Supplementary Material to:

A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols

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	Calc. C	205	388	419	632	637	709	773	606	979	1005	1017	1029	1054	1082	1073	1180	1235	1315	1370	1460	1482	1593	1627		
Ag colloid)	Calc. B	203	390	419	631	636	206	773	200	978	992	1016	1027	1056	1071	1062	1175	1227	1285	1368	1450	1474	1573	1607		
$\frac{1}{N}$	Calc. A	208	391	420	637	641	704	775	904	977	992	1015	1033	1061	1077	1066	1189	1237	1295	1379	1459	1481	1571	1602	d the	
I	Raman	$210^{b} \mathrm{\ br}$			623 m	$649 \mathrm{~w/m}$	708 w			942 vw	1008 vvs		1036 vvs			$1069 \mathrm{~m}$	$1197 { m \ sh}$	$1221 \mathrm{~m}$	1299 vw		1452 vw	1487 vw	$1575 \mathrm{ w/m}$	1599 m	complex and	
	Calc. C		383	397	608	640	724	766	912	976	992	1017	1019	1042	1070	1070	1164	1224	1312	1358	1446	1473	1598	1612	dine/water	- X - X - X -
ieous sol.)	Calc. B		385	395	007	640	722	766	918	277	679	1020	1014	1044	1058	1062	1159	1218	1279	1356	1436	1465	1579	1593	e, the pyrid	
ridine (aqı	Calc. A		382	394	613	646		769	921	978	978	1018	1022	1046	1064	1068		1227	1290	1369	1444	1473	1575	1588	ie molecule	
py	Raman				615 w/m	649 m	726				1000 vvs		1032 vs			1069 w	1172	$1216 \mathrm{~m}$				1480 vw	1574 w/m	$1592 \mathrm{~m}$	or the pyridir	
	Calc. C		377	409	593	643	727	762	916	971	971	1013	1018	1038	1059	1070	1160	1223	1301	1356	1439	1467	1596	1600	equencies fo	
(liq.)	Calc. B		381	411	594	642	725	761	915	968	962	1011	1013	1040	1050	1062	1156	1215	1273	1353	1431	1459	1577	1581	rational fre	or of number
pyridine	Calc. A		376	410	599	648	729	762	918	967	959	1008	1020	1041	1054	1068	1169	1224	1282	1367	1438	1466	1574	1576	asured vib	netry sher
	Raman		379^a	407 w	604 w/m	653 m	709 vvw	750 vvw	885 w	942 vw	992 vvs	$980 \mathrm{sh}$	1031 vs	1020 vvw	1052 vvw	1069 w	1150 w	$1217 \mathrm{~m}$	1290^a	1356 vvw	1438 w	1483 w	$1573 \mathrm{ w/m}$	$1582 \mathrm{~m}$	outed and me	
	Assignment	$Ag \cdots N$ stretch	u(13)	u(27)	u(10)	$\nu(22)$	u(26)	$\nu(25)$	u(12)	u(24)	$\nu(9)$	u(11)	$\nu(8)$	$ \nu(23) $	$ \nu(21) $	$\nu(7)$	u(20)	$\nu(6)$	u(19)	u(18)	u(17)	u(5)	u(16)	u(4)	Table 1S: Comp 1: 1 + 1	$\pi n n o T n o T n o n o n o n o n o n o n$
	\mathbf{s}		A_2	\mathbf{B}_1	\mathbf{A}_{1}	B_2	B_1	B_1	A_2	B_1	\mathbf{A}_1	\mathbf{A}_2	\mathbf{A}_{1}	\mathbf{B}_1	B_2	\mathbf{A}_1	B_2	\mathbf{A}_1	B_2	B_2	B_2	\mathbf{A}_1	B_2	\mathbf{A}_1		DVT

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1	5																								
	Calc. C	202	387	422	639	644	705	766	887	957	1002	995	1033	1033	1076	1067	1183	1228	1309	1364	1451	1475	1582	1609	
g colloid)	Calc. B	200	389	423	638	644	703	764	885	955	991	966	1030	1036	1068	1058	1179	1222	1285	1363	1442	1468	1565	1592	
yridine (A	Calc. A	208	391	420	637	641	704	775	904	277	992	1015	1033	1061	1077	1066	1189	1237	1295	1379	1459	1481	1571	1602	nd the Calc. C =
d	Raman	$210^{b} \mathrm{\ br}$			623 w	649 w/m	708 w			942 vw	1008 vvs		1036 vvs			$1069 \mathrm{~m}$	$1197 { m ~sh}$	$1221 \mathrm{~m}$	1299 vw		1452 vw	1487 vw	1575 w/m	$1599 \mathrm{~m}$	er complex a /LanL2DZ; (
	Calc. C		381	397	614	648	716	762	896	952	988	966	1021	1020	1064	1066	1168	1220	1300	1357	1440	1469	1587	1601	ridine/wate = B3LYP
ieous sol.)	Calc. B		383	393	613	648	716	761	897	952	978	998	1015	1023	1056	1060	1164	1215	1276	1356	1432	1462	1570	1579	ule, the py Z; Calc. B
<u>ridine (aqu</u>	Calc. A		382	391	613	646	726	769	921	978	978	1018	1022	1046	1064	1068	1172	1227	1290	1369	1444	1473	1575	1588	dine molec P/LanL2D
py	Raman				615 w/m	$649 \mathrm{~m}$					1000 vvs		1032 vs			1069 w		$1216 \mathrm{~m}$				1480 vw	1574 w/m	$1592 \mathrm{m}$	for the pyric $A = BLY$
	U U				_																				iencies e. Cal
	Cald		374	414	597	650	716	758	895	942	968	066	1018	1017	1054	1066	1165	1220	1293	1357	1435	1463	1584	1586	frequ
(liq.)	Calc. B Calc		377 374	416 414	598 597	650 650	715 716	757 758	894 895	939 942	961 968	989 990	1013 1018	1019 1017	1047 1054	1060 1066	1161 1165	1214 1220	1271 1293	1355 1357	1428 1435	1457 1463	1568 1584	1570 1586	ibrational frequecies of pyridin
pyridine (liq.)	Calc. A Calc. B Calc		373 377 374	418 416 414	607 598 597	660 650 650	723 715 716	764 757 758	903 894 895	943 939 942	966 961 968	991 989 990	1026 1013 1018	1025 1019 1017	1060 1047 1054	1072 1060 1066	1182 1161 1165	1231 1214 1220	1291 1271 1293	1378 1355 1357	1445 1428 1435	1473 1457 1463	1574 1568 1584	1576 1570 1586	neasured vibrational frequ mmetry species of pyridin
pyridine (liq.)	Raman Calc. A Calc. B Cald		379 a 373 377 374	407 w 418 416 414	604 w/m 607 598 597	653 m 660 650 650	709 vvw 723 715 716	750 vvw 764 757 758	885 w 903 894 895	942 vw 943 939 942	992 vvs 966 961 968	980 sh 991 989 990	1031 vs 1026 1013 1018	1020 vvw 1025 1019 1017	1052 vvw 1060 1047 1054	1069 w 1072 1060 1066	1150 w 1182 1161 1165	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	1290 a 1291 1271 1293	1356 vvw 1378 1355 1357	1438 vvw 1445 1428 1435	1483 w 1473 1457 1463	$\left \begin{array}{ccc}1573 \text{ w/m}\\\end{array}\right 1574 \\ 1568 \\ 1584 \\ 158$	1582 m 1576 1570 1586	mputed and measured vibrational frequiplex. S = symmetry species of pyridin
pyridine (liq.)	Assignment Raman Calc. A Calc. B Cald	Ag-N stretch	u(13) 379 a 373 377 374	u(27) 407 w 418 416 414	u(10) 604 w/m 607 598 597	$ \nu(22)$ 653 m 660 650 650	$\nu(26)$ 709 vvw 723 715 716	u(25) 750 vvw 764 757 758	u(12) 885 w 903 894 895	u(24) 942 vw 943 939 942	$\nu(9)$ 992 vvs 966 961 968	$ \nu(11)$ 980 sh 991 989 990	$ \nu(8)$ 1031 vs 1026 1013 1018	$ \nu(23)$ 1020 vvw 1025 1019 1017	u(21) 1052 vvw 1060 1047 1054	u(7) 1069 w 1072 1060 1066	$ \nu(20)$ 1150 w 1182 1161 1165	$\nu(6)$ 1217 m 1231 1214 1220	u(19) 1290 a 1291 1271 1293	u(18) 1356 vvw 1378 1355 1357	u(17) 1438 vvw 1445 1428 1435	u(5) 1483 w 1473 1457 1463	u(16) 1573 w/m 1574 1568 1584	$ \nu(4)$ 1582 m 1576 1570 1586	able 2S: Computed and measured vibrational frequine/ Ag^+ complex. S = symmetry species of pyridin

oid)	Calc. B	199	382	417	653	661	702	741	847	883	991	891	1069	928	1083	1082	1218	1261	1316	1414	1481	1511	1586	1622	ex and the
ne (Ag coll	Calc. A	204	384	419	644	647	697	747	882	904	988	920	1065	941	1080	1074	1209	1255	1324	1402	1476	1500	1586	1627	ater compl
pyridir	Raman	$210 \ bbr$			623 m	649 w/m	708 w			942 vw	1008 vvs		1036 vvs			$1069 \mathrm{~m}$	$1197 \mathrm{~sh}$	$1221 \mathrm{m}$	1299 vw		1452 vw	1487 vw	1575 w/m	$1599 \mathrm{~m}$	pyridine/w
sol.)	Calc. B		378	393	629	662	704	736	847	869	976	893	1045	911	1071	1088	1202	1247	1295	1401	1468	1502	1585	1599	olecule, the
e (aqueous	Calc. A		382	398	618	649	706	744	889	902	973	923	1040	919	1067	1076	1192	1240	1305	1386	1458	1487	1583	1603	pyridine m
pyridine	Raman				615 w/m	649 m					1000 vvs		1032 vs			1069 w		1216 m				1480 vw	1574 w/m	1592 m	ncies for the
	Calc. B		373	406	613	663	702	733	843	872	956	894	1039	908	1061	1088	1199	1245	1285	1396	1463	1494	1582	1588	nal freque
ridine (liq.)	Calc. A		377	408	605	605	707	742	885	904	954	920	1034	915	1056	1077	1189	1237	1294	1380	1451	1479	1580	1591	ed vibratic
IXd	Raman		379 a	407 w	604 w/m	653 m	709 vvw	750 vvw	885 w	942 vw	992 vvs	980 m sh	1031 vs	1020 vvw	1052 vvw	1069 w	1150 w	$1217 \mathrm{~m}$	1290 a	1356 vvw	1438 vvw	1483 w	1573 w/m	$1582 \mathrm{m}$	l and measur
	Assignment	Ag-N stretch	u(13)	$\nu(27)$	u(10)	u(22)	u(26)	u(25)	u(12)	$ \nu(24) $	$\nu(9)$	u(11)	$\nu(8)$	u(23)	u(21)	$\nu(7)$	u(20)	$\nu(6)$	u(19)	u(18)	u(17)	u(5)	u(16)	u(4)	S: Computed
	S	7	A_2	B_1	\mathbf{A}_1	B_2	B_{1}	B_1	A_2	B_1	\mathbf{A}_1	A_2	\mathbf{A}_1	B_{1}	B_2	\mathbf{A}_1	B_2	\mathbf{A}_1	B_2	B_2	B_2	\mathbf{A}_1	B_2	A_1	able 3

anions.
chloride a
without
iydrosol

22	LanL2DZ	120	375	412	632	662	700	735	845	870	886	606	677	1047	1071	1086	1205	1248	1298	1402	1469	1499	1584	1602	
IM	CEP-31G	128	379	414	623	649	702	743	889	902	916	921	976	1045	1070	1075	1195	1243	1312	1390	1462	1489	1583	1608	g(0) complex
W91	LanL2DZ	97	374	417	611	648	713	758	893	948	982	992	1020	1020	1061	1065	1169	1218	1299	1355	1440	1466	1586	1595	e pyridine/A
B3P	CEP-31G	108	376	412	605	640	720	764	916	977	987	1017	1018	1043	1067	1069	1165	1223	1310	1358	1447	1472	1596	1613	encies for the
YP	LanL2DZ	94	377	419	611	648	712	757	892	946	974	992	1015	1022	1053	1058	1164	1212	1275	1354	1432	1459	1569	1578	ational freque
B3I	CEP-31G	103	380	414	605	640	718	764	915	975	976	1014	1016	1044	1058	1060	1160	1216	1279	1356	1438	1465	1577	1593	nputed vibra
YP	LanL2DZ	96	371	421	620	657	719	761	006	950	978	993	1028	1028	1065	1070	1186	1229	1296	1375	1450	1475	1575	1584	ble 4S: Cor
BL	CEP-31G	106	372	411	611	645	720	763	917	974	974	1013	1021	1045	1063	1065	1173	1225	1290	1368	1446	1471	1573	1589	Та

References

[1] T. D. Klots, Spectrochim. Acta Part. A, 1998, **54**, 1481–1498.