Evidences of Deprotonation of Aromatic Acids and Amides Adsorbed on Silver Colloids by Surface-Enhanced Raman Scattering

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SUPPORTING INFORMATION

Table S1. Calculated B3LYP/LanL2DZ vibrational wavenumbers (cm^{-1}) for different structures modelling the molecular environment of benzoic acid (BA): a) solid (BA_2), b) aqueous solution (BA^--$(H_2O)_2$-Na^+) and c) SERS (BA^--Ag^+).

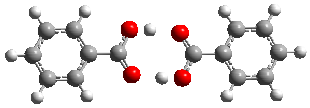
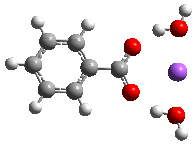
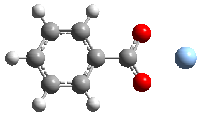
BA_2		**BA^--$(H_2O)_2$-Na^+**		**BA^--Ag^+**	
					
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_{2v})**	**Wavenumber (cm^{-1})**	**Symmetry (C_{2v})**
421	A_u	424	A_2	423	A_2
421	B_g	431	A_1	435	A_1
436	A_g	456	B_1	462	B_1
453	A_u	546	B_2	499	B_2
457	B_g	615	B_2	635	B_2
514	A_g	635	B_2	687	A_1
570	B_u	651	A_1	708	B_1
634	A_g	675	A_1	732	B_1
634	B_u	706	B_1	**827 (1; ν_{ring})**	A_1
653	A_g	733	B_1	828	B_1
671	B_u	**820 (1; ν_{ring})**	A_1	899	A_1
706	A_u	831	B_1	996	B_1
707	B_g	843	A_2	1016	A_1
732	B_g	861	B_1	1040	A_2
732	A_u	898	A_2	1047	A_1
792 (1; ν_{ring})	A_g	994	B_1	1051	B_1
803	B_u	1017	A_1	1101	B_2
833	B_g	1039	A_2	1143	A_1
834	A_u	1046	A_1	1203	B_2
899	A_u	1048	B_1	1211	A_1
900	B_g	1098	B_2	1352	B_2
1001	B_g	1157	A_1	1380	B_2
1001	A_u	1202	B_2	1386	A_1
1017	B_u	1207	A_1	1414	B_2
1017	A_g	1348	B_2	1484	B_2
1042	A_u	1381	B_2	1522	A_1
1042	B_g	1401	A_1	1632	B_2
1047	B_u	1469	B_2	1650	A_1
1047	A_g	1507	B_2		
1055	B_g	1520	A_1		
1055	A_u	1595	A_1		
1106	B_u	1601	B_2		
1106	A_g	1638	B_2		
1121	B_g	1651	A_1		
1141	B_u				
1149	A_g				
1165	A_u				
1207	B_u				
1207	A_g				
1215	B_u				

Table S1. Continued.

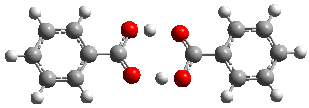
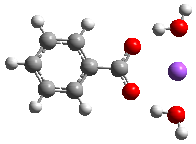
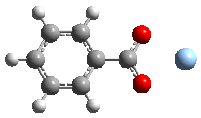
BA_2		BA^--$(H_2O)_2$-Na^+		BA^--Ag^+	
					
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_{2v})**	**Wavenumber (cm^{-1})**	**Symmetry (C_{2v})**
1216	A_g				
1321	A_g				
1334	B_u				
1361	Ag				
1362	B_u				
1388	A_g				
1388	B_u				
1439	A_g				
1478	B_u				
1484	A_g				
1491	B_u				
1520	A_g				
1528	B_u				
1606	B_u				
1629	A_g				
1646	B_u				
1648	A_g				
1654	B_u				
1670	A_g				

Table S2. Calculated B3LYP/LanL2DZ vibrational wavenumbers (cm^{-1}) for different structures modelling the molecular environment of benzamide (BM): a) solid (BM_2), and b) SERS (BM^--Ag^+).

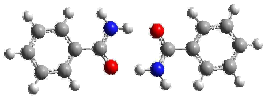
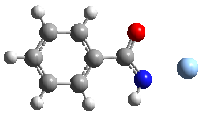
BM_2		**BM^--Ag^+**	
			
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**
412	B_g	422	A’
413	A_u	459	A’’
423	A_g	465	A’’
450	A_u	504	A’
454	B_g	636	A’
492	A_g	654	A’’
521	B_u	678	A’
557	B_g	711	A’’
562	A_u	724	A’’
629	A_g	807	A’’
636	B_u	**833 (1; ν_{ring})**	A’
636	A_g	876	A’’
642	B_u	960	A’’
702	A_u	965	A’
705	B_g	990	A’
724	B_g	1013	A’’
724	A_u	1035	A’’
773 (1; ν_{ring})	A_g	1052	A’
779	B_u	1115	A’
826	A_u	1182	A’
827	B_g	1190	A’
885	A_u	1233	A’
885	B_g	1286	A’
976	B_u	1339	A’
976	A_u	1374	A’
1000	B_g	1443	A’
1017	B_u	1504	A’
1017	A_g	1509	A’
1030	A_u	1555	A’
1030	B_g	1640	A’
1049	B_u		
1049	A_g		
1050	A_u		
1054	B_g		
1055	A_u		
1102	B_u		
1103	A_g		
1128	B_u		
1130	A_g		
1177	B_u		

Table S2. Continued.

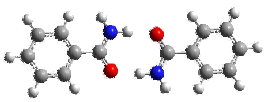
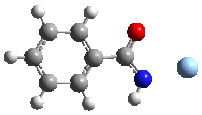
BM_2		BM^--Ag^+	
			
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**
1180	A_g		
1206	B_u		
1206	A_g		
1227	B_u		
1227	A_g		
1360	A_g		
1360	B_u		
1383	A_g		
1383	B_u		
1432	B_u		
1446	A_g		
1475	B_u		
1477	A_g		
1531	B_u		
1532	A_g		
1566	A_g		
1605	B_u		
1639	A_g		
1651	B_u		
1654	B_u		
1654	A_g		
1720	B_u		
1753	A_g		

Table S3. Calculated B3LYP/LanL2DZ vibrational wavenumbers (cm^{-1}) for different structures modelling the molecular environment of salicylic acid (SA): a) solid (SA_2), b) aqueous solution pH=7 (SA^--$(H_2O)_2$-Na^+), c) aqueous solution pH=14 (SA^{2-}-$(H_2O)_2$-Na^+) and d) SERS (SA^--Ag^+).

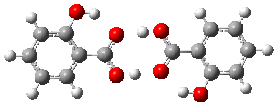
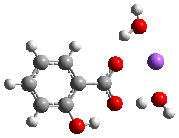
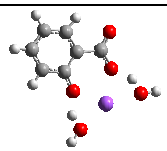
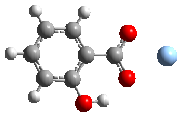
SA_2		SA^--$(H_2O)_2$-Na^+		SA^{2-}-$(H_2O)_2$-Na^+		SA^--Ag^+	
							
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**
392	A_g	421	A’	384	A’	408	A’
445	A_u	445	A’’	452	A’’	450	A’’
447	B_g	483	A’	471	A’	453	A’
474	A_g	542	A’	557	A’’	540	A’
483	B_u	546	A’’	573	A’	545	A’’
531	A_g	575	A’	602	A’	567	A’
541	A_u	613	A’	658	A’	681	A’
541	B_g	669	A’	682	A’	705	A’’
549	B_u	708	A’’	704	A’	785	A’’
570	A_g	714	A’	707	A’’	**805 (1; ν_{ring})**	A’
589	B_u	749	A’’	775	A’’	806	A’’
662	A_g	787	A’’	**801 (1; ν_{ring})**	A’	864	A’
673	B_u	809	A’’	803	A’’	877	A’’
705	B_g	**813 (1; ν_{ring})**	A’	869	A’’	908	A’’
706	A_u	868	A’	886	A’	1011	A’’
764 (1; ν_{ring})	A_g	904	A’’	956	A’’	1035	A’’
782	B_u	925	A’’	979	A’’	1047	A’
786	B_g	1002	A’’	1018	A’’	1107	A’
787	A_u	1028	A’’	1022	A’’	1157	A’
798	B_g	1046	A’’	1050	A’	1198	A’
799	A_u	1047	A’	1091	A’	1269	A’
828	B_g	1112	A’	1151	A’	1276	A’
829	A_u	1165	A’	1180	A’	1340	A’
859	A_g	1196	A’	1259	A’	1368	A’
860	B_u	1268	A’	1296	A’	1428	A’
914	B_g	1278	A’	1363	A’	1459	A’
914	A_u	1365	A’	1364	A’	1508	A’
1018	B_g	1368	A’	1461	A’	1533	A’
1018	A_u	1435	A’	1495	A’	1626	A’
1041	B_g	1482	A’	1545	A’	1674	A’
1041	A_u	1510	A’	1581	A’		
1049	B_u	1562	A’	1624	A’		
1049	A_g	1600	A’	1641	A’		
1107	B_u	1628	A’	1661	A’		
1111	A_g	1674	A’				
1128	B_g	1716	A’				
1167	B_u						

Table S3. Continued.

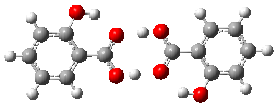
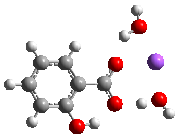
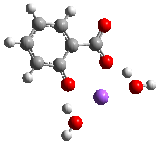
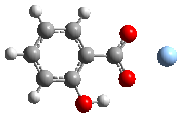
SA_2		SA^--$(H_2O)_2$-Na^+		SA^{2-}-$(H_2O)_2$-Na^+		SA^--Ag^+	
							
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**
1171	A_g						
1180	A_u						
1203	B_u						
1204	A_g						
1253	A_g						
1258	B_u						
1276	B_u						
1277	A_g						
1346	A_g						
1358	B_u						
1366	A_g						
1384	B_u						
1405	A_g						
1419	B_u						
1439	A_g						
1468	Bu						
1507	A_g						
1508	B_u						
1521	A_g						
1531	B_u						
1580	B_u						
1620	A_g						
1623	B_u						
1643	A_g						
1678	B_u						
1689	A_g						

Table S4. Calculated B3LYP/LanL2DZ vibrational wavenumbers (cm^{-1}) for different structures modelling the molecular environment of salicylamide (SM): a) solid (SM_2), b) aqueous solution (SM^--$(H_2O)_2$-Na^+) and c) SERS (SM^--Ag^+).

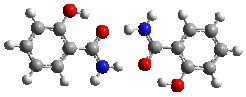
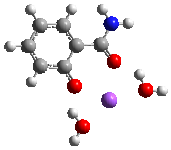
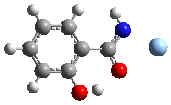
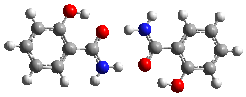
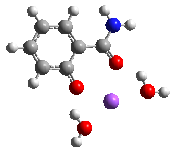
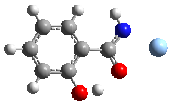
SM_2		SM^--$(H_2O)_2$-Na^+		SM^--Ag^+	
					
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**
404	A_g	404	A''	435	A'
432	A_u	449	A'	442	A''
434	B_g	474	A''	445	A'
452	A_g	537	A'	540	A''
462	B_u	545	A''	547	A'
515	A_g	549	A''	567	A'
524	B_u	581	A'	633	A''
534	B_g	592	A'	681	A'
534	A_u	626	A'	697	A''
568	A_g	662	A'	774	A''
570	B_u	709	A''	794	A''
575	B_g	721	A''	**806 (1; ν_{ring})**	A'
580	A_u	**729 (1; ν_{ring})**	A'	864	A'
651	A_g	768	A''	892	A''
659	B_u	805	A''	951	A''
698	A_u	838	A''	980	A''
700	B_g	880	A'	1024	A''
745 (1; ν_{ring})	A_g	880	A''	1052	A'
757	B_u	958	A''	1090	A'
778	B_g	1019	A''	1149	A'
778	A_u	1050	A'	1183	A'
801	B_g	1069	A'	1203	A'
802	A_u	1118	A'	1280	A'
855	A_g	1172	A'	1290	A'
856	B_u	1209	A'	1359	A'
892	A_u	1292	A'	1382	A'
892	B_g	1316	A'	1437	A'
899	B_g	1392	A'	1475	A'
900	A_u	1423	A'	1517	A'
981	B_g	1466	A'	1561	A'
981	A_u	1507	A'	1628	A'
991	B_g	1555	A'	1674	A'
1030	A_u	1577	A'		
1030	B_g	1598	A'		
1046	A_u	1602	A'		
1055	B_u	1662	A'		
1055	A_g	1670	A'		
1094	B_u				
1097	A_g				
1148	B_u				

Table S4. Continued.

SM_2		$SM^-\text{-}(H_2O)_2\text{-}Na^+$		$SM^-\text{-}Ag^+$	
					
Wavenumber (cm^{-1})	**Symmetry (C_{2h})**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**	**Wavenumber (cm^{-1})**	**Symmetry (C_s)**
1150	A_g				
1176	B_u				
1179	A_g				
1210	B_u				
1211	A_g				
1282	B_u				
1282	A_g				
1285	B_u				
1287	A_g				
1369	A_g				
1371	B_u				
1426	A_g				
1432	B_u				
1453	B_u				
1456	A_g				
1484	B_u				
1493	A_g				
1522	B_u				
1526	A_g				
1577	A_g				
1605	B_u				
1626	A_g				
1627	B_u				
1679	A_g				
1682	B_u				
1727	B_u				
1757	A_g				