about 1 mg of each phenylboronic acids. Each of the investigated compound's samples were dispersed in KBr at room temperature. The Bruker spectrometer (EQUINOX 55) equipped with a DT-GS detector and Nernst rod as a excitation source was used to perform the FT-IR measurements.

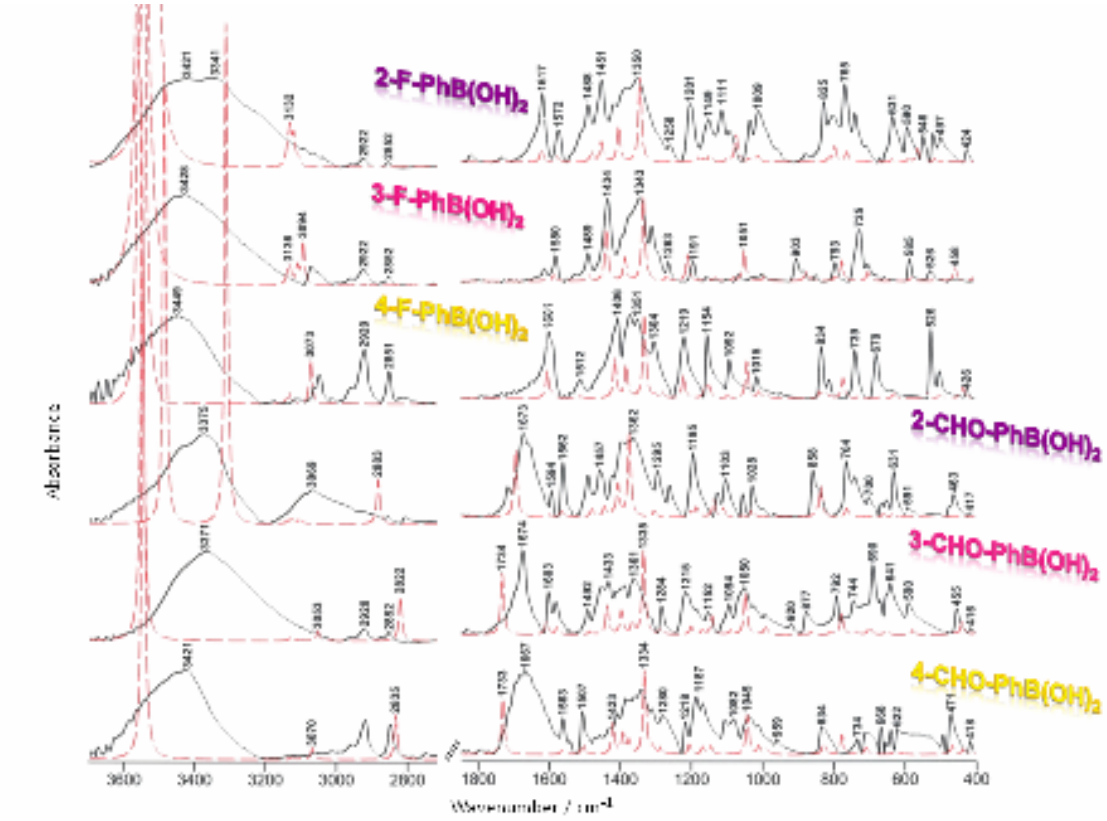

Figure S1 The experimental (black solid line) and theoretical (red dashed line) FT-IR spectra of the investigated phenylboronic acid analogues in the spectral range of 3650 – 400 cm^{-1}.

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Table S1 The calculated wavenumbers and potential energy distribution (PED, %) for the FT-Raman and FT-IR spectra of the investigated fluorophenylboronic acid analogues

calculated wavenumbers / cm^{-1}			Assignment		experimental wavenumbers / cm^{-1}					
					2-F-PhB$(OH)_2$		3-F-PhB$(OH)_2$		4-F-PhB$(OH)_2$	
2-F-PhB $(OH)_2$	3-F-PhB $(OH)_2$	4-F-PhB $(OH)_2$	B3LYP/6-311G(d,p) (PED %; > 5%)	Literature [36, 66,67,70-76]	FT-IR	FT-Raman	FT-IR	FT-Raman	FT-IR	FT-Raman
		398	$\gamma_{as}(_{bridge})(38)$, $\gamma_{s}(_{bridge})$, $\gamma_{as}(\phi)$, $\delta_{p}(_{bridge})$							
	406		**$\gamma_{as}(\phi)(34)$, $\delta_{oop}(BO(H)H)_{bridge}$, $\delta_{p}(_{bridge})$, $\delta_{oop}(CC_L(B)C)_{\phi}$, $\gamma_{as}(_{bridge})$**							
	408	403	**$\delta_{p}(_{bridge})(38)$, $\gamma_{s}(_{bridge})$, $\gamma_{as}(\phi)$, $\gamma_{as}(_{bridge})$**							
421		425	**$\gamma_{as}(_{bridge})(28)$, $\gamma_{s}(_{bridge})$, $\delta_{oop}(BO(H)H)_{bridge}$, $\gamma_{as}(\phi)$**	γ(OBCC), γ(HOBC)	424	427			426	
422		435	**$\delta_{p}(_{bridge})(42)$, $\gamma_{s}(_{bridge})$, $\delta_{oop}(BO(H)H)_{bridge}$, $\gamma_{as}(_{bridge})$**							
		445	$\delta_{p}(_{bridge})(20)$, $\rho_{r}(CC_F(F)C)_{\phi}$, $\rho_{r}(OB(C_L)O)$, $\gamma_{s}(_{bridge})$, $\rho_{r}(CC_L(B)C)_{\phi}$							
		452	$\delta_{p}(_{bridge})(26)$, $\gamma_{as}(_{bridge})$, $\rho_{r}(OB(C_L)O)$, $\rho_{r}(CC_F(F)C)_{\phi}$, $\gamma_{s}(_{bridge})$							
	453		**$\gamma_{s}(_{bridge})(47)$, $\gamma_{as}(_{bridge})$, $\delta_{oop}(BO(H)H)_{bridge}$**							

	457		**$\rho_r(CC_F(F)C)_\phi$(31), $\rho_r(CC_L(B)C)_\phi$, $\rho_r(OB(C_L)O)$**							
	458 461		$\delta_p(_{bridge})$(42), $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							
480			**$\rho_r(C_LC_F(F)C)_\phi$(34), $\delta_{as}(_{bridge})$, $\rho_r(OB(C_L)O)$, $\rho_r(CC_L(B)C_F)_\phi$**	γ(FCC)	497	492				
491			$\rho_r(C_LC_F(F)C)_\phi$(36), $\rho_r(CC_L(B)C_F)_\phi$, $\delta_{as}(_{bridge})$, $\rho_r(OB(C_L)O)$							
		498	**$\gamma_{as}(_{bridge})$(40), $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$**							
		499 506	**$\delta_p(_{bridge})$(47), $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**	δ(OBO), δ(CBO)					502	499
	504		**$\gamma_s(_{bridge})$(51), $\delta_{oop}(CC_F(F)C)_\phi$, $\gamma_{as}(_{bridge})$**							
510			$\delta_{oop}(C_LC_F(F)C)_\phi$(35), $\gamma_{as}(\phi)$, $\delta_{oop}(BO(H)H)_{bridge}$	Phe(ν_{6a}), δ(FCC)	518	521	526	522	526	
	517		**$\delta_p(_{bridge})$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
	519		$\delta_{as}(\phi)$(32), $\delta_p(_{bridge})$, $\gamma_s(_{bridge})$							
531			**$\delta_{as}(\phi)$(40), $\delta_{as}(_{bridge})$, $\rho_r(C_LC_F(F)C)_\phi$, $\rho_r(CC_L(B)C_F)_\phi$**							
536			$\delta_{as}(\phi)$(42), $\delta_{as}(_{bridge})$, $\rho_r(CC_L(B)C_F)_\phi$							
	544	534	**$\delta_p(_{bridge})$(48), $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$**							
544			**$\gamma_{as}(_{bridge})$(40), $\gamma_s(_{bridge})$, $\delta_{oop}(BO(H)H)_{bridge}$, $\delta_p(_{bridge})$**	γ(HOBC), γ(HOBO)	546	545				

562			$\delta_p(_{bridge})(48)$, $\gamma_s(_{bridge})$, $\delta_{oop}(BO(H)H)_{bridge}$, $\gamma_{as}(_{bridge})$		590	578	585			
564			**$\delta_{as}(\phi)(38)$, $\delta_{as}(_{bridge})$**							
	580		**$\delta_p(_{bridge})(44)$, $\gamma_{as}(_{bridge})(33)$, $\gamma_s(_{bridge})(22)$**							
587			$\delta_{as}(_{bridge})(41)$, $\delta_{as}(\phi)$							
632		627	$\gamma_{as}(_{bridge})(42)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$	Phe(ν_{6b})	631				632	629
		628	**$\delta_p(_{bridge})(52)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$**							
634		634	$\delta_p(_{bridge})(47)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$							
	650		**$\gamma_{as}(_{bridge})(31)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$, $\delta_p(\phi)$, $\delta_{oop}(CC_F(F)C)_\phi$**							
		655	**$\delta_p(_{bridge})(40)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**				655	658		
		671	$\delta_p(_{bridge})(34)$, $\gamma_s(_{bridge})$, $\delta_{as}(_{bridge})$, $\gamma_{as}(_{bridge})$	ν(CB), γ(HOBO), γ(OBCC)	668				679	675
689			**$\delta_{as}(\phi)(40)$, $\nu(C_LB)$, $\nu(C_LC_F)_\phi$, $\delta_{as}(_{bridge})$**							
	694 699		**$\delta_p(_{bridge})(38)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**	γ(OBCC)			681			
698			$\delta_{as}(\phi)(30)$, $\delta_{as}(_{bridge})(13)$, $\nu(C_LB)(18)$, $\nu(C_LC_F)_\phi(10)$	Phe(ν_4), ν(CB)	708	700	703	698		
	702		**$\gamma_s(_{bridge})(38)$, $\delta_p(\phi)(22)$, $\gamma_{as}(_{bridge})(6)$, $\delta_{oop}(OB(C_L)O)(10)$**							
	703		$\delta_p(_{bridge})(41)$, $\gamma_s(_{bridge})$							

		722	$\gamma_{as}(_{bridge})(50)$, $\gamma_{s}(_{bridge})$, $\delta_{p}(_{bridge})$							
	727		**$\gamma_{s}(_{bridge})(71)$, $\gamma_{as}(_{bridge})$, $\delta_{p}(_{bridge})$**							
		729	$\delta_{p}(_{bridge})(45)$, $\gamma_{s}(_{bridge})$, $\gamma_{as}(_{bridge})$							
		731	**$\gamma_{as}(_{bridge})(49)$, $\gamma_{s}(_{bridge})$, $\delta_{p}(_{bridge})$**	γ(OBCC)			725		739	727
740			**$\gamma_{as}(_{bridge})(49)$, $\gamma_{s}(_{bridge})$, $\delta_{p}(_{bridge})$**	γ(OBCC), γ(FCCB)						
742			$\delta_{p}(_{bridge})(34)$, $\gamma_{s}(_{bridge})$, $\delta_{p}(\phi)$, $\gamma_{as}(_{bridge})$		737	741				
745			$\gamma_{as}(_{bridge})(53)$, $\gamma_{s}(_{bridge})$, $\delta_{p}(_{bridge})$							
760			$\delta_{oop}(CC(H)C)_{\phi}(51)$, $\delta_{oop}(C_{F}C(H)C)_{\phi}$, $\delta_{p}(_{bridge})$, $\gamma_{s}(_{bridge})$, $\delta_{oop}(CC(H)C_{L})_{\phi}$	Phe(ν_{11})	765					
761			$\gamma_{as}(_{bridge})(32)$, $\gamma_{s}(_{bridge})$, $\delta_{oop}(CC(H)C)_{\phi}$, $\delta_{p}(_{bridge})$, $\delta_{oop}(C_{F}C(H)C)_{\phi}$							
	775	772	**$\delta_{p}(_{bridge})(56)$, $\gamma_{s}(_{bridge})$, $\gamma_{as}(_{bridge})$**							
	794		$\delta_{oop}(C_{F}C(H)C)_{\phi}(26)$, $\delta_{oop}(CC(H)C)_{\phi}$, $\delta_{oop}(CC(H)C_{L})_{\phi}$, $\delta_{p}(\phi)$, $\delta_{p}(_{bridge})$, $\gamma_{s}(_{bridge})$							
794			**$\delta_{p}(_{bridge})(58)$, $\gamma_{s}(_{bridge})$, $\gamma_{as}(_{bridge})$**							
	795		$\delta_{p}(_{bridge})(34)$, $\gamma_{s}(_{bridge})$, $\delta_{oop}(C_{F}C(H)C)_{\phi}$, $\delta_{oop}(CC(H)C)_{\phi}$, $\delta_{oop}(CC(H)C_{L})_{\phi}$	ν(CB), ν(OB)	798		793	800		
		809	**$\delta_{p}(_{bridge})(27)$, $\gamma_{s}(_{bridge})$, $\delta_{oop}(C_{F}C(H)C)_{\phi}$, $\delta_{oop}(CC(H)C_{L})_{\phi}$**						812	809
		810	$\delta_{oop}(C_{F}C(H)C)_{\phi}$, $\delta_{oop}(CC(H)C_{L})_{\phi}$							

811			**$\nu(C_FF)_\phi(27)$, $\delta_{as}(\phi)$, $\delta_{trig}(\phi)$**	ν(CF)	825	824				
		820	**$\nu(C_FC)_\phi(24)$, $\nu(C_FF)_\phi$, $\delta_{as}(\phi)$**							822
		837	$\delta_{oop}(C_FC(H)C)_\phi(45)$, $\delta_{oop}(CC(H)C_L)_\phi$, $\delta_{oop}(CC_F(F)C)_\phi$, $\gamma_{as}(\phi)$	Phe(ν_{10a})			848	845	834	
	859		$\delta_{oop}(C_LC(H)C_F)_\phi(66)$, $\delta_p(\phi)$							
862			$\delta_{oop}(C_FC(H)C)_\phi(41)$, $\delta_{oop}(CC(H)C_L)_\phi$, $\delta_{oop}(CC(H)C)_\phi$, $\delta_p(\phi)$							
	878		$\nu(C_FF)_\phi(20)$,$\delta_p(_{bridge})$	γ(HCCF), γ(HCCB)	875		884			
	910		$\delta_{oop}(C_FC(H)C)_\phi(47)$, $\delta_{oop}(CC(H)C_L)_\phi$	Phe(ν_{17b})			903			
		923	$\delta_{oop}(CC(H)C_L)_\phi(40)$, $\delta_{oop}(C_FC(H)C)_\phi$, $\delta_p(\phi)$							
953			$\delta_{oop}(CC(H)C)_\phi(42)$, $\delta_{oop}(CC(H)C_L)_\phi$, $\delta_{oop}(C_FC(H)C)_\phi$	Phe(ν_5), (ν_{17a})	955				948	
		969	$\delta_{oop}(CC(H)C_L)_\phi(57)$, $\delta_{oop}(C_FC(H)C)_\phi$							
	973		$\delta_{oop}(CC(H)C)_\phi(43)$, $\delta_{oop}(CC(H)C_L)_\phi$							
	978		$\delta_p(_{bridge})(48)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							
981			$\delta_{oop}(CC(H)C)_\phi(49)$, $\delta_{oop}(CC(H)C_L)_\phi$, $\delta_p(\phi)$							
		987	$\rho_r(BO(H)H)_{bridge}(48)$, ν(BO)							
	991		$\delta_p(_{bridge})(37)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							

	995		**$\delta_{trig}(\phi)(56)$**	Phe(ν_{12})	1009	997	1000	1001		
1001			**$\nu(BO)(33)$, $\delta_{trig}(\phi)$, $\delta_{as}(_{bridge})$, $\rho_r(BO(H)H)_{bridge}$, $\delta_{trig}(_{bridge})$**							
		1009	$\delta_{trig}(\phi)(28)$, $\delta_p(_{bridge})$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							
		1010	**$\delta_{trig}(\phi)(48)$, $\nu(C_FC)_\phi$**	Phe(ν_{12})					1015	1012
1010			$\nu(BO)(34)$, $\delta_{trig}(\phi)$, $\rho_r(BO(H)H)_{bridge}$							
1032			**$\nu(CC)_\phi(62)$, $\rho_r(C_FC(H)C)_\phi$**	Phe(ν_{18a})	1033	1034				1020
	1049	1042	**$\delta_p(_{bridge})(40)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
	1070		$\delta_p(_{bridge})(33)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							
1071			$\delta_s(_{bridge})(42)$, $\delta_{as}(_{bridge})$, $\rho_r(BO(H)H)_{bridge}$	δ(BOH)		1068	1067			
	1079		$\delta_p(_{bridge})(44)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							
1085			**$\delta_{trig}(\phi)(30)$, $\rho_r(BO(H)H)_{bridge}$, $\delta_{trig}(_{bridge})$**							
		1085	**$\rho_r(BO(H)H)_{bridge}(24)$, $\nu(BO)$, $\delta_p(_{bridge})$**	δ(BOH)	1090	1089	1095		1092	1097
1093			$\delta_{trig}(\phi)(16)$, $\nu(CC)_\phi$, $\delta_s(_{bridge})$, $\delta_{as}(_{bridge})$							
		1097	**$\rho_r(C_FC(H)C)_\phi(38)$, $\nu(CC)_\phi$, $\rho_r(CC(H)C_L)_\phi$, $\delta_p(_{bridge})$**							
	1100		**$\rho_r(BO(H)H)_{bridge}(18)$, $\nu(BO)$, $\rho_r(C_LC(H)C_F)_\phi$**							
1118			**$\rho_r(BO(H)H)_{bridge}(22)$, $\rho_r(C_FC(H)C)_\phi$**		1111	1117				
	1131		**$\delta_p(_{bridge})(45)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							

1145			$\delta_s(_{bridge})(16)$, $\rho_r(C_FC(H)C)_\phi$, $\delta_{as}(_{bridge})$							
		1148	$\delta_p(_{bridge})(40)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$							
	1154		**$\delta_p(_{bridge})(47)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
1156			**$\rho_r(CC(H)C)_\phi(58)$, $\nu(CC)_\phi$**		1149	1153				
		1158	**$\delta_p(_{bridge})(35)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$**							
		1159	$\rho_r(C_FC(H)C)_\phi(32)$, $\nu(C_FF)_\phi$, $\rho_r(CC(H)C_L)_\phi$, $\delta_p(_{bridge})$	Phe(ν_{9b})		1153	1155	1160	1154	1161
	1160 1169		**$\delta_p(_{bridge})(48)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
1163			$\rho_r(CC(H)C)_\phi(38)$, $\delta_s(_{bridge})$, $\delta_{as}(_{bridge})$							
1175			**$\nu(C_FF)_\phi(32)$, $\delta_{trig}(_{bridge})$, $\delta_{as}(_{bridge})$, $\rho_r(CC(H)C)_\phi$**							
1178			$\nu(C_FF)_\phi(38)$, $\delta_{trig}(\phi)$, $\rho_r(CC(H)C)_\phi$, $\nu(CC)_\phi$	Phe(ν_{9a})	1201	1195	1191			
		1180	**$\delta_p(_{bridge})(48)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
1195			**$\delta_{trig}(_{bridge})(38)$, $\delta_{as}(_{bridge})$, $\rho_r(BO(H)H)_{bridge}$**							
	1208		**$\delta_p(_{bridge})(48)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
		1221	**$\nu(C_FF)_\phi(47)$, $\rho_r(CC(H)C_L)_\phi$, $\nu(CC)_\phi$, $\delta_{trig}(\phi)$**	Phe(ν_{7a})					1219	1217
1247			**$\rho_r(CC(H)C_L)_\phi(24)$, $\delta_{trig}(_{bridge})$, $\rho_r(C_FC(H)C)_\phi$, $\nu(CC_L)_\phi$**			1236				
1254			$\rho_r(CC(H)C_L)_\phi(28)$, $\rho_r(C_FC(H)C)_\phi$, $\nu(CC_L)_\phi$	Phe(ν_3)	1258	1250	1263	1264		1264
	1266	1273	**$\delta_p(_{bridge})(38)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							

		1282	$\delta_p(_{bridge})(15)$, $\nu(CC_L)_\phi$, $\gamma_{as}(_{bridge})$							
1301			**$\nu(CC)_\phi(27)$, $\nu(C_LC_F)_\phi$, $\nu(C_FC)_\phi$, $\nu(CC_L)_\phi$**							
		1301	**$\delta_p(_{bridge})(26)$, $\rho_r(CC(H)C_L)_\phi$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
		1302	$\rho_r(CC(H)C_L)_\phi(36)$, $\rho_r(C_FC(H)C)_\phi$, $\nu(C_FC)_\phi$							
	1304		**$\delta_p(_{bridge})(47)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**	ν(BO), δ(BOH)					1304	1298
1302	1315		$\nu(CC)_\phi(26)$, $\rho_r(C_LC(H)C_F)_\phi$, $\rho_r(C_FC(H)C)_\phi$, $\nu(C_LC_F)_\phi$, $\nu(C_LC)_\phi$, $\rho_r(CC(H)C_L)_\phi$	Phe(ν_{14})			1310			
1316			**$\delta_{trig}(_{bridge})(26)$, ν(BO), $\delta_{as}(_{bridge})$**							
	1316 1333	1308 1331	**$\delta_p(_{bridge})(39)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
1342			$\delta_s(_{bridge})(32)$, ν(BO), $\nu(C_LB)$, $\delta_{as}(_{bridge})$	ν(BO), ν (BC), δ(BOH), $\nu_s(BO_2)$	1350	1347	1343	1341	1351	1348
	1382		**$\delta_p(_{bridge})(46)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
		1383	$\nu(CC)_\phi(26)$, ν(BO), $\delta_p(_{bridge})$							
		1384	**$\delta_p(_{bridge})(32)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
	1385	1406	ν(BO)(18), $\delta_p(_{bridge})$, $\gamma_s(_{bridge})$							
1396			**ν(BO)(47), $\delta_{trig}(_{bridge})$, $\nu(C_LB)$**	ν(BO)	1383	1370	1380		1372	1372

1402			ν(BO)(47), $\rho_r(CC_L(B)C_F)_\phi$	$\nu_{as}(BO_2)$	1416				1406	
		1415	ν(BO)(38)							
	1433		**$\delta_p(_{bridge})$(33), $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
	1437		ν(BO)(21), $\nu(CC_F)_\phi$, $\rho_r(C_FC(H)C)_\phi$				1434	1434		
1444			**$\rho_r(CC(H)C)_\phi$(44), $\nu(C_FC)_\phi$, $\nu(CC)_\phi$**							
1451			$\rho_r(CC(H)C)_\phi$(38), ν(BO)	ν(BO)	1451	1446			1456	
1479			**$\rho_r(CC(H)C_L)_\phi$(18), $\rho_r(C_FC(H)C)_\phi$, $\nu(C_LC_F)_\phi$, $\rho_r(CC(H)C)_\phi$**	Phe(ν_{19a})	1488	1484	1489			
	1487		**$\rho_r(CC(H)C)_\phi$(20), $\nu(CC)_\phi$, $\rho_r(CC(H)C_L)_\phi$, $\nu(CC_L)_\phi$, $\rho_r(C_LC(H)C_F)_\phi$, $\delta_p(_{bridge})$, $\nu(C_FC)_\phi$**							
		1511	**$\rho_r(CC(H)C_L)_\phi$(24), $\rho_r(C_FC(H)C)_\phi$, $\nu(C_FC)_\phi$**				1526 1547		1512	1512
1574	1585	1590	**$\nu(CC)_\phi$(16), $\nu(C_FC)_\phi$, $\nu(CC_F)_\phi$, $\nu(C_LC)_\phi$, $\rho_r(CC(H)C)_\phi$, $\rho_r(C_FC(H)C)_\phi$, $\nu(C_LC_F)_\phi$**	Phe(ν_{8b})	1572	1569	1580		1591	
1620	1614	1606	**$\nu(CC_F)_\phi$(23), $\nu(CC)_\phi$, $\nu(C_LC_F)_\phi$, $\delta_{as}(\phi)$, $\nu(CC_L)_\phi$, $\nu(C_LC)_\phi$, $\rho_r(C_LC(H)C_F)_\phi$, $\rho_r(CC(H)C_L)_\phi$, $\nu(C_FC)_\phi$, $\delta_{as}(\phi)$**	Phe(ν_{8a})	1617	1616	1613	1616	1601	1600
		3073	$\nu(CH)_\phi$(98)	Phe(ν_2)						3055
	3094		**$\nu(CH)_\phi$(>93)**							
3107	3110		**$\nu(CH)_\phi$(>90)**			3072		3061		3067

3120		3121	**$\nu(CH)_{\phi}$(>86)**				
3131	3130	3134	**$\nu(CH)_{\phi}$(>89)**		3091	3075	3075
3138	3136	3136	**$\nu(CH)_{\phi}$(>89)**		3109		
3492	3520	3521	**$\nu(OH)_{BOHbrigde}$(>94)**	3341			
3746	3796	3798	**$\nu(OH)$(>97)**				

Abbreviations: ν, stretching; ρ_r, rocking; ρ_b, bending; ρ_s, scissoring; ρ_t, twisting; ρ_w, wagging; δ, deformation; γ, torsion; p, puckering; δ_{trig}, trigonal deformation; s, symmetric; as, antisymmetric; oop, out-of-plane; i.p., in-plane; ϕ, aromatic ring; bridge, HOBO···H hydrogen-bonds; C_F, the ring carbon atom bounded with the fluorine atom; C_L, the ring carbon atom bounded with the aliphatic chain; bold, vibrations with Raman Intensity > 0.4 [%]

Table S2 The calculated wavenumbers and potential energy distribution (PED, %) for the FT-Raman and FT-IR spectra of the investigated formylphenylboronic acid analogues

calculated wavenumbers / cm^{-1}			Assignment		experimental wavenumbers / cm^{-1}					
					2-CHO-PhB$(OH)_2$		3-CHO-PhB$(OH)_2$		4-CHO-PhB$(OH)_2$	
2-CHO-PhB$(OH)_2$	3-CHO-PhB$(OH)_2$	4-CHO-PhB$(OH)_2$	B3LYP/6-311G(d,p) (PED %; > 5%)	Literature [36, 66,67,70-76]	FT-IR	FT-Raman	FT-IR	FT-Raman	FT-IR	FT-Raman
		400	$\gamma_{as}(\phi)(69)$, $\delta_{oop}(BO(H)H)_{bridge}$							
		417	$\gamma_{as}(_{bridge})(30)$, $\rho_r(OB(C_L)O)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$							
418		428	$\delta_p(_{bridge})(34)$, $\gamma_{as}(_{bridge})$, $\gamma_{as}(\phi)$, $\gamma_s(_{bridge})$, $\delta_{oop}(CC_L(B)C_{CHO})_\phi$	δ(OBC)	417		416		418	
428			**$\rho_r(OB(C_L)O)(43)$, $\rho_r(CC_L(B)C_{CHO})_\phi$**			434				
		429	**$\delta_{oop}(BO(H)H)_{bridge}(37)$, $\gamma_{as}(\phi)$, $\delta_p(_{bridge})$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$**							
	434		**$\gamma_{as}(_{bridge})(32)$, $\gamma_s(_{bridge})$, $\delta_{oop}(BO(H)H)_{bridge}$, $\delta_p(_{bridge})$, $\gamma_{as}(\phi)$**							
		437	$\delta_p(_{bridge})(49)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$							
	441		$\delta_p(_{bridge})(24)$, $\delta_{oop}(BO(H)H)_{bridge}$, $\gamma_{as}(\phi)$, $\gamma_s(_{bridge})$							
451			$\rho_r(OB(C_L)O)(46)$, $\rho_r(CC_L(B)C_{CHO})_\phi$	δ(OBC),	463		455			

				δ(OBO), γ(HOBO), γ(HOBC), γ(CCBO)						
		465	**$\gamma_{s(bridge)}$(17), $\gamma_{as(bridge)}$, $\gamma_{as}(\phi)$, $\delta_{as(bridge)}$, $\delta_{p(bridge)}$**							
466			**$\delta_{as(bridge)}$(25), $\rho_r(C_LC_{CHO}(C)C)_\phi$, $\delta_{as}(\phi)$, $\nu(C_{CHO}C)$**		477	475	480	476	471	
469			$\rho_r(C_LC_{CHO}(C)C)_\phi$(22), $\delta_{s(bridge)}$, $\delta_{as}(\phi)$, $\nu(C_{CHO}C)$							
	475		**$\delta_{p(bridge)}$(45), $\gamma_{s(bridge)}$, $\gamma_{as(bridge)}$**							
	477	468	$\gamma_{as(bridge)}$(28), $\gamma_{s(bridge)}$, $\delta_{p(bridge)}$							
		469	$\gamma_{as}(\phi)$(33), $\delta oop(CC_{CHO}(C)C)_\phi$, $\delta_{oop}(BO(H)H)_{bridge}$, $\delta_{p(bridge)}$							
471		479	$\delta_{p(bridge)}$(50), $\gamma_{s(bridge)}$, $\gamma_{as(bridge)}$							
472			$\delta_{p(bridge)}$(31), $\gamma_{as(bridge)}$, $\gamma_{as}(\phi)$, $\delta_{oop}(CC_L(B)C_{CHO})_\phi$, $\gamma_{s(bridge)}$							
	540		**$\delta_{p(bridge)}$(41), $\gamma_{s(bridge)}$, $\delta_{as(bridge)}$, $\gamma_{as(bridge)}$**	δ(OBO), δ(CBO)					494	497
	578	580	$\gamma_{as(bridge)}$(35), $\gamma_{s(bridge)}$, $\delta_{as(bridge)}$, $\delta_{p(bridge)}$	γ(HOBC), γ(HOBO)	591	575	590	570		
570			**$\delta_{as(bridge)}$(46), $\delta_{as}(\phi)$**							

596			$\delta_s(_{bridge})(45)$, $\delta_{as}(\phi)$						
		605	$\delta_p(_{bridge})(52)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$						
634		627	$\gamma_{as}(_{bridge})(40)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$, $\delta_{oop}(OB(C_L)O)$, $\delta_p(\phi)$	Phe(ν_{6b})	631				622	631
635			$\delta_p(_{bridge})(56)$, $\gamma_s(_{bridge})$						
	648		$\gamma_{as}(_{bridge})(41)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$						
	649	629	$\delta_p(_{bridge})(39)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$	γ(HOBC), γ(HOBO)	650		641	649	640	646
		634	**$\delta_{as}(\phi)(74)$**						
	652		**$\delta_p(_{bridge})(47)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$**						656	
	653		$\gamma_{as}(_{bridge})(26)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$, $\delta_{as}(\phi)$						
659			**$\delta_{as}(\phi)(44)$, $\delta(C_{CHO}C(=O)H)$**	δ(BOH), γ(HOBO), γ(OBCC), δ(C=O)	666	662	671		668	
686			**$\delta_{as}(\phi)(26)$, $\delta(C_{CHO}C(=O)H)$, $\nu(C_LB)$, $\nu(C_LC_{CHO})_\phi$, $\delta_{as}(_{bridge})$**	γ(OBCC)	689		690			
694			$\delta_{as}(\phi)(18)$, $\nu(C_LB)$, $\delta_s(_{bridge})$, $\nu(C_LC_{CHO})_\phi$, $\delta(C_{CHO}C(=O)H)$	Phe(ν_4), ν(CB)	700	697			710	718
	699		$\delta_p(\phi)(24)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$						
	700		$\delta_p(_{bridge})(43)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$						

		704	**γ_{as}(bridge)(31), γ_{s}(bridge), δ_{p}(bridge), $\delta(C_{CHO}C(=O)H)$**							
		710	δ_{p}(bridge)(44), γ_{s}(bridge), γ_{as}(bridge)							
	728	729	**γ_{as}(bridge)(44), γ_{s}(bridge), δ_{p}(bridge)**							
		731	γ_{s}(bridge)(22), γ_{as}(bridge), $\delta_{p}(\phi)$, δ_{p}(bridge)							
		732	$\delta_{p}(\phi)$(43), δ_{p}(bridge), γ_{s}(bridge)							
	733		**$\delta(C_{CHO}C(=O)H)$(24), $\nu(C_{L}B)$, $\delta_{as}(\phi)$**							
	737		γ_{as}(bridge)(45), γ_{s}(bridge), δ_{p}(bridge)	γ(OBCC)	740		744	747		
745			δ_{p}(bridge)(25), γ_{as}(bridge), $\delta_{oop}(CC_{L}(B)C_{CHO})_{\phi}$, $\delta_{p}(\phi)$, γ_{s}(bridge), $\delta_{oop}(OB(C_{L})O)$						734	
762 787			δ_{p}(bridge)(49), γ_{as}(bridge), γ_{s}(bridge)	Phe(ν_{11})	764	771	772			
	778	778	δ_{p}(bridge)(56), γ_{s}(bridge), γ_{as}(bridge)	ν(CB), ν(OB)			792			
	808		$\delta_{oop}(CC(H)C)_{\phi}$(26), $\delta_{oop}(CC(H)C_{CHO})_{\phi}$, $\delta_{p}(\phi)$, $\delta_{oop}(CC(H)C_{L})_{\phi}$							
	809		δ_{p}(bridge)(33), γ_{s}(bridge), $\delta_{oop}(CC(H)C)_{\phi}$, $\delta_{oop}(CC(H)C_{CHO})_{\phi}$							
		825	**$\delta_{oop}(CC(H)C_{L})_{\phi}$(37), $\delta_{oop}(C_{CHO}C(H)C)_{\phi}$**	Phe(ν_{10a}), ρ_{w}(CHO)	838				834	840

		831	$\nu(C_{CHO}C)_{\phi}(19)$, $\nu(C_{CHO}C)$, $\delta(C_{CHO}C(=O)H)$, $\delta_{as}(\phi)$					
836			$\delta_p(_{bridge})(64)$, $\gamma_s(_{bridge})$					
843			$\delta_p(_{bridge})(50)$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$		858	859		
		848	$\delta_{oop}(C_{CHO}C(H)C)_{\phi}(47)$, $\delta_{oop}(CC(H)C_L)_{\phi}$					
850			**$\delta(C_{CHO}C(=O)H)(33)$, $\delta_{trig}(\phi)$, $\nu(C_{CHO}C)$, $\delta_{as}(\phi)$**					
852			$\delta_p(_{bridge})(64)$, $\gamma_s(_{bridge})$					
	862		**$\nu(CC_{CHO})\phi(16)$, $\nu(C_{CHO}C)$, $\delta_{as}(\phi)$**					
	863		$\nu(C_{CHO}C)(22)$, $\nu(CC_{CHO})_{\phi}$, $\delta_{as}(\phi)$					
	884		$\delta_{oop}(C_{CHO}C(H)C_L)_{\phi}(72)$, $\delta_p(\phi)$	γ(HCCB)			877	
892			$\delta_p(_{bridge})(56)$, $\gamma_s(_{bridge})$	Phe(ν_{17b})			920	
	954		$\delta_{oop}(CC(H)C_L)_{\phi}(44)$, $\delta_{oop}(CC(H)C_{CHO})$	Phe(ν_5), (ν_{17a})	965			959
967		963	$\delta_{oop}(CC(H)C)_{\phi}(30)$, $\delta_{oop}(CC(H)C_L)_{\phi}$, $\delta_{oop}(CC(H)C_{CHO})_{\phi}$, $\gamma_{as}(\phi)$, $\delta_p(\phi)$, $\delta_{oop}(CC_L(B)C_{CHO})_{\phi}$					
	977	976	$\delta_p(_{bridge})(35)$, $\gamma_s(_{bridge})$, $\rho_r(BO(H)H)_{bridge}$, $\gamma_{as}(_{bridge})$					

		983	$\delta_{oop}(CC(H)C_L)_\phi(41)$, $\delta_{oop}(C_{CHO}C(H)C)_\phi$							
	990	989	$\rho_r(BO(H)H)_{bridge}(31)$, $\delta_p(_{bridge})$, $\gamma_s(_{bridge})$							
	993		**$\delta_{trig}(\phi)(54)$**	Phe(ν_{12})	995	999	993	998		
	994		$\delta_{trig}(\phi)(36)$, $\rho_r(BO(H)H)_{bridge}$, $\nu(CC_L)_\phi$							
	999		$\delta_{oop}(CC(H)C)_\phi(36)$, $\delta_{oop}(CC(H)C_L)_\phi$, $\delta_{oop}(C_{CHO}C(=O)H)$							
1004			**$\delta_p(\phi)(17)$, $\delta_{oop}(CC(H)C_L)_\phi$, $\delta_{oop}(C_{CHO}C(=O)H$, $\delta_{oop}(CC(H)C)_\phi$**							
1007			$\delta_{oop}(CC(H)C_L)_\phi(39)$, $\delta_{oop}(CC(H)C)_\phi$, $\delta_{oop}(C_{CHO}C(=O)H)$, $\gamma_{as}(\phi)$							
	1009	1008	**$\delta_{oop}(C_{CHO}C(=O)H)(49)$, $\delta_{oop}(CC(H)C_{CHO})_\phi$, $\delta_{oop}(CC(H)C)_\phi$, $\delta_p(\phi)$**							
		1011	$\delta_p(_{bridge})(45)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$							
		1012	**$\delta_{trig}(\phi)(48)$**	Phe(ν_{12})					1014	1017
1029			**$\nu(BO)(26)$, $\delta_{trig}(\phi)$, $\nu(CC)_\phi$, $\delta_{as}(_{bridge})$**	Phe(ν_{18a})	1028	1033	1025	1027	1039	
		1044	$\delta_p(_{bridge})(53)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$							
	1048		$\gamma_{as}(_{bridge})(28)$, $\gamma_s(_{bridge})$, $\delta_{as}(_{bridge})$, $\delta_p(_{bridge})$							

1054			**$\nu(CC)_{\phi}(34)$, $\delta_{trig}(\phi)$, $\delta_{as}(_{bridge})$, $\rho_r(CC(H)C_L)_{\phi}$**		1055	1059	1050			
	1078		**$\nu(CC)_{\phi}(24)$, $\rho_r(CC(H)C_{CHO})_{\phi}$**					1077		
		1087	**$\rho_r(BO(H)H)_{bridge}(24)$, $\nu(BO)$, $\delta_p(_{bridge})$**	δ(BOH)			1094		1082	1081
	1088		$\nu(CC)_{\phi}(24)$, $\rho_r(CC(H)C_{CHO})_{\phi}$, $\gamma_{as}(_{bridge})$, $\gamma_s(_{bridge})$, $\delta_s(_{bridge})$, $\delta_{as}(_{bridge})$							
		1107	$\delta_p(_{bridge})(26)$, $\gamma_s(_{bridge})$, $\rho_r(C_{CHO}C(H)C)_{\phi}$							
	1108		**$\rho_r(BO(H)H)_{bridge}(18)$, $\nu(BO)$**		1103	1113				
		1108	**$\nu(CC)_{\phi}(31)$, $\rho_r(C_{CHO}C(H)C)_{\phi}$, $\rho_r(CC(H)C_L)_{\phi}$**							
1110			**$\nu(CC)_{\phi}(12)$, $\delta_{as}(_{bridge})$, $\delta_{trig}(_{bridge})$**							
1111			$\delta_{as}(_{bridge})(17)$, $\delta_s(_{bridge})$, $\nu(CC)_{\phi}$							
1137			$\delta_{as}(_{bridge})(51)$, $\delta_s(_{bridge})$	δ(BOH)	1126					
	1142		$\gamma_{as}(_{bridge})(18)$, $\delta_s(_{bridge})$, $\gamma_s(_{bridge})$, $\delta_{as}(_{bridge})$, $\delta_p(_{bridge})$							
1153			**$\delta_{trig}(_{bridge})(29)$, $\delta_{as}(_{bridge})$, $\nu(C_LB)$**							
	1159	1146	**$\delta_p(_{bridge})(38)$, $\gamma_s(_{bridge})$, $\delta_{trig}(_{bridge})$, $\delta_{as}(_{bridge})$, $\gamma_{as}(_{bridge})$**							
		1167	**$\gamma_{as}(_{bridge})(43)$, $\gamma_s(_{bridge})$, $\delta_p(_{bridge})$**							

1168	1168		**ρ_r(CC(H)C)$_\phi$(56), ρ_r(CC(H)C$_{CHO}$)$_\phi$**	Phe(ν_{9b})		1157	1152	1163		
		1169	**δ_p($_{bridge}$)(29), γ_s($_{bridge}$), ρ_r(C$_{CHO}$C(H)C)$_\phi$, γ_{as}($_{bridge}$)**							
	1171		**δ_p($_{bridge}$)(20), ρ_r(CC(H)C)$_\phi$, γ_s($_{bridge}$), (CC(H)C$_L$)$_\phi$**			1170			1170	1172
		1179	**γ_{as}($_{bridge}$)(49), γ_s($_{bridge}$), δ_p($_{bridge}$)**							
1185			**ν(C$_{CHO}$C)(36), ν(CC$_{CHO}$)$_\phi$, δ_{trig}(ϕ)**	Phe(ν_{9a}), ν(C-CHO)	1195	1193	1187	1187	1187	
1198			ρ_r(BO(H)H)$_{bridge}$(34), ν(C$_L$B)(24), ν(BO)(10)							
	1200		ν(C$_{CHO}$C)(16), γ_{as}($_{bridge}$), δ_s($_{bridge}$), γ_s($_{bridge}$), δ_p($_{bridge}$)							
	1205		**δ_p($_{bridge}$)(39), γ_s($_{bridge}$), δ_{trig}($_{bridge}$), γ_{as}($_{bridge}$)**							
		1207	ρr(CC(H)CL)$_\phi$(28), ν(C$_{CHO}$C), ν(CC)$_\phi$, δ_{trig}(ϕ)							
		1208	**ν(C$_{CHO}$C)(18), γ_{as}($_{bridge}$), γ_s($_{bridge}$), δ_p($_{bridge}$)**	Phe(ν_{7a})			1215		1218	1218
1258			**δ_{trig}($_{bridge}$)(17), ρ_r(CC(H)C$_L$)$_\phi$, ρ_r(CC(H)C$_{CHO}$)$_\phi$, ν(CC$_L$)$_\phi$, δ_{as}($_{bridge}$)**					1231		
1262			ρ_r(CC(H)C$_L$)$_\phi$(27), ν(CC$_L$)$_\phi$, ρ_r(CC(H)C$_{CHO}$)$_\phi$	Phe(ν_3)	1261	1263	1268			

1267			**ρ_r(BO(H)H)$_{bridge}$(34), δ_{trig}(bridge), δ_{as}(bridge)**					
		1276	γ_{as}(bridge)(39), γ_s(bridge), δ_p(bridge)					
	1282		**δ_p(bridge)(13), $\nu(C_LC)_\phi$, γ_s(bridge)**					
		1285	δ_p(bridge)(38), γ_s(bridge), γ_{as}(bridge)			1284		1280
1303	1286		**$\nu(C_LC_{CHO})_\phi$(24), $\nu(C_LC)_\phi$, $\nu(CC_L)_\phi$, $\nu(CC_{CHO})_\phi$, $\nu(CC)_\phi$**					
	1306		**δ_p(bridge)(30), γ_s(bridge), δ_{trig}(bridge)**	ν(BO), δ(BOH)	1295	1297		
		1308 1311	**γ_{as}(bridge)(38), γ_s(bridge), δ_p(bridge)**					
		1310	$\rho_r(CC(H)C_L)_\phi$(32), $\nu(C_{CHO}C)_\phi$	Phe(ν_{14})			1312	1312
	1325		$\rho_r(C_{CHO}C(H)C_L)_\phi$(20), $\rho_r(CC(H)C_{CHO})_\phi$, $\rho_r(CC(H)C_L)_\phi$, $\nu(CC)_\phi$					
	1326		**$\rho_r(C_{CHO}C(H)C_L)_\phi$(16), $\nu(CC)_\phi$, $\rho_r(CC(H)C_{CHO})_\phi$, δ_p(bridge)**					
		1332	δ_p(bridge)(52), γ_s(bridge), γ_{as}(bridge)					
1335	1334		**ν(BO)(25), δ_{trig}(bridge), δ_s(bridge), γ_{as}(bridge), γ_s(bridge), δ_p(bridge)**	ν(BO), ν(BC), δ(BOH), $\nu_s(BO_2)$		1336		1342	1342

	1366		$\rho_r(C_{CHO}C(=O)H)(28)$, $\rho_r(CC(H)C_L)_\phi$							
	1368		**$\rho_r(C_{CHO}C(=O)H)(24)$, $\delta_p(_{bridge})$, $\rho_r(CC(H)C_L)_\phi$, $\gamma_s(_{bridge})$, $\delta_{trig}(_{bridge})$**		1362		1361		1364	
1374			$\rho_r(BO(H)H)_{bridge}(32)$, $\delta_{as}(_{bridge})$, $\nu(BO)$							
		1377	$\nu(CC)_\phi(24)$, $\rho_r(C_{CHO}C(=O)H)$, $\delta_p(_{bridge})$, $\rho_r(CC(H)C_L)_\phi$, $\gamma_s(_{bridge})$							
		1378	**$\gamma_s(_{bridge})(11)$, $\gamma_{as}(_{bridge})$, $\rho_r(C_{CHO}C(=O)H)$, $\nu(CC)_\phi$, $\delta_p(_{bridge})$**							
1392			**$\nu(BO)(40)$, $\rho r(BO(H)H)_{bridge}$, $\delta_{trig}(_{bridge})$**				1388	1382	1385	
		1392	**$\gamma_{as}(_{bridge})(29)$, $\gamma_s(_{bridge})$, $\rho_r(C_{CHO}C(=O)H)$, $\nu(BO)$, $\delta_p(_{bridge})$**							
	1392 1397	1393	**$\rho_r(C_{CHO}C(=O)H)(30)$, $\nu(BO)$, $\delta_p(_{bridge})$, $\delta_{trig}(_{bridge})$, $\gamma_s(_{bridge})$**							
1406		1414	**$\nu(BO)(16)$, $\rho_r(C_{CHO}C(=O)H)$, $\gamma_s(_{bridge})$, $\gamma_{as}(_{bridge})$**	$\nu(BO)$, $\nu_{as}(BO_2)$	1396		1398		1409	1407
1418			**$\rho_r(C_{CHO}C(=O)H)(70)$**							
		1421	$\nu(BO)(30)$, $\delta_p(_{bridge})$							
	1434		**$\nu(CC_{CHO})_\phi(14)$, $\nu(BO)$, $\rho_r(C_{CHO}C(=O)H)$**							
	1437		**$\nu(BO)(22)$, $\nu(C_{CHO}C)_\phi$, $\nu(CC_{CHO})_\phi$**		1457	1429	1433 1453	1431	1433 1459	

1440			$\rho_r(CC(H)C)_\phi(36)$, $\rho_r(C_{CHO}C(=O)H)$, $\nu(CC_{CHO})_\phi$							
1444			$\rho_r(CC(H)C)_\phi(30)$, $\rho_r(CC_L(B)C_{CHO})_\phi$							
	1485		$\rho_r(CC(H)C)_\phi(28)$, $\rho_r(C_{CHO}C(H)C_L)_\phi$, $\nu(CC)_\phi$, $\nu(CC_{CHO})_\phi$	Phe(ν_{19a})	1490	1489	1492			
1479		1506	**$\rho_r(CC(H)C_L)_\phi(18)$, $\nu(C_LC_{CHO})_\phi$, $\rho_r(CC(H)C_{CHO})_\phi$**				1523 1547		1507 1539	1505
1562	1578	1564	**$\nu(CC_{CHO})_\phi(24)$, $\nu(CC_L)_\phi$, $\nu(CC)_\phi$, $\rho_r(CC(H)C_{CHO})_\phi$, $\nu(C_LC_{CHO})_\phi$, $\rho_r(CC(H)C)_\phi$**	Phe(ν_{8b})	1562	1564	1579	1582	1563	1567
1597	1608	1614	**$\nu(CC)_\phi(32)$, $\nu(CC_{CHO})_\phi$, $\rho_r(C_{CHO}C(H)C_L)_\phi$, $\delta_{as}(\phi)$, $\nu(C_{CHO}C)_\phi$, $\nu(CC_L)_\phi$, $\rho_r(CC(H)C_L)_\phi$, $\rho_r(C_{CHO}C(H)C)_\phi$**	Phe(ν_{8a})	1594	1593	1603	1603		1611
1693	1733	1732	**$\nu(C=O)(>76)$**	$\nu(C=O)$	1673	1657	1674	1670	1667	1670
2883	2821	2834	**$\nu(CH)_{CHO}(99)$**	$\nu(CH)_{CHO}$		2810		2881		2835
3096	3053	3069	**$\nu(CH)_\phi(>93)$**	Phe(ν_2)		3034		3025		3006
3106	3108	3094	**$\nu(CH)_\phi(>90)$**					3051		3051
3124	3124		**$\nu(CH)_\phi(>86)$**							
3137	3130	3128	**$\nu(CH)_\phi(>89)$**			3067		3070		3067
3325			**$\nu(OH)(96)$**							

3445			**$\nu(OH)_{BOHbrigde}$(94)**	3375	3371
	3521	3518	**$\nu(OH)_{BOHbrigde}$(>94)**		
	3796	3794	**ν(OH)(>97)**		

Abbreviations: ν, stretching; ρ_r, rocking; ρ_b, bending; ρ_s, scissoring; ρ_t, twisting; ρ_w, wagging; δ, deformation; γ, torsion; p, puckering; δ_{trig}, trigonal deformation; s, symmetric; as, antisymmetric; oop, out-of-plane; i.p., in-plane; ϕ, aromatic ring; bridge, HOBO···H hydrogen-bonds; C_{CHO}, the ring carbon atom bonded with the formyl group; C_L, the ring carbon atom bonded with the aliphatic chain; bold, vibrations with Raman Intensity > 0.4 [%]