Electronic Supplementary Material for PCCP

The Mono- and Di-hydrates of Acetic Acid: A High-resolution Microwave Spectroscopic Study

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Supplementary Data

A. Cartesian coordinates

Table S.1-S.2 show the artesian coordinates of atoms of the fully optimized ACE–(H_2O) and ACE–(H_2O)$_2$ in their principal axis systems on the level of MP2/6-311++G(2df,2pd) calculations.

Table S.1: Cartesian coordinates of atoms in ACE–(H_2O) in its principal axis system from MP2/6-311++G(2df,2pd) calculation.

	a	*b*	*c*
C	2.1840	-0.0322	0.0166
C	0.6929	0.0849	0.0077
O	0.0989	-1.1136	0.0188
H	-0.8714	-0.9675	0.0271
O	0.0833	1.1390	0.0143
H	2.5181	-0.6144	0.8386
H	2.6314	0.9538	0.0012
H	2.4888	-0.5657	-0.9139
O	-2.4523	-0.0404	-0.0628
H	-1.8786	0.7380	0.0023
H	-3.1145	0.0660	0.6219

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Table S.2: Cartesian coordinates of atoms in ACE–$(H_2O)_2$ in its principal axis system from MP2/6-311++G(2df,2pd) calculation.

	a	*b*	*c*
C	2.6974	-0.2500	0.0084
C	1.2061	-0.1147	-0.0017
O	0.8216	1.1548	0.0141
H	-0.1672	1.2198	0.0003
O	0.4416	-1.0657	-0.0024
H	2.9745	-1.2969	0.0102
H	3.1109	0.2463	-0.8663
H	3.1012	0.2479	0.8866
H	-1.3811	-1.3385	0.0240
O	-2.3484	-1.2464	0.0693
H	-2.6915	-1.8304	-0.6081
H	-2.2550	0.5525	-0.0414
O	-1.8678	1.4475	-0.0671
H	-2.3041	1.9369	0.6316

B. Observed Transitions of *A* and *E* states of ACE–(H_2O)

Table S.3: Fit to the observed transitions of A and E states of ACE–(H_2O).

	$\nu_{\rm obs}$ [a]/MHz		$\Delta\nu_{\rm SPFIT}$ [b]/MHz		$\Delta\nu_{\rm XIAM}$ [c]/MHz	
Transition	A	E	A	E	A	E
$2_{1,2}\leftarrow1_{1,1}$	8967.2202	9294.8626	0.0035	0.0059	0.0010	0.0101
$2_{0,2}\leftarrow1_{0,1}$	9406.2866	9405.5812	0.0010	0.0009	−0.0002	0.0006
$2_{1,1}\leftarrow1_{1,0}$	9880.7641	9552.9173	0.0001	0.0010	−0.0005	0.0012
$3_{1,3}\leftarrow2_{1,2}$	13439.8984	13747.6331	0.0016	0.0053	−0.0009	0.0115
$3_{0,3}\leftarrow2_{0,2}$	14065.2292	14062.9384	−0.0054	−0.0026	−0.0055	−0.0083
$3_{2,2}\leftarrow2_{2,1}$	14135.8498	14174.9172	0.0019	−0.0055	0.0017	0.0008
$3_{2,1}\leftarrow2_{2,0}$	14206.5362	14169.1290	−0.0040	0.0013	−0.0084	0.0017
$3_{1,2}\leftarrow2_{1,1}$	14809.7598	14501.1863	0.0050	−0.0009	0.0051	−0.0065
$1_{1,0}\leftarrow1_{0,1}$	9055.8936	10193.9641	−0.0003	0.0079	0.0016	0.0032
$1_{1,1}\leftarrow0_{0,0}$	13311.1282	–	−0.0029	–	−0.0030	–
$1_{1,0}\leftarrow0_{0,0}$	–	14905.8587	–	−0.0013	–	−0.0020
$2_{1,1}\leftarrow2_{0,2}$	9530.3733	10341.2847	0.0010	−0.0075	0.0035	−0.0116
$3_{1,2}\leftarrow3_{0,3}$	10274.8859	10779.5624	−0.0066	0.0240	−0.0039	0.0200
$4_{0,4}\leftarrow3_{1,3}$	11137.4698	12001.9908	−0.0009	0.0010	0.0051	−0.0026
$4_{1,3}\leftarrow4_{0,4}$	11327.1882	11617.3009	0.0039	−0.0055	0.0055	−0.0080
$5_{1,4}\leftarrow5_{0,5}$	12733.3782	12892.2752	0.0127	−0.0178	0.0121	−0.0167
$6_{1,5}\leftarrow6_{0,6}$	14541.9676	14625.0445	−0.0087	0.0106	0.0131	−0.0020

[a] $\nu_{\rm obs}$ of the transitions are the intensity-weighted average frequencies of hyperfine splittings of the order of 20–120 kHz.

[b] $\Delta\nu_{\rm SPFIT} = \nu_{\rm obs} - \nu_{\rm calc,SPFIT}$.

[c] $\Delta\nu_{\rm XIAM} = \nu_{\rm obs} - \nu_{\rm calc,XIAM}$.

C. Observed Transitions of *A* and *E* states of ACE–(H_2O)$_2$

Table S.4: List of observed transitions of A and E states of ACE–$(H_2O)_2$.

	$\nu_{\rm obs}{}^a$/MHz		$\Delta\nu_{\rm SPFIT}{}^b$/MHz		$\Delta\nu_{\rm XIAM}{}^c$/MHz	
Transition	A	E	A	E	A	E
$3_{1,3}\leftarrow2_{1,2}$	7800.7853	7947.0258	−0.0005	0.0004	−0.0026	−0.0025
$3_{0,3}\leftarrow2_{0,2}$	8286.0733	8280.7742	0.0013	−0.0016	0.0003	0.0009
$3_{1,2}\leftarrow2_{1,1}$	9054.2784	8906.3055	0.0000	0.0012	−0.0022	0.0013
$4_{1,4}\leftarrow3_{1,3}$	10357.0658	10433.4980	0.0007	0.0001	−0.0011	−0.0014
$4_{0,4}\leftarrow3_{0,3}$	10868.8808	10858.6329	0.0006	−0.0026	0.0028	−0.0022
$4_{2,3}\leftarrow3_{2,2}$	11239.0536	11439.5078	0.0027	−0.0017	0.0037	0.0070
$4_{2,2}\leftarrow3_{2,1}$	11642.5860	11449.9794	−0.0006	−0.0018	−0.0007	−0.0076
$4_{1,3}\leftarrow3_{1,2}$	12015.6353	11934.8160	−0.0003	−0.0015	−0.0016	−0.0013
$5_{1,5}\leftarrow4_{1,4}$	12882.9759	12921.9811	0.0008	0.0018	0.0003	0.0020
$5_{0,5}\leftarrow4_{0,4}$	13342.8559	13327.8744	−0.0007	0.0025	0.0059	-0.0035
$5_{2,4}\leftarrow4_{2,3}$	13995.4410	14289.1762	0.0020	0.0011	0.0024	0.0000
$5_{2,3}\leftarrow4_{2,2}$	14742.0561	14459.1446	−0.0008	0.0011	0.0034	0.0050
$5_{1,4}\leftarrow4_{1,3}$	14920.0789	14872.6183	0.0004	0.0021	0.0014	0.0016
$6_{0,6}\leftarrow5_{0,5}$	15739.6353	15722.4168	−0.0006	0.0030	−0.0065	0.0026
$6_{1,6}\leftarrow5_{1,5}$	15378.6718	15398.3503	−0.0005	−0.0009	0.0017	0.0011
$6_{2,5}\leftarrow5_{2,4}$	16717.2575	–	−0.0030	–	−0.0036	–

[a] $\Delta\nu_{\rm SPFIT} = \nu_{\rm obs} - \nu_{\rm calc,SPFIT}$.

[b] $\Delta\nu_{\rm XIAM} = \nu_{\rm obs} - \nu_{\rm calc,XIAM}$.