Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Microwave Spectroscopic and Theoretical Studies on Phenylacetylene···H_2O Complex: C-H•••O and O-H•••π Hydrogen Bonds as Equal Partners

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Supporting Information

Table I-S. Experimentally observed rotational transitions and their assignments for C_6H_5CCH•••H_2O complex.

Transitions	Strong /MHz	Residue(kHz)	Weak/MHz	Residue(kHz)
4_{14}-5_{15}	-	-	7313.3681	-0.3
3_{12}-4_{13}	7377.2239	-0.8	7377.1167	-1.5
3_{03}-4_{14}	7469.9099	-3.1	-	-
4_{14}-5_{15}	7871.0364	-0.2	7870.0680	0.2
4_{04}-5_{05}	8143.0807	1.0	8142.2742	0.8
4_{23}-5_{24}	8575.9471	5.3	8575.4126	1.2
4_{04}-5_{15}	8699.4556	2.5	8698.9750	2.2
1_{10}-2_{21}	8747.9047	-2.8	8750.8803	-0.1
5_{15}-6_{06}	9041.4890	-1.8	9041.1213	1.2
1_{11}-2_{20}	9042.5188	-1.1	9044.6475	0.2
4_{22}-5_{23}	9072.0932	0.3	9071.8680	-0.6
4_{13}-5_{14}	9153.4035	-0.1	9153.2243	0.8
5_{15}-6_{16}	9391.9782	-2.6	9390.7862	1.1
6_{25}-7_{16}	9574.4927	1.4	9572.3070	-0.1
5_{05}-6_{06}	9598.8931	-0.3	9597.8176	-1.9
5_{05}-6_{16}	9948.3535	-0.8	9947.4832	-1.3
2_{11}-3_{22}	10211.3150	5.9	10214.0197	-0.2
5_{24}-6_{25}	10239.0055	-2.9	-	-
5_{33}-6_{34}	10477.6610	-0.0	-	-
6_{16}-7_{07}	10687.3803	0.2	10685.8271	1.6
5_{14}-6_{15}	10874.3312	-0.2	10874.0427	1.0
6_{16}-7_{17}	10895.7674	1.6	10894.3327	-0.4
5_{23}-6_{24}	11004.1483	-1.8	-	-
6_{06}-7_{07}	11036.8388	-2.2	11035.9982	-5.6
6_{06}-7_{17}	11245.2288	2.1	11243.9982	0.1
6_{25}-7_{26}	11875.5196	-0.5	11874.6923	-0.7
7_{17}-8_{08}	12266.3368	1.9	12264.5854	-1.5
7_{17}-8_{18}	12385.8729	-1.3	-	-
7_{07}-8_{08}	-	-	12473.0986	4.0

Table II-S. Experimentally observed rotational transitions and their assignments for $C_6H_5CCH\cdots D_2O$ complex

Transitions	Strong/(MHz)	Residue(kHz)	Weak/(MHz)	Residue(kHz)
2_{02}-3_{03}	4879.8129	-1.9	4879.8129	0.4
3_{13}-4_{14}	6103.4511	-3.7	6103.4997	2.1
3_{03}-4_{04}	6402.7017	7.3	-	-
4_{14}-5_{05}	6989.9181	2.5	6990.0177	-3.8
3_{03}-4_{14}	7275.0634	2.5	7274.9904	-4.2
4_{14}-5_{15}	7592.6171	-0.1	7592.6758	2.0
4_{04}-5_{05}	7862.2781	-4.0	7862.3142	2.6
4_{04}-5_{15}	8464.9861	2.4	-	-
5_{15}-6_{06}	8673.9217	-5.0	8674.0249	-4.1
4_{13}-5_{14}	8779.0901	-1.2	8779.0213	-0.8
5_{15}-6_{16}	9064.2232	-1.2	9064.2950	-1.3
5_{05}-6_{06}	9276.6291	0.8	9276.6831	1.7
5_{05}-6_{16}	9666.9220	-4.0	9666.9474	-1.3
5_{24}-6_{25}	9843.5036	6.3	-	-
2_{11}-3_{22}	9997.9802	-0.2	9997.9608	0.0
6_{16}-7_{07}	10279.9605	0.9	10280.0727	5.9
5_{14}-6_{15}	10442.6530	-4.4	10442.5923	4.5
5_{23}-6_{24}	10517.8896	0.9	10517.8104	-0.5
6_{16}-7_{17}	10520.0474	-0.1	10520.1344	-1.4
6_{06}-7_{07}	10670.2610	3.7	10670.3336	-0.5
6_{25}-7_{26}	10910.3453	0.1	10910.4061	2.9
7_{17}-8_{08}	11423.8391	-2.9	-	-
7_{17}-8_{18}	11820.8681	3.1	11820.9801	-2.6
6_{15}-7_{16}	11962.9115	-1.5	11963.0191	0.7
7_{07}-8_{08}	12045.4611	0.9	12045.4026	-2.3
7_{07}-8_{18}	12060.9550	2.0	12061.0535	1.8
6_{06}-7_{17}	12202.9978	-3.1	12203.0850	-2.4

Table III-S. Experimentally observed rotational transitions and their assignments for $C_6H_5CCH{\cdots}HOD$ complex

Transitions	Frequency(MHz)	Residue(kHz)
1_{01}-2_{02}	3376.0999	-3.1
2_{02}-3_{03}	4998.5991	0.9
3_{13}-4_{04}	5383.1567	3.6
2_{02}-3_{13}	6167.9561	-7.3
3_{13}-4_{14}	6244.0877	2.8
3_{03}-4_{04}	6552.5189	0.5
4_{14}-5_{05}	7178.5777	-1.7
3_{12}-4_{13}	7259.4733	-3.6
4_{14}-5_{15}	7765.4392	0.9
4_{04}-5_{05}	8039.5094	-1.8
4_{04}-5_{15}	8626.3761	6.0
1_{10}-2_{21}	8740.6683	-2.7
5_{15}-6_{06}	8893.5292	-5.5
4_{22}-5_{23}	8914.9734	-3.8
4_{13}-5_{14}	9011.2874	0.3
5_{15}-6_{16}	9268.0845	4.4
5_{05}-6_{06}	9480.4020	8.5
5_{05}-6_{16}	9854.9380	-1.0
5_{24}-6_{25}	10088.5637	-3.2
2_{11}-3_{22}	10185.6857	-4.8
6_{16}-7_{07}	10527.0795	-0.0
5_{14}-6_{15}	10712.0944	-1.6
6_{16}-7_{17}	10754.0969	-0.6
5_{23}-6_{24}	10813.6711	1.1
6_{06}-7_{07}	10901.6439	0.9
2_{12}-3_{21}	11088.2486	10.0
6_{06}-7_{17}	11128.6413	-1.7
3_{12}-4_{23}	11499.2399	-2.7
7_{17}-8_{08}	12094.3226	-3.1
6_{15}-7_{16}	12346.2835	4.6

Table IV-S. Experimentally observed rotational transitions and their assignments for $C_6H_5CCD{\bullet}{\bullet}{\bullet}H_2O$ complex

Transitions	Strong/MHz	Residue(kHz)	Weak/MHz	Residue(kHz)
3_{13}-4_{14}	6197.1539	-0.6	-	-
3_{03}-4_{04}	6500.7486	1.9	6500.1811	-4.2
4_{14}-5_{05}	7173.1047	-0.8	7171.8512	1.5
5_{24}-6_{15}	7188.8364	-0.0	-	-
3_{03}-4_{14}	7296.2949	0.6	-	-
4_{14}-5_{15}	7704.5633	0.8	7703.6020	-2.6
4_{04}-5_{05}	7968.6556	2.5	7967.8513	-0.2
4_{04}-5_{15}	8500.1102	0.0	8499.6057	-0.8
5_{15}-6_{06}	8860.7195	2.3	8859.3511	0.1
4_{13}-5_{14}	8965.9070	-2.9	8965.7311	0.2
5_{15}-6_{16}	9192.6244	-0.6	9191.4411	-0.0
5_{05}-6_{06}	9392.1737	-0.5	9391.1077	1.8
5_{05}-6_{16}	9724.0808	-1.2	9723.1923	-3.8
6_{16}-7_{07}	10467.0288	0.1	10465.4972	-4.9
5_{14}-6_{15}	10649.2319	2.0	10648.9449	2.3
6_{06}-7_{07}	10798.9321	-4.4	10797.5874	-4.8
6_{06}-7_{17}	10995.7069	-1.6	10994.4706	0.5
7_{17}-8_{08}	12009.3631	-1.9	12007.6409	1.3
7_{07}-8_{08}	12206.1385	1.4	12204.5192	1.8
7_{07}-8_{18}	12318.3659	3.5	12316.8098	7.9

Table V-S. Experimentally observed rotational transitions and their assignments for $C_6H_5CCH{\cdot}{\cdot}{\cdot}H_2{}^{18}O$ complex

Transitions	Frequency (MHz)	Residue (kHz)	Frequency (MHz)	Residue (kHz)
4_{14}-5_{15}	-	-	7587.6948	-0.4
5_{15}-6_{06}	-	-	8688.1026	1.0
4_{13}-5_{14}	8805.1067	2.3	8805.3708	0.1
5_{15}-6_{16}	9054.7981	-2.4	9055.9917	4.0
5_{05}-6_{06}	-	-	9264.0632	-1.4
5_{05}-6_{16}	9631.0682	-3.9	-	-
6_{16}-7_{07}	-	-	10284.8832	-2.2
6_{15}-5_{14}	10467.1563	-1.6	-	-
6_{06}-7_{17}	-	-	10652.7705	0.3
6_{06}-7_{07}	10874.6966	5.1	10875.9179	-0.9

Table VI-S. The cartesian co-ordinates (Å) of the $C_6H_5CCH{\bullet\bullet\bullet}H_2O$ complex in the *abc* principal axes system of the complex derived from the fitting of the r_0 structure to the experimentally derived moments of inertia of all the isotopologues. Labeling of the atoms are shown in Figure 3.

Atoms	*a*	*b*	c
C_1	0.091	-0.516	0.045
C_2	1.261	1.253	0.120
C_3	0.136	0.136	0.136
C_4	2.490	0.594	0.156
C_5	1.368	1.368	1.368
C_6	2.546	0.027	2.547
C_7	-1.184	-1.195	0.082
C_8	-2.248	-1.763	0.113
H_9	-3.179	-2.259	0.140
H_{10}	1.215	2.325	0.219
H_{11}	-0.773	1.433	0.302
H_{12}	3.401	1.163	0.284
H_{13}	1.409	2.600	0.238
H_{14}	3.499	0.055	3.499
O_{15}	-3.278	1.502	-0.144
H_{16}	-2.990	0.642	0.186
H_{17}	-3.666	1.318	-1.008

Table VII-S. The equilibrium cartesian co-ordinates (Å) of $C_6H_5CCH{\bullet\bullet\bullet}H_2O$ complex in the *abc* principal axes system calculated at MP2/aug-cc-pVDZ level. Labeling of the atoms are shown in Figure 3.

Atoms	*a*	*b*	*c*
C_1	0.055	0.502	-0.015
C_2	1.235	1.281	0.054
C_3	0.142	-0.910	-0.071
C_4	2.490	0.650	0.066
C_5	1.404	-1.527	-0.060
C_6	2.579	-0.754	0.008
C_7	-1.227	1.160	-0.033
C_8	-2.317	1.748	-0.054
H_9	-3.253	2.276	-0.084
H_{10}	1.158	2.371	0.097
H_{11}	-0.774	-1.505	-0.121
H_{12}	3.399	1.256	0.119
H_{13}	1.470	-2.618	-0.105
H_{14}	3.558	-1.241	0.016
O_{15}	-3.205	-1.508	0.025
H_{16}	-2.976	-0.565	0.043
H_{17}	-3.652	-1.655	0.870