Supplementary Material

Interaction of Aromatic Compounds with Xenon: Spectroscopic and Computational Characterization for the Cases of *p*-Cresol and Toluene

Qian Cao,[1,2] Natalya Andrijchenko,[3] Alexander Ermilov,[3] Markku Räsänen,[1] Alexander Nemukhin,[3] Leonid Khriachtchev[1,a)]

[1] Department of Chemistry, P. O. Box 55, University of Helsinki, Helsinki, FI-00014, Finland

[2] School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, China

[3] Department of Chemistry, M. V. Lomonosov Moscow State University, Leninskie Gory 1/3, Moscow, 119991, Russia

Table S1. Vibrational frequencies (ω, in cm^{-1}), shifts ($\Delta\omega$, in cm^{-1}), assignment, and intensities (I, in $D^2Å^{-2}\,amu^{-1}$) of *p*-cresol-d3.

Assignment	Experiment	Calculation							
	Monomer	Monomer		π structure			H-bonded structure		
	ω	ω	I	ω	I	$\Delta\omega$	ω	I	$\Delta\omega$
$\delta(CCH)_{methyl}$ + $\delta(CCH)_{ring,\ oop}$		505.3	0.4	504.4	0.4	−0.9	505.5	0.4	+0.2
$\delta(CCC)_{ring}$		645.4	0.0	644.7	0	−0.7	645.3	0	−0.1
$\delta(CCH)_{methyl}$ + $\delta(CCH)_{ring,\ oop}$	679.5	688.6	0.2	687.4	0.2	−1.2	689.3	0.1	+0.7
$\nu(CC)_{ring}$ + $\nu(CC)_{methyl}$	711.5	724.0	0.2	724.8	0.1	+0.8	724.3	0.2	+0.2
$\delta(CCH)_{methyl}$ + $\delta(CCH)_{ring,\ oop}$	788.0	797.6	0.8	798.3	0.8	0.7	798.8	0.7	+1.2
$\delta(CCH)_{methyl}$		808.9	0.0	808.4	0	−0.5	808.9	0	0
$\delta(CCH)_{ring,\ oop}$		824.3	0.0	826.5	0	+2.2	825.7	0	+1.4
$\nu(CC)$	839.0	843.8	0.3	843.5	0.3	−0.3	843.8	0.3	0
$\delta(CCH)_{ring,\ oop}$ + $\delta(CCH)_{methyl}$	875.0	886.1	0.4	886.9	0.5	+0.9	886.7	0.3	+0.7

$\delta(CCH)_{ring,\ oop}$		947.0	0.0	947.4	0	+0.5	947.6	0	+0.6
$\delta(CCH)_{ring,\ oop}$		965.5	0.0	965.9	0	+0.4	965.2	0	−0.3
$\delta(CCH)_{methyl} + \nu(CC)_{ring}$		1032.2	0.0	1031.7	0	−0.5	1032	0	−0.2
$\delta(CCH)_{methyl} + \nu(CC)_{ring}$		1067.9	0.0	1067.1	0	−0.9	1068	0	0
$\delta(HCH)_{methyl}$	1054.2	1079.3	0.1	1079.3	0.1	0	1079.2	0.1	−0.1
$\delta(HCH)_{methyl}$	1083.0	1083.0	0.1	1081.2	0.1	−1.8	1083.2	0.1	+0.1
$\delta(CCH)_{ring}$	1106.5	1117.1	0.3	1117	0.3	−0.2	1117.2	0.3	+0.1
$\delta(CCH)_{ring}$	1161.5	1189.9	0.6	1189.5	0.6	−0.3	1189.6	0.3	−0.2
$\delta(CCH)_{ring} + \delta(COH)$	1178.5 1164.2	1193.9	3.3	1193.9	3.2	0	1200.8	3.3	+6.9
$\delta(CCH)_{ring} + \nu(CC)_{ring}$	1200.5	1265.7	0.1	1266.3	0.1	0.6	1265.6	0.1	−0.1
$\nu(CC)_{ring} + \nu(CO)$	1265.01258.8	1287.8	2.0	1288	1.8	+0.2	1288.6	2	+0.8
$\delta(CCH)_{ring} + \delta(COH)$	1330.8	1338.7	0.3	1337.9	0.2	−0.8	1339.3	0.2	+0.6
$\nu(CC)_{ring} + \delta(COH)$	1435.5 1430.5	1447.3	0.5	1448.5	0.6	+1.2	1447.9	0.5	+0.6
$\nu(CC)$	1463.0	1478.1	0.0	1483.2	0.0	+5.1	1478.7	0.0	+0.6

ν(CC)	1522.5 1510.0	1549.3	2.5	1548.7	2.4	−0.6	1549.2	2.8	−0.1
$\nu(CC)_{ring} + \delta$(COH)	1601.5 1600.0	1637.3	0.2	1635.9	0.2	−1.4	1636.3	0.2	−0.9
ν(CC)	1630.5 1623.7	1661.5	0.7	1660.2	0.6	−1.3	1661.1	0.8	−0.4
$\nu(CD)_{sym}$	2075.3 2065.0	2203.8	0.3	2201.5	0.3	−2.4	2203.7	0.4	−0.2
$\nu(CD)_{asym}$	2144.8 2140.0	2325.9	0.1	2322.4	0.2	−3.5	2325.7	0.1	−0.2
$\nu(CD)_{asym}$	2239.5 2217.0	2342.2	0.1	2342.9	0.1	+0.7	2341.7	0.1	−0.5
ν(CH)	3014.0 3017.3	3185.9	0.3	3184.7	0.3	−1.3	3189.8	0.3	+3.9
ν(CH)	3033.5	3194.7	0.2	3194.6	0.2	−0.1	3193.6	0.2	−1
ν(CH)	3042.6	3205.5	0.2	3203.8	0.2	−1.7	3206.6	0.2	+1.1
ν(CH)	3078.8	3227.1	0.1	3226.1	0.1	−0.9	3226.2	0.1	−0.9

	3066.5								
v(OH)	3661.5 3657.8	3824.7	1.7	3823.5	1.7	−1.1	3801.4	5.5	−23.3

Table S2. Vibrational frequencies (ω, in cm^{-1}), shifts ($\Delta\omega$, in cm^{-1}), assignment, and intensities (I, in $D^2Å^{-2}\,amu^{-1}$) of *p*-cresol.

Assignment	Experiment (monomer)	Calculation							
		Monomer		π structure			H-bonded structure		
	ω	ω	I	ω	I	$\Delta\omega$	ω	I	$\Delta\omega$
$\delta(CCH)_{ring,\ oop}$ + $\delta(CCH)_{methyl}$		512.0	0.48	511.1	0.51	–0.9	512.2	0.43	+0.2
$\delta(CCC)_{ring}$	688.2	648.0	0.01	647.3	0.01	–0.7	647.9	0.01	0.0
$\delta(CCH)_{ring,\ oop}$ + $\delta(CCH)_{methyl}$	730.4 740.4	711.6	0.04	711.0	0.04	–0.6	712.3	0.03	+0.6
$\nu(CC) + \nu(CO)$	750.5	753.6	0.21	754.1	0.18	+0.5	753.9	0.23	+0.3
$\delta(CCH)_{ring,\ oop}$	805.4	813.3	0.59	815.2	0.67	+2.0	816.1	0.49	+2.8
$\delta(CCH)_{ring,\ oop}$	812.7	834.9	0.58	835.4	0.56	+0.6	835.0	0.59	+0.1
$\nu(CC) + \nu(CO)$	821.4 841.6	849.8	0.22	849.6	0.22	–0.2	849.7	0.21	0.0
$\delta(CCH)_{ring,\ oop}$		933.8	0.00	935.1	0.01	+1.4	934.8	0.00	+1.0
$\delta(CCH)_{ring,\ oop}$		964.2	0.00	964.8	0.00	+0.5	964.1	0.00	–0.2

$\delta(CCH)_{methyl}$		1008.4	0.01	1008.5	0.01	+0.1	1008.3	0.01	–0.1
$\nu(CC)_{ring}$ + $\delta(CCH)_{methyl}$	1072.2	1034.3	0.03	1033.6	0.02	–0.7	1034.2	0.03	0.0
$\delta(CCH)_{methyl}$	1100.4	1061.9	0.06	1060.4	0.13	–1.4	1061.8	0.05	0.0
$\delta(CCH)_{ring}$	1118.4	1122.2	0.38	1122.2	0.31	0.0	1122.2	0.31	0.0
$\nu(CC)_{ring}$ + $\delta(CCH)_{ring}$	1151.7 1169.5	1189.8	0.58	1189.5	0.56	–0.4	1189.6	0.28	–0.3
$\nu(CC)_{ring}$ + $\delta(CCH)_{ring}$ + $\delta(CCH)_{methyl}$ + $\delta(COH)$	1172.5	1193.8	3.31	1193.8	3.23	0.0	1200.7	3.27	+6.9
$\nu(CC)$ + $\delta(CCH)_{ring}$		1246.0	0.08	1246.3	0.06	+0.3	1246.0	0.07	0.0
$\nu(CC)$ + $\delta(CCH)_{ring}$ + $\nu(CO)$	1261.9	1287.8	2.01	1287.9	1.92	+0.1	1288.6	2.02	+0.8
$\delta(CCH)_{ring}$ + $\delta(COH)$	1328.5 1338.5	1341.7	0.28	1341.0	0.25	–0.7	1342.3	0.18	+0.6

	1344.4								
$\delta(CCH)_{ring,\ sym}$		1412.9	0.00	1411.7	0.01	−1.1	1412.8	0.00	−0.1
$\nu(CC)_{ring}$ + $\delta(CCH)_{ring}$ + $\delta(COH)$	1428.4	1446.0	0.40	1446.6	0.42	+0.5	1446.6	0.34	+0.6
$\nu(CC)_{ring}$		1478.2	0.02	1483.1	0.01	+4.9	1478.8	0.04	+0.6
$\delta(CCH)_{ring,\ asym}$	1473.7	1498.7	0.14	1499.4	0.12	0.8	1498.4	0.14	−0.2
$\delta(CCH)_{ring,\ asym}$	1503.2	1512.7	0.29	1510.2	0.32	−2.5	1512.9	0.33	+0.2
$\nu(CC)_{ring}$ + $\delta(CCH)_{ring}$	1519.3 1525.6	1550.1	2.43	1549.4	2.37	−0.7	1550.0	2.71	0.0
$\nu(CC)_{ring}$ + $\delta(CCH)_{ring}$ + $\delta(CCH)_{methyl}$ + $\delta(COH)$	1603.0	1639.9	0.31	1638.6	0.24	−1.3	1638.9	0.28	−1.0
$\nu(CC)_{ring}$ + $\delta(CCH)_{ring}$ + $\delta(COH)$	1612.5	1662.1	0.63	1660.6	0.62	−1.4	1661.7	0.74	−0.4

$\nu(CH)_{methyl,\ sym}$	2884.0 2881.0	3065.4	0.70	3061.5	0.66	–4.0	3065.2	0.75	–0.2
$\nu(CH)_{methyl,\ asym}$	2941.1 2947.2	3141.6	0.25	3138.1	0.29	–3.5	3141.2	0.25	–0.3
$\nu(CH)_{methyl,\ asym}$	2984.5	3161.5	0.27	3162.1	0.24	0.5	3161.0	0.27	–0.6
$\nu(CH)_{ring}$	3017.6	3186.0	0.30	3184.7	0.26	–1.3	3189.8	0.28	+3.9
$\nu(CH)_{ring}$	3036.5	3194.7	0.20	3194.6	0.18	0.0	3193.7	0.22	–1.0
$\nu(CH)_{ring}$	3065.7	3205.6	0.22	3203.8	0.18	–1.7	3206.7	0.21	+1.1
$\nu(CH)_{ring}$	3078.3	3227.1	0.07	3226.1	0.05	–0.9	3226.2	0.07	–0.9
$\nu(OH)$	3656.5	3824.7	1.66	3823.5	1.66	–1.1	3801.4	5.51	–23.3

Table S3. Vibrational frequencies (ω), shifts ($\Delta\omega$, in cm^{-1}), assignment, of and intensities (I in $D^2Å^{-2}\,amu^{-1}$) toluene-d3.

Assignment	Experiment	Calculation				
	Monomer	Monomer		Complex		
	ω	ω	I	ω	I	$\Delta\omega$
$\delta(CCC)_{ring}$		499.8	0.01	499.7	0.01	–0.1
$\delta(CCC)_{ring}$		623.5	0.00	622.9	0.00	–0.6
$\delta(CCH)_{ring,\ oop} + \delta(CCD)_{methyl}$		697.1	0.01	695.7	0.00	–1.4
$\delta(CCH)_{ring,\ oop} + \delta(CCD)_{methyl}$	708.6	720.8	1.72	720.60	1.78	–0.2
$\delta(CCC)_{ring} + \nu(CC)_{ring\text{-}methyl}$		771.2	0.02	771.2	0.02	0.0
$\delta(CCD)_{asym}$		808.1	0.00	808	0.00	–0.1
$\delta(CCH)_{ring,\ oop}$		857.8	0.00	859	0.00	+1.2
$\delta(CCH)_{ring,\ oop} + \delta(CCD)_{methyl}$	844.5	859.2	0.09	860	0.11	+0.8
$\delta(CCH)_{ring,\ oop}$	927.4	941.3	0.10	940.8	0.10	–0.5
$\delta(CCH)_{ring,\ oop}$		976.5	0.00	978.7	0.00	+2.2
$\delta(CCH)_{ring,\ oop}$		999.9	0.00	1000.1	0.00	+0.2

$\delta(CCC)_{ring}$		1020.7	0.00	1020.7	0.00	0.0
$\delta(CCH)_{ring} + \delta(CCC)$	1028.0	1046.0	0.06	1045.4	0.03	–0.6
$\delta(CCD)_{methyl, sym} + \delta(CCH)_{ring}$	1056.5	1073.0	0.03	1072	0.04	–1.0
$\delta(DCD)_{methyl. asym}$	1075.0	1083.3	0.12	1082.3	0.09	–1.0
$\delta(DCD)_{methyl, sym}$	1094.5	1084.6	0.08	1083.8	0.06	–0.8
$\delta(CCH)_{ring} + \delta(CCD)_{methyl}$		1101.6	0.09	1101.5	0.08	–0.1
$\delta(CCH)_{ring}$		1175.4	0.00	1175.5	0.00	0.1
$\delta(CCH)_{ring}$		1199.1	0.00	1198.7	0.00	–0.4
$\delta(CCH)_{ring} + \nu(CC)_{ring, methyl} + \delta(CCD)_{methyl}$	1230.0	1265.9	0.03	1266.5	0.03	+0.6
$\delta(CCH)$	1300.5	1342.7	0.01	1342.3	0.02	–0.4
$\nu(CC)_{ring} + \delta(CCH)_{ring}$		1455.3	0.04	1459.7	0.06	+4.4
$\nu(CC)_{ring} + \delta(CCH)_{ring}$	1452.0	1477.7	0.07	1479.3	0.07	+1.6
$\nu(CC)_{ring} + \delta(CCH)_{ring}$	1505.51498.5	1524.9	0.27	1524.4	0.29	–0.5
$\nu(CC)_{ring} + \delta(CCH)_{ring}$	1604.1	1624.0	0.01	1622.8	0.01	–1.2
$\nu(CC)_{ring} + \delta(CCH)_{ring}$	1630.5	1648.3	0.14	1647.2	0.13	–1.1

$\nu(CD)_{sym}$	2066.0	2203.8	0.25	2201.1	0.24	–2.7
$\nu(CD)_{asym}$	2138.0	2325.8	0.13	2322	0.15	–3.8
$\nu(CD)_{asym}$	2217.3 2241.0	2343.9	0.14	2343.9	0.13	0.0
$\nu(CH)_{ring}$	3037.7	3191.1	0.15	3190.2	0.13	–0.9
$\nu(CH)_{ring}$	3039.9	3191.7	0.12	3190.6	0.10	–1.1
$\nu(CH)_{ring}$	3071.5	3207.1	0.07	3206.5	0.05	–0.6
$\nu(CH)_{ring}$	3096.2	3216.3	0.52	3215.4	0.44	–0.9
$\nu(CH)_{ring}$	3120.0	3229.0	0.24	3228.3	0.22	–0.7

Table S4. Vibrational frequencies (ω, in cm^{-1}), shifts (Δω, in cm^{-1}), assignment, of toluene and relative intensities (*I*, in $D^2Å^{-2}\,amu^{-1}$).

Assignment	Experiment	Calculation				
	Monomer	Monomer		Complex		
	ω	ω	I	ω	I	$\Delta\omega$
$\delta(CCC)_{ring}$		521.1	0.01	520.9	0.01	–0.2
$\delta(CCC)_{ring}$		624.3	0.00	623.6	0.00	–0.7
$\delta(CCH)_{ring,\,oop} + \delta(CCH)_{methyl}$	695.5	708.7	0.46	707.2	0.46	–1.5
$\delta(CCH)_{ring,\,oop} + \delta(CCH)_{methyl}$	730.6	741.3	1.30	741.1	1.36	–0.2
$\delta(CCC)_{ring} + \nu(CC)_{ring\text{-}methyl}$		800.3	0.01	800.6	0.02	+0.3
$\delta(CCH)_{ring\cdot oop}$		857.6	0.00	858.7	0.00	+1.1
$\delta(CCH)_{ring,\,oop} + \delta(CCH)_{methyl}$		911.5	0.02	912.2	0.02	+0.7
$\delta(CCH)_{ring,\,oop}$		976.5	0.00	978.7	0.00	+2.2
$\delta(CCH)_{ring,\,oop}$		999.8	0.00	1000.0	0.00	+0.2
$\delta(CCH)_{methyl} + \delta(CCC)_{ring}$		1007.3	0.01	1006.9	0.01	–0.4

$\delta(CCH)_{methyl} + \delta(CCC)_{ring}$.		1020.7	0.00	1020.6	0.00	–0.1
$\delta(CCH)_{methyl} + \delta(CCC)_{ring}$		1050.8	0.07	1050.4	0.06	–0.4
$\delta(CCH)_{methyl}$	1032.4	1064.8	0.13	1063.4	0.13	–1.4
$\delta(CCH)_{ring} + \delta(HCH)_{methyl}$	1083.5	1110.5	0.12	1110.5	0.10	0.0
$\delta(CCH)_{ring}$		1175.4	0.00	1175.4	0.00	0.0
$\delta(CCH)_{ring}$		1199.0	0.00	1198.6	0.00	–0.4
$\delta(CCH)_{ring} + \delta(HCH)_{methyl} + \nu(CC)_{ring,methyl}$		1245.2	0.02	1245.5	0.01	+0.3
$\delta(CCH)_{ring}$		1346.5	0.00	1346.0	0.00	–0.5
$\delta(CCH)_{methyl, sym}$	1384.5	1416.8	0.02	1415.3	0.04	–1.5
$\delta(CCH)_{ring} + \delta(HCH)_{methyl} + \nu(CC)_{ring}$		1453.6	0.00	1456.8	0.01	+3.2
$\delta(CCH)_{ring} + \delta(HCH)_{methyl} + \nu(CC)_{ring}$		1475.7	0.01	1478.0	0.02	+2.3
$\delta(CCH)_{methyl}$		1506.6	0.15	1505.4	0.12	–1.2
$\delta(CCH)_{ring} + \delta(HCH)_{methyl}$	1473.4	1514.0	0.28	1513.0	0.26	–1.0
$\delta(CCH)_{ring}$	1498.5	1525.3	0.27	1524.9	0.28	–0.4
$\nu(CC)_{ring} + \delta(CCH)_{ring}$		1627.9	0.00	1626.7	0.00	–1.2
$\nu(CC)_{ring} + \delta(CCH)_{ring}$	1610.6	1648.6	0.14	1647.5	0.13	–1.1

$\nu(CH)_{methyl}$	2890.7	3065.3	0.55	3061.1	0.52	–4.2
$\nu(CH)_{methyl}$	2932.1	3142.6	0.24	3138.3	0.28	–4.3
$\nu(CH)_{methyl}$	2970.8 2993.3	3163.6	0.24	3163.4	0.22	–0.2
$\nu(CH)_{ring}$	3035.7	3191.1	0.16	3190.2	0.14	–0.9
$\nu(CH)_{ring}$	3051.4	3191.7	0.13	3190.7	0.11	–1.0
$\nu(CH)_{ring}$	3064.8	3207.1	0.07	3206.5	0.06	–0.6
$\nu(CH)_{ring}$	3078.4	3216.3	0.52	3215.4	0.44	–0.9
$\nu(CH)_{ring}$	3098.2	3229.0	0.24	3228.3	0.22	–0.7