TABLE I: Geometry (Å, degrees) and Rotational Constants A, B, C (GHz) of the m1, m2, m3, m4 Minima and sp1, sp2 Saddle Points of the $C_2H_2(H_2O)_2$ (AW_2) at the MP2/aug–cc–pVDZ (avdz) and aug–cc–pVTZ (avtz) Level.

AW_2	m1		m2		sp1	m3		sp2	m4	
	avdz	avtz	avdz	avtz	avdz	avdz	avtz	avdz	avdz	avtz
R_1 (C_1–C_2)	1.2339	1.2147	1.2325	1.2135	1.2329	1.2335	1.2148	1.2335	1.2331	1.2140
R_2 (H_1–C_1)	1.0825	1.0690	1.0786	1.0650	1.0764	1.0796	1.0666	1.0795	1.0765	1.0636
R_3 (H_2–C_2)	1.0755	1.0626	1.0751	1.0623	1.0764	1.0796	1.0666	1.0791	1.0765	1.0636
ϕ_1 ($H_1C_1C_2$)	176.07	177.11	179.16	178.86	179.40	179.82	179.78	179.92	180	180
ϕ_2 ($H_2C_2C_1$)	177.22	178.36	179.69	179.55	179.40	179.82	179.78	179.91	180	180
δ_1 ($H_1C_1C_2H_2$) [a]	−172.63	−169.27	180	180	0	180	180	180	0	0
R_4 (O_a–C_1)	3.1293	3.1253	3.2861	3.2960	3.5843	3.2944	3.3000	3.2949	3.4236	3.3925
R_5 (O_a–H_{1a})	0.9760	0.9720	0.9666	0.9627	0.9660	0.9660	0.9618	0.9660	0.9680	0.9639
R_6 (O_a–H_{2a})	0.9646	0.9605	0.9666	0.9627	0.9708	0.9660	0.9618	0.9660	0.9658	0.9614
ϕ_3 ($H_{1a}O_aH_{2a}$)	105.05	105.18	104.36	104.68	102.60	104.07	104.35	104.10	103.95	104.27
ϕ_4 ($O_aC_1C_2$)	152.65	151.88	164.07	161.29	80.10	178.34	177.80	178.69	79.63	79.69
ϕ_5 ($H_{1a}O_aC_1$)	77.51	76.51	126.27	126.52	29.41	118.45	118.23	119.35	11.06	11.27
δ_2 ($O_aC_1C_2H_2$) [a]	−178.93	−177.39	180	180	−60.40	180	180	180	0	0
δ_3 ($H_{1a}O_aC_1C_2$) [a]	4.79	3.86	−101.55	−99.89	71.95	63.72	63.71	−64.78	−20.52	−24.14
δ_4 ($H_{2a}O_aH_{1a}C_1$) [a]	−144.43	−142.49	160.95	163.67	20.51	133.97	133.75	−136.15	110.17	113.73
R_7 (O_b–C_2)	3.5709	3.5074	3.9802	3.8767	3.3182	3.2944	3.3000	3.2804	3.4236	3.3925
R_8 (H_{1b}–O_b)	0.9718	0.9681	0.9670	0.9627	0.9681	0.9660	0.9618	0.9656	0.9680	0.9639
R_9 (H_{2b}–O_b)	0.9663	0.9620	0.9701	0.9660	0.9651	0.9660	0.9618	0.9657	0.9658	0.9614
ϕ_6 ($H_{2b}O_bH_{1b}$)	104.14	104.61	103.10	103.15	105.38	104.07	104.35	104.28	103.95	104.27
ϕ_7 ($O_bC_2O_a$)	41.64	41.83	52.71	41.35	50.85	179.55	179.41	179.95	159.25	159.39
ϕ_8 ($H_{1b}O_bC_2$)	8.60	7.62	22.10	20.60	28.91	118.45	118.23	130.23	11.06	11.27
δ_5 ($O_bC_2O_aC_1$) [a]	178.26	178.25	180	180	−84.20	0	0	180	0	0
δ_6 ($H_{1b}O_bC_2C_1$) [a]	−176.22	178.26	180	180	69.98	63.72	63.71	180	20.52	24.14
δ_7 ($H_{2b}O_bH_{1b}C_2$) [a]	114.71	122.31	0	0	−157.40	133.97	133.74	180	−110.17	−113.73
A	6.5534	6.6598	6.0000	6.1309	5.3149	177.032	177.240	194.943	30.6510	31.5430
B	2.9548	3.0089	2.5641	2.6113	3.2567	0.8687	0.8713	0.8667	1.2535	1.2753
C	2.0514	2.0876	1.8115	1.8470	2.2922	0.8660	0.8686	0.8664	1.2134	1.2350

[a] Dihedral angle between the two planes defined from the first and the last three designated atoms.

TABLE II: Harmonic Vibrational Frequencies ω (cm^{-1}), IR Intensities IR–I (km/mol), Zero Point Energies ZPE (kcal/mol) of the m1, m2, m3 and m4 Minima and of the sp1 and sp2 Saddle Points of the $C_2H_2(H_2O)_2$ (AW_2) at the MP2/avdz and avtz Level.

AW_2	m2				sp1			m3		
	avdz		avtz		avdz			avdz		avtz
	ω	IR–I	ω		ω	IR–I		ω	IR–I	ω
$\omega_1(a')$	51	0.921	53	$\omega_1(a'')$	133i	145	$\omega_1(a_u)$	12	69.1	19
$\omega_2(a'')$	63	15.5	54	$\omega_2(a'')$	45i	12.3	$\omega_2(a_u)$	28	9.06	25
$\omega_3(a')$	106	2.18	93	$\omega_3(a')$	65	2.72	$\omega_3(b_u)$	33	41.9	30
$\omega_4(a'')$	111	0.628	97	$\omega_4(a'')$	87	17.1	$\omega_4(b_g)$	75	0	69
$\omega_5(a')$	123	6.98	124	$\omega_5(a')$	109	2.05	$\omega_5(a_g)$	86	0	86
$\omega_6(a')$	157	2.19	156	$\omega_6(a')$	151	4.98	$\omega_6(a_g)$	97	0	91
$\omega_7(a'')$	194	9.52	191	$\omega_7(a')$	171	8.48	$\omega_7(b_u)$	111	424	122
$\omega_8(a')$	207	204	199	$\omega_8(a'')$	231	38.4	$\omega_8(b_u)$	143	3.54	135
$\omega_9(a'')$	260	85.5	271	$\omega_9(a')$	322	170	$\omega_9(a_u)$	151	55.8	163
$\omega_{10}(a')$	349	72.8	348	$\omega_{10}(a'')$	325	4.11	$\omega_{10}(a_g)$	159	0	166
$\omega_{11}(a'')$	456	5.26	550	$\omega_{11}(a'')$	420	4.70	$\omega_{11}(b_g)$	186	0	213
$\omega_{12}(a')$	458	0.835	572	$\omega_{12}(a')$	442	18.4	$\omega_{12}(a_g)$	550	0	677
$\omega_{13}(a'')$	553	73.1	623	$\omega_{13}(a'')$	474	67.5	$\omega_{13}(b_g)$	568	0	696
$\omega_{14}(a')$	751	110	789	$\omega_{14}(a')$	709	97.1	$\omega_{14}(b_u)$	820	90.6	840
$\omega_{15}(a'')$	761	104	791	$\omega_{15}(a')$	721	94.5	$\omega_{15}(a_u)$	833	89.3	859
$\omega_{16}(a')$	1629	82.9	1629	$\omega_{16}(a')$	1609	86.9	$\omega_{16}(b_u)$	1624	139	1629
$\omega_{17}(a')$	1652	83.6	1661	$\omega_{17}(a')$	1656	85.6	$\omega_{17}(a_g)$	1624	0	1629
$\omega_{18}(a')$	1939	2.58	1959	$\omega_{18}(a')$	1938	0.438	$\omega_{18}(a_g)$	1931	0	1949
$\omega_{19}(a')$	3402	195	3403	$\omega_{19}(a'')$	3419	116	$\omega_{19}(b_u)$	3367	425	3357
$\omega_{20}(a')$	3501	0.844	3512	$\omega_{20}(a')$	3507	0.334	$\omega_{20}(a_g)$	3459	0	3476
$\omega_{21}(a')$	3749	147	3763	$\omega_{21}(a')$	3756	116	$\omega_{21}(b_u)$	3800	19.5	3818
$\omega_{22}(a')$	3792	15.4	3809	$\omega_{22}(a')$	3776	57.0	$\omega_{22}(a_g)$	3800	0	3818
$\omega_{23}(a')$	3882	123	3888	$\omega_{23}(a')$	3894	72.9	$\omega_{23}(b_g)$	3932	0	3942
$\omega_{24}(a'')$	3921	95.4	3929	$\omega_{24}(a')$	3922	165	$\omega_{24}(a_u)$	3962	154	3942
ZPE	45.84		46.50		45.33			44.77		45.40

TABLE II (Continued)

AW_2	sp2			m4		
	avdz			avdz		avtz
	ω	IR–I		ω	IR–I	ω
$\omega_1(a'')$	62i	196	$\omega_1(b_u)$	9	4.11	7
$\omega_2(a'')$	17	44.8	$\omega_2(a_u)$	12	15.5	16
$\omega_3(a')$	30	26.1	$\omega_3(b_g)$	19	0	25
$\omega_4(a'')$	32	0.893	$\omega_4(a_g)$	82	0	83
$\omega_5(a')$	74	66.8	$\omega_5(a_u)$	115	226	117
$\omega_6(a')$	96	1.61	$\omega_6(b_u)$	124	3.28	126
$\omega_7(a'')$	105	28.2	$\omega_7(b_g)$	126	0	128
$\omega_8(a')$	118	195	$\omega_8(b_u)$	150	164	179
$\omega_9(a')$	144	4.01	$\omega_9(a_g)$	158	0	183
$\omega_{10}(a')$	175	7.30	$\omega_{10}(b_g)$	339	0	362
$\omega_{11}(a'')$	178	9.71	$\omega_{11}(a_u)$	352	87.0	366
$\omega_{12}(a')$	570	0.0494	$\omega_{12}(b_g)$	405	0	608
$\omega_{13}(a'')$	570	0.112	$\omega_{13}(b_g)$	509	0	628
$\omega_{14}(a'')$	827	85.8	$\omega_{14}(b_u)$	709	87.4	755
$\omega_{15}(a')$	828	91.4	$\omega_{15}(b_u)$	741	112	774
$\omega_{16}(a')$	1624	111	$\omega_{16}(b_u)$	1625	86.2	1630
$\omega_{17}(a')$	1624	22.0	$\omega_{17}(a_g)$	1626	0	1630
$\omega_{18}(a')$	1932	0.0064	$\omega_{18}(a_g)$	1937	0	1959
$\omega_{19}(a')$	3371	415	$\omega_{19}(a_u)$	3418	123	3418
$\omega_{20}(a')$	3464	0.469	$\omega_{20}(a_g)$	3506	0	3513
$\omega_{21}(a')$	3800	9.43	$\omega_{21}(b_u)$	3778	169	3790
$\omega_{22}(a')$	3803	8.17	$\omega_{22}(a_g)$	3781	0	3794
$\omega_{23}(a'')$	3932	76.7	$\omega_{23}(b_u)$	3915	309	3922
$\omega_{24}(a')$	3936	78.0	$\omega_{24}(a_g)$	3918	0	3925
ZPE	44.67			44.82		45.68

TABLE III: Cartesian Coordinates X, Y, Z (Å) and Rotational Constants RC (A, B, C in GHz) of the m1, m2, m3, m4, m5, m6, m7, m8, m9, and m10 Minima and of the sp1, sp2, and sp3 Saddle Points of the $C_2H_2(H_2O)_3$ (AW_3) at the MP2/avdz Level.

AW_3_m1

Atoms	X	Y	Z
C	−1.661906	−0.937551	−0.048489
C	−2.745060	−0.357647	−0.171023
O	1.283349	−1.885350	0.110701
O	2.163875	0.747958	−0.178874
O	−0.334359	1.962740	0.165564
H	−0.690802	−1.415391	0.055487
H	−3.706266	0.110869	−0.286354
H	1.841550	−2.363756	0.734889
H	1.708927	−1.007110	0.014183
H	2.533610	1.037516	−1.022067
H	1.325165	1.247909	−0.088192
H	−0.489263	2.315834	1.051566
H	−0.984043	1.242533	0.078431

RC(A, B, C): 3.1198030 1.9351033 1.2192589

AW_3_m2

Atoms	X	Y	Z
C	−1.942076	0.552060	−0.310596
C	−2.914096	−0.200355	−0.411769
O	0.352394	−1.200255	1.149407
O	1.003400	1.540018	0.387250
O	2.093925	−0.612208	−0.960915
H	−1.070391	1.182420	−0.200790
H	−3.777377	−0.833666	−0.512184
H	−0.584427	−1.256369	0.908843
H	0.478052	−0.247361	1.307463
H	1.581065	2.264519	0.655710
H	1.536666	0.992902	−0.228122
H	1.877823	−0.930233	−1.846053
H	1.497862	−1.102885	−0.356613

RC(A, B, C): 3.8452759 1.6273519 1.4630162

AW_3_m3

C	−2.942807	−0.213979	−0.396380
C	−1.962649	0.532860	−0.345888
O	0.985830	1.543896	0.407027
O	2.057919	−0.578705	−0.999751
O	0.330566	−1.207593	1.094204
H	−3.812441	−0.843443	−0.458289
H	−1.082997	1.157287	−0.276067
H	1.487934	2.328614	0.656970
H	1.578003	1.027506	−0.178907
H	2.906418	−1.036329	−1.037646
H	1.524488	−1.073540	−0.341873
H	−0.588154	−1.276840	0.793315
H	0.424961	−0.257322	1.284254

RC(A, B, C): 3.9291605 1.6176654 1.4421495

AW_3_m4

C	−2.736681	−0.365616	−0.213276
C	−1.650229	−0.930166	−0.053602
O	−0.340755	1.968144	0.219077
O	2.104325	0.724146	−0.393547
H	−3.699817	0.090912	−0.357139
H	−0.675117	−1.394021	0.077465
H	2.855514	1.228271	−0.058983
H	1.315003	1.260263	−0.169237
H	−0.978001	1.251165	0.050276
H	−0.491506	2.192347	1.146953
O	1.301271	−1.858720	0.309060
H	1.760576	−2.516875	−0.226434
H	1.716090	−1.005933	0.061646

RC(A, B, C): 3.0944372 1.9383801 1.2316304

AW_3_m5

C	−2.852213	−0.304488	−0.314999
C	−1.901548	0.448759	−0.537569
O	1.086913	1.554509	0.065007
O	1.842734	−0.981513	−0.924839
O	0.333091	−0.700846	1.461776
H	−3.697147	−0.948002	−0.146445
H	−1.047483	1.089537	−0.697384
H	1.871028	−0.009969	−0.843738
H	2.713540	−1.238314	−1.250801
H	−0.591024	−0.802506	1.186790

AW_3_m6

C	−0.617080	1.787889	0.072961
C	0.617123	1.787880	0.072985
O	−2.782711	−0.521424	−0.209791
O	0.000000	−1.301282	0.312995
O	2.782700	−0.521449	−0.209784
H	−1.693420	1.728969	0.049801
H	1.693458	1.728814	0.049877
H	−3.427571	−1.081353	−0.658796
H	−1.961575	−1.042685	−0.205279
H	−0.000093	−1.585983	1.237886

Table III (continued)

Atoms	X	Y	Z
H	0.833893	−1.160902	0.761512
H	1.508670	2.299016	0.510763
H	0.829186	0.928312	0.779165
RC(A, B, C):	3.7299661	1.6621155	1.5638343

AW_3_m7

C	−3.220758	−0.953458	0.143960
C	−2.010060	−1.104496	−0.042242
O	0.900527	−0.192372	−0.385071
O	−1.026732	1.922539	0.146295
H	−4.281243	−0.869811	0.301319
H	−0.937099	−1.161039	−0.189428
H	1.839967	−0.121445	−0.148493
H	0.505005	0.669470	−0.168400
H	−1.703667	1.227247	0.193289
H	−1.277049	2.437491	−0.632085
O	3.759427	−0.268593	0.197377
H	4.210947	−0.658606	−0.563035
H	3.962274	−0.868165	0.927721
RC(A, B, C):	4.9063787	1.0198182	0.8597597

AW_3_sp1

C	2.034579	0.593530	0.616602
C	2.034579	0.593530	−0.616602
O	−2.128491	−0.659876	0.000000
O	0.234282	−2.367724	0.000000
H	2.037256	0.575049	1.693079
H	2.037256	0.575049	−1.693079
H	0.887375	−1.656548	0.000000
H	−0.612615	−1.887607	0.000000
H	−1.952975	0.297267	0.000000
O	−0.946752	1.919133	0.000000
H	−3.088064	−0.749036	0.000000
H	0.000000	1.708601	0.000000
H	−0.995488	2.882600	0.000000
RC(A, B, C):	2.6356962	2.1783538	1.2828859

AW_3_m9

C	−1.832357	1.456760	−0.616459
C	−1.832357	1.456760	0.616459
O	1.579081	1.420283	0.00000
O	1.941864	−1.543804	0.000000
O	−1.027706	−1.858586	0.000000
H	−0.000023	−0.325105	0.367641
H	3.427493	−1.081339	−0.658932
H	1.961554	−1.042694	−0.205226
RC(A, B, C):	3.8469378	1.6856355	1.2041702

AW_3_m8

C	0.986167	−0.774056	−0.020310
C	−0.178245	−1.485112	−0.028809
H	2.018521	−0.453633	−0.015133
H	−1.219694	−1.474622	−0.025639
O	4.065337	0.239527	0.002337
H	4.752035	−0.116062	−0.576531
H	4.533972	0.458415	0.818185
H	−0.745908	1.057487	0.067157
O	−1.514435	1.654377	0.064482
H	−1.422286	2.149517	−0.760197
O	−3.279270	−0.595126	−0.036750
H	−2.858219	0.281913	0.046808
H	−4.079004	−0.538236	0.499508
RC(A, B, C):	5.9376015	0.8965535	0.7836058

AW_3_sp2

C	−1.064516	1.479538	0.000000
C	−2.281584	1.673993	0.000000
O	2.273862	1.127450	0.000000
O	−1.572162	−1.915936	0.000000
H	0.000000	1.306716	0.000000
H	−3.343607	1.841938	0.000000
H	2.702493	1.534473	0.764790
H	2.702493	1.534473	−0.764790
H	−0.601123	−1.875642	0.000000
H	−1.826524	−0.983200	0.000000
O	1.367291	−1.615455	0.000000
H	1.831192	−0.761956	0.000000
H	2.059748	−2.286453	0.000000
RC(A, B, C):	2.5271530	1.8805473	1.0836624

AW_3_sp3

C	2.081148	0.594670	0.616660
C	2.081148	0.594670	−0.616660
O	−0.960373	1.916182	0.000000
O	−2.461711	−0.703402	0.000000
H	2.077447	0.593611	1.693469

Table III (continued)

Atoms	X	Y	Z
H	–1.835443	1.459190	–1.692745
H	–1.835443	1.459190	1.692745
H	–1.352098	–0.947447	0.000000
H	–0.062458	–1.760528	0.000000
H	0.618270	1.530983	0.000000
H	1.701081	0.457764	0.000000
H	2.404528	–1.911581	–0.764870
H	2.404528	–1.911581	0.764870
RC(A, B, C):	3.0536444	1.7879471	1.2148280

AW_3_m10

C	0.000000	1.032883	0.000000
C	–1.181557	0.678445	0.000000
O	3.308494	0.846781	0.000000
O	1.789767	–1.760142	0.000000
H	1.039766	1.315973	0.000000
H	–2.218162	0.373564	0.000000
H	3.888975	0.966974	0.763365
H	3.888975	0.966974	–0.763365
H	0.888384	–1.408004	0.000000
H	2.332442	–0.956001	0.000000
O	–4.276770	–0.329904	0.000000
H	–4.651486	–0.790661	0.761859
H	–4.651486	–0.790661	–0.761859
RC(A, B, C):	5.5734018	0.8084774	0.7107127

Atoms	X	Y	Z
H	2.077447	0.593611	–1.693469
H	–1.674193	–1.268713	0.000000
H	–2.091826	0.192670	0.000000
H	0.000000	1.797958	0.000000
H	–1.097356	2.871565	0.000000
O	0.197001	–2.134315	0.000000
H	0.949972	–1.526593	0.000000
H	0.585399	–3.017869	0.000000
RC(A, B, C):	2.7627822	1.9819368	1.2383632

TABLE IV: Harmonic Vibrational Frequencies ω (cm^{-1}), Zero Point Energies ZPE (kcal/mol), and IR Intensities IR–I (km/mol) of the m2, m3, m4, m5, m6, m7, m8, m9, and m10 Minima and of the sp1, sp2, and sp3 Saddle Points of the $C_2H_2(H_2O)_3$ (AW_3) at the MP2/avdz Level.

AW_3	m2		m3		m4		m5		m6	
	ω	IR–I	ω	IR–I	ω	IR–I	ω	IR–I	ω	IR–I
ω_1	23	1.22	30	1.76	21	4.33	31	0.633	35	1.58
ω_2	68	0.224	70	0.804	53	5.62	74	0.412	81	35.1
ω_3	99	2.18	92	0.533	113	13.8	78	3.48	81	7.05
ω_4	109	1.82	106	0.507	118	6.25	104	3.78	87	8.05
ω_5	134	1.92	131	5.93	147	58.1	138	85.3	114	0.910
ω_6	173	6.27	172	14.5	161	21.6	156	0.403	116	136.
ω_7	191	30.2	184	33.5	165	38.0	169	30.1	126	39.7
ω_8	208	105	202	18.1	192	70.2	186	5.84	132	2.81
ω_9	212	64.8	223	44.9	203	7.10	232	14.1	173	4.96
ω_{10}	225	9.28	224	64.0	213	63.9	250	30.5	174	16.1
ω_{11}	319	20.9	314	61.4	236	23.7	334	61.8	215	65.7
ω_{12}	331	22.9	334	87.0	286	13.2	383	193.	244	242.
ω_{13}	398	120	398	89.2	384	84.6	407	123.	285	143.
ω_{14}	456	17.3	449	22.7	429	124.	444	15.3	376	19.1
ω_{15}	475	35.3	464	171.	471	15.8	458	62.6	433	0.295
ω_{16}	492	170	480	7.43	510	11.3	486	33.4	464	0.116
ω_{17}	540	128	606	201.	584	47.0	540	83.3	561	146.
ω_{18}	682	267	617	83.5	690	150.	678	263.	611	84.4
ω_{19}	769	83.4	763	96.2	746	76.0	744	95.6	723	120.
ω_{20}	771	98.1	770	104.	820	97.4	760	61.0	725	4.30
ω_{21}	853	5.81	859	47.6	850	73.8	912	63.1	755	109.
ω_{22}	1633	85.5	1634	62.7	1639	50.0	1630	56.0	1623	43.5
ω_{23}	1647	71.3	1649	136.	1649	61.1	1646	111.	1641	4.75
ω_{24}	1667	37.2	1664	17.7	1672	28.2	1654	14.2	1644	117.
ω_{25}	1933	4.74	1933	4.39	1921	17.9	1935	1.96	1932	0.467
ω_{26}	3372	221.	3377	220.	3289	391.	3392	146.	3397	160.
ω_{27}	3490	4.98	3492	3.82	3478	11.0	3486	333.	3488	1.77
ω_{28}	3535	172	3539	173.	3546	536.	3498	41.3	3618	319.
ω_{29}	3591	547.	3593	566.	3591	506.	3658	167.	3703	318.
ω_{30}	3705	171	3711	158.	3695	275.	3679	309.	3718	85.7
ω_{31}	3843	134	3839	146.	3880	128.	3827	201.	3858	130.
ω_{32}	3889	75.3	3891	104.	3890	92.2	3886	93.6	3902	194.
ω_{33}	3889	116	3892	91.0	3893	98.6	3901	108.	3905	23.6
ZPE	62.50		62.47		62.24		62.55		61.39	61.39

	m6	
	ω	IR–I
ω_1(a')	35	1.58
ω_2(a')	81	35.1
ω_3(a")	81	7.05
ω_4(a")	87	8.05
ω_5(a")	114	0.910
ω_6(a')	116	136.
ω_7(a')	126	39.7
ω_8(a")	132	2.81
ω_9(a')	173	4.96
ω_{10}(a")	174	16.1
ω_{11}(a')	215	65.7
ω_{12}(a")	244	242.
ω_{13}(a")	285	143.
ω_{14}(a')	376	19.1
ω_{15}(a")	433	0.295
ω_{16}(a")	464	0.116
ω_{17}(a')	561	146.
ω_{18}(a")	611	84.4
ω_{19}(a')	723	120.
ω_{20}(a")	725	4.30
ω_{21}(a')	755	109.
ω_{22}(a')	1623	43.5
ω_{23}(a")	1641	4.75
ω_{24}(a')	1644	117.
ω_{25}(a')	1932	0.467
ω_{26}(a")	3397	160.
ω_{27}(a')	3488	1.77
ω_{28}(a')	3618	319.
ω_{29}(a")	3703	318.
ω_{30}(a')	3718	85.7
ω_{31}(a')	3858	130.
ω_{32}(a")	3902	194.
ω_{33}(a')	3905	23.6
	61.39	61.39

Table IV (continued)

AW_3	m7		m8			sp1			sp2	
	ω	IR–I	ω	IR–I		ω	IR–I		ω	IR–I
ω_1	16	4.20	28	3.37	ω_1(a")	171i	4.34	ω_1(a")	127i	94.6
ω_2	37	10.1	33	4.86	ω_2(a")	140i	275.	ω_2(a")	16i	1.09
ω_3	59	52.1	44	15.9	ω_3(a")	54i	20.3	ω_3(a')	46	0.024
ω_4	87	7.20	93	50.4	ω_4(a")	12	1.35	ω_4(a")	78	12.9
ω_5	105	1.62	103	17.8	ω_5(a')	39	0.061	ω_5(a')	81	5.20
ω_6	109	5.23	109	138.	ω_6(a")	89	7.39	ω_6(a')	107	0.553
ω_7	143	20.2	126	59.4	ω_7(a')	93	1.63	ω_7(a')	108	4.08
ω_8	152	47.6	130	51.7	ω_8(a')	122	1.51	ω_8(a')	146	1.95
ω_9	162	73.3	154	8.45	ω_9(a')	164	0.896	ω_9(a")	172	55.5
ω_{10}	172	24.1	177	13.3	ω_{10}(a')	193	10.9	ω_{10}(a')	191	1.29
ω_{11}	200	109.	184	29.0	ω_{11}(a')	240	97.1	ω_{11}(a")	228	4.03
ω_{12}	212	119.	195	2.56	ω_{12}(a")	270	34.3	ω_{12}(a')	249	158.
ω_{13}	223	18.4	197	115.	ω_{13}(a')	346	7.93	ω_{13}(a")	271	38.5
ω_{14}	421	191.	251	62.8	ω_{14}(a")	376	6.16	ω_{14}(a')	307	49.2
ω_{15}	477	18.9	355	134.	ω_{15}(a")	431	0.121	ω_{15}(a')	417	155.
ω_{16}	497	26.8	503	65.6	ω_{16}(a')	466	142.	ω_{16}(a")	450	9.58
ω_{17}	563	47.1	561	8.64	ω_{17}(a")	476	0.158	ω_{17}(a')	457	3.02
ω_{18}	628	171.	582	31.0	ω_{18}(a")	507	15.7	ω_{18}(a")	489	83.1
ω_{19}	666	19.8	712	107.	ω_{19}(a")	535	112.	ω_{19}(a")	598	68.7
ω_{20}	791	86.2	822	92.1	ω_{20}(a')	710	96.5	ω_{20}(a')	753	96.3
ω_{21}	816	95.9	826	97.5	ω_{21}(a')	728	97.3	ω_{21}(a")	766	99.9
ω_{22}	1623	73.0	1625	67.6	ω_{22}(a')	1620	42.9	ω_{22}(a')	1619	105.
ω_{23}	1631	56.8	1631	68.5	ω_{23}(a')	1643	60.5	ω_{23}(a')	1644	17.4
ω_{24}	1651	23.6	1647	27.9	ω_{24}(a')	1667	53.0	ω_{24}(a')	1665	68.2
ω_{25}	1928	10.7	1924	1.15	ω_{25}(a')	1937	0.784	ω_{25}(a')	1938	2.54
ω_{26}	3337	318.	3351	400.	ω_{26}(a")	3416	122.	ω_{26}(a')	3403	209.
ω_{27}	3485	3.14	3445	11.0	ω_{27}(a')	3505	0.636	ω_{27}(a')	3499	0.899
ω_{28}	3674	53.9	3637	300.	ω_{28}(a')	3693	274.	ω_{28}(a')	3716	334.
ω_{29}	3737	184.	3714	207.	ω_{29}(a')	3713	233.	ω_{29}(a')	3735	110.
ω_{30}	3787	475.	3800	11.2	ω_{30}(a')	3750	164.	ω_{30}(a')	3791	14.4
ω_{31}	3800	118.	3887	132.	ω_{31}(a')	3886	129.	ω_{31}(a')	3873	164.
ω_{32}	3893	131.	3899	97.6	ω_{32}(a')	3913	181.	ω_{32}(a')	3911	147.
ω_{33}	3926	85.5	3931	81.0	ω_{33}(a')	3915	140.	ω_{33}(a")	3920	100.
ZPE	61.50		61.01			60.69			60.94	

Table IV (continued)

AW_3	m9		sp3		m10	
	ω	IR–I	ω	IR–I	ω	IR–I
ω_1(a")	15	0.001	146i	0	18	17.8
ω_2(a")	32	24.3	128i	269.	23	10.1
ω_3(a')	45	0.767	23i	8.04	24	24.0
ω_4(a")	52	4.10	41	1.31	78	0.058
ω_5(a')	96	1.76	65	39.7	82	41.4
ω_6(a')	107	0.752	99	0	88	1.77
ω_7(a")	129	6.08	102	0.009	107	141.
ω_8(a")	138	0.001	116	1.48	111	6.39
ω_9(a')	139	9.46	137	0.145	132	10.7
ω_{10}(a')	157	0.140	148	0.033	146	29.2
ω_{11}(a')	209	140.	170	69.6	166	1.71
ω_{12}(a")	325	0.001	259	65.4	174	45.5
ω_{13}(a")	346	75.2	327	0	195	2.77
ω_{14}(a')	356	126.	331	9.20	207	217.
ω_{15}(a')	375	67.5	420	0	303	67.7
ω_{16}(a")	439	0.001	430	125.	349	64.5
ω_{17}(a")	449	12.9	435	43.6	525	4.86
ω_{18}(a")	553	0	463	110.	532	27.6
ω_{19}(a")	586	181.	472	0	566	65.0
ω_{20}(a')	714	92.6	714	97.6	802	104.
ω_{21}(a')	717	107.	730	96.9	821	96.7
ω_{22}(a')	1627	80.1	1611	31.8	1625	70.3
ω_{23}(a')	1631	102.	1617	56.6	1628	78.9
ω_{24}(a')	1665	1.09	1675	67.5	1657	87.1
ω_{25}(a')	1938	0.711	1936	0.511	1931	3.04
ω_{26}(a")	3420	116.	3414	125.	3372	369.
ω_{27}(a')	3508	0.600	3503	0.377	3470	2.23
ω_{28}(a')	3739	198.	3749	144.	3750	139.
ω_{29}(a')	3748	76.0	3777	21.8	3793	16.8
ω_{30}(a')	3793	26.4	3781	76.9	3800	10.9
ω_{31}(a')	3866	0.243	3855	233.	3871	142.
ω_{32}(a')	3880	489.	3921	256.	3923	91.6
ω_{33}(a")	3920	102.	3924	95.1	3931	79.8
ZPE	61.06		60.36		60.32	

TABLE V: Cartesian Coordinates X, Y, Z (Å) and Rotational Constants RC (A, B, C in GHz) of 27 Minima and 1 Saddle point of the $C_2H_2(H_2O)_4$ AW_4 at the MP2/avdz and 3 Minima and 2 Saddle Points of AW_4 at the MP2/4-31G Level.

AW_4_m1

Atoms	X	Y	Z
C	2.520445	−0.472284	−0.441728
C	3.359099	0.368435	−0.774439
O	0.234116	1.133533	1.212631
O	−0.164895	−1.634159	0.848341
O	−2.253120	−1.050880	−0.799784
O	−1.924410	1.633343	−0.397533
H	1.761929	−1.175502	−0.128167
H	4.105431	1.080032	−1.079231
H	1.100951	1.258051	0.799004
H	0.142362	0.158869	1.253907
H	−0.431251	−2.285765	1.508324
H	−0.939109	−1.548220	0.240759
H	−2.198394	−1.228741	−1.746853
H	−2.248969	−0.067339	−0.725212
H	−2.563401	2.188450	0.065723
H	−1.140347	1.588561	0.199507

RC(A, B, C): 2.3461483 1.0976926 0.9318485

AW_4_m2

Atoms	X	Y	Z
C	−1.935216	0.087898	−0.868252
C	−3.022820	−0.226628	−0.378623
O	0.753995	1.750638	1.165000
O	1.158022	0.809812	−1.435769
O	1.624375	−1.646238	−0.396662
O	−0.072753	−0.891497	1.602175
H	−0.970349	0.360044	−1.274178
H	−3.981465	−0.497822	0.026016
H	0.148766	2.501604	1.205441
H	0.937710	1.622891	0.211134
H	1.739900	1.099651	−2.148350
H	1.478869	−0.088833	−1.177521
H	−2.449783	−2.000858	−0.044569
H	1.049472	−1.496001	0.393848
H	−0.956267	−0.916016	1.204406
H	0.142687	0.065999	1.607073

RC(A, B, C): 1.9720490 1.3266345 1.2867195

AW_4_m3

O	−1.278966	−1.860154	0.371871
O	0.139886	−0.029514	1.822285
O	−1.134478	1.959109	0.320653
O	−1.189380	−0.039271	−1.628296
H	−0.737233	−1.310014	0.990175
H	−0.865006	−2.731714	0.378788
H	−1.302006	−0.816631	−1.028570
H	−1.779851	−0.196068	−2.374753
H	−0.305506	0.764884	1.456701
H	−1.310167	1.382583	−0.451881
H	−1.985004	2.360878	0.536085
H	1.027198	0.021500	1.435030
C	3.043654	−0.093184	−0.287877
C	1.951594	0.042959	−0.859522
H	0.982143	0.081904	−1.336998
H	4.007450	−0.037338	0.187705

RC(A, B, C): 1.9559502 1.3285481 1.2898800

AW_4_m4

C	−3.167442	−0.474730	−0.815387
C	−2.418677	0.463023	−0.531583
O	0.225410	1.699258	0.839361
O	2.154781	0.916313	−0.992888
O	1.765385	−1.727726	−0.293565
O	−0.246027	−0.901739	1.410125
H	−3.836506	−1.273293	−1.082017
H	−1.737236	1.253410	−0.254884
H	0.439422	2.235811	1.612529
H	0.057724	0.785461	1.187045
H	1.912617	1.231238	−1.872545
H	1.503716	1.332136	−0.385390
H	−1.073448	−1.087324	0.941643
H	0.447696	−1.333724	0.862150
H	2.011223	−0.835062	−0.625492
H	2.595124	−2.127259	−0.005488

RC(A, B, C): 2.2101087 1.1610297 1.0131789

AW_4_m5

O	−1.365244	−1.859236	−0.023414
O	0.124003	−0.433272	1.760588
O	−0.874504	1.952664	0.684021
O	−1.234425	0.363375	−1.562750
H	−0.844768	−1.448998	0.711087
H	−2.115986	−2.287578	0.404935

AW_4_m6

C	3.360949	0.282060	−0.740276
C	2.435822	−0.513948	−0.562641
O	0.312853	0.952095	1.391583
O	−0.279067	−1.707358	0.666677
O	−1.725439	1.764890	−0.273339
O	−2.364784	−0.828747	−0.855700

Table V (Continued)

Atoms	X	Y	Z
H	−1.433262	−0.502107	−1.131258
H	−1.724681	0.365438	−2.393090
H	−0.203427	0.466699	1.549256
H	−1.153417	1.567329	−0.171997
H	−1.624119	2.480171	0.984785
H	1.024484	−0.430371	1.401184
C	3.042684	−0.123885	−0.327417
C	1.940526	0.066572	−0.847164
H	0.962096	0.230034	−1.276953
H	4.015168	−0.284988	0.101977
RC(A, B, C):	1.9485143	1.3431604	1.2822552

AW_4_m7

C	3.059920	0.393069	−0.806429
C	2.215265	−0.498314	−0.693009
O	−0.383460	−1.779915	0.729903
O	−2.050724	−0.653013	−1.165675
O	−1.554089	1.845974	−0.089268
O	0.309234	0.685570	1.609464
H	3.812070	1.151060	−0.933643
H	1.458994	−1.255561	−0.550895
H	−0.148890	−0.935887	1.194375
H	−0.586796	−2.413234	1.428723
H	−1.564375	−1.199492	−0.509902
H	−2.939559	−1.027273	−1.197225
H	−0.302160	1.229241	1.062916
H	−1.810485	1.025400	−0.566507
H	−1.306330	2.469294	−0.783203
H	1.168739	0.798990	1.176602
RC(A, B, C):	2.0968636	1.2297895	1.0940218

AW_4_m8

C	−2.377077	0.601856	−0.031690
C	3.303159	−0.211767	−0.099143
O	−0.422753	2.024763	0.083452
O	−1.659083	−0.293320	1.408648
O	−1.943630	−0.172460	−1.363002
O	0.165138	−1.703105	−0.034130
H	1.516870	1.263982	0.021260
H	4.139518	−0.885515	−0.154583
H	−0.857919	1.701875	−0.720809
H	−0.838237	1.475211	0.769804
H	−2.717463	−0.321747	−1.920185
H	−2.267423	−0.234084	−0.444238
H	1.038152	−1.278280	−0.079165
H	−0.299496	−1.377232	−0.824628
H	−0.935569	−0.900593	1.123623
H	−1.977217	−0.631174	2.254172
RC(A, B, C):	2.4654598	1.2035405	1.0590899

AW_4_m9

C	2.148218	0.986491	−0.155095
C	3.207442	0.369024	−0.303431
O	−0.565869	2.410409	0.212543
O	−2.660031	0.604418	−0.016814
O	−1.602493	−1.918600	−0.340516
O	1.058221	−1.984660	0.451748
H	1.208144	1.522950	−0.032341
H	4.142177	−0.145108	−0.440086
H	−0.823181	3.186009	−0.300220
H	−1.335034	1.803710	0.139218
H	−3.271403	0.516266	0.724547
H	−2.311898	−0.304231	−0.158608
H	−1.661561	−2.376487	−1.187674
H	−0.653280	−1.960511	−0.094406
H	1.172809	−2.090867	1.405213
H	1.560672	−1.177356	0.239819

AW_4_m10

C	3.315550	−0.047553	−0.060605
C	2.312395	0.665668	0.024528
O	−0.593220	1.964900	0.158381
O	−1.910000	−0.086823	−1.241336
O	−1.699664	−0.613705	1.410674
O	0.290122	−1.825719	−0.185702
H	−1.336678	0.265491	1.602238
H	−0.912321	−1.131399	1.142655
H	−0.189915	−1.427798	−0.930634
H	1.148145	−1.372188	−0.192501
H	−2.737587	−0.191804	−1.726383
H	−2.104579	−0.347458	−0.307996
H	−1.098292	1.484554	−0.527369
H	−0.849088	2.889965	0.057964
H	4.206896	−0.645361	−0.129036
H	1.407850	1.258085	0.091395

Table V (Continued)

RC(A, B, C): 1.8243129 1.2259723 0.7587176

AW_4_m11

Atoms	X	Y	Z
C	–3.125732	–0.779167	–0.127664
C	–2.399794	0.210807	–0.256800
O	–0.147312	2.407112	–0.342926
O	1.636735	0.661214	1.023410
O	0.087825	–1.536762	0.762175
O	2.137872	–1.091617	–1.165971
H	–3.785747	–1.621797	–0.024036
H	–1.727783	1.058027	–0.357047
H	2.978153	–1.485327	–1.430336
H	2.368473	–0.410395	–0.509293
H	0.553656	1.906525	0.118495
H	0.272936	2.721805	–1.152730
H	–0.806265	–1.312498	0.454292
H	0.591474	–1.728558	–0.050271
H	1.016828	–0.102402	1.138483
H	1.970460	0.865203	1.905718

RC(A, B, C): 2.0482166 1.2611736 0.9568222

RC(A, B, C): 2.4036283 1.2292349 1.0312783

AW_4_m12

Atoms	X	Y	Z
C	–2.858949	–1.183521	0.456874
C	–1.714683	–1.329620	0.017785
O	1.281796	–1.425033	–0.958701
O	2.516177	–0.164170	1.153541
O	1.159596	1.511417	–0.548790
H	–3.857419	–1.088809	0.845362
H	–0.704655	–1.449473	–0.360545
H	1.811872	–2.062336	–1.452179
H	1.810477	–1.210267	–0.158326
H	2.243418	–0.178611	2.078975
H	2.066123	0.618123	0.760625
H	0.227458	1.737746	–0.362699
H	1.098780	0.724932	–1.115995
O	–1.601900	1.910271	0.035402
H	–1.946233	1.003307	0.104880
H	–2.153382	2.326759	–0.639677

RC(A, B, C): 2.1210369 1.2091668 0.9187659

AW_4_m13

C	1.748206	–1.308916	–0.073309
C	2.861235	–1.193328	0.447383
O	–1.211633	–1.165869	–1.157478
O	–1.189469	1.457673	–0.520584
O	1.535787	1.913262	0.162051
H	0.763524	–1.392226	–0.520810
H	3.833447	–1.124382	0.902197
H	–1.658482	–1.403196	–1.979096
H	–1.202974	–0.175265	–1.183853
H	–0.284689	1.714190	–0.254149
H	–1.638481	1.229372	0.312351
H	1.903440	1.018013	0.172116
H	2.076442	2.387514	–0.483022
O	–2.504314	–0.382599	1.273257
H	–2.334915	–0.843695	2.103704
H	–2.156931	–0.971591	0.578152

RC(A, B, C): 2.1197421 1.1864432 0.9497794

AW_4_m14

C	–2.793303	–1.250124	0.466751
C	–1.641617	–1.349379	0.034340
O	1.350661	–1.353744	–1.036063
O	2.323072	–0.194248	1.254992
O	1.118374	1.540230	–0.488464
O	–1.658091	1.885652	0.002395
H	–3.794423	–1.195977	0.855972
H	–0.627773	–1.427714	–0.343322
H	1.837648	–2.035278	–1.514340
H	1.872941	–1.178736	–0.222804
H	3.198510	0.066823	1.565097
H	1.953026	0.605645	0.815262
H	0.176718	1.750621	–0.330214
H	1.091807	0.791462	–1.106104
H	–1.957181	0.967486	0.120034
H	–2.213883	2.229566	–0.709003

RC(A, B, C): 2.0940829 1.2368243 0.9430258

AW_4_m15

C	1.681106	–1.322907	–0.092573
C	2.805973	–1.239482	0.408201
O	–1.273677	–1.087907	–1.225192
O	–1.191099	1.497664	–0.453406

AW_4_m16

C	–3.456321	–0.795731	0.169148
C	–2.788165	0.221822	–0.029282
O	0.122395	–1.020193	–0.361923
O	1.359989	0.431031	1.615161

Table V (Continued)

Atoms	X	Y	Z
O	1.552234	1.898322	0.163492
O	−2.261910	−0.450040	1.361372
H	0.688992	−1.377579	−0.526483
H	3.785358	−1.198953	0.850686
H	−1.694488	−1.270022	−2.073979
H	−1.243154	−0.100446	−1.147960
H	−0.275937	1.735444	−0.204056
H	−1.617516	1.241489	0.382689
H	1.884501	0.984572	0.193208
H	2.092752	2.327677	−0.512397
H	−3.016313	−0.843888	1.815110
H	−2.131055	−0.988265	0.559279
RC(A, B, C):	2.0804055	1.2276592	0.9831211

Atoms	X	Y	Z
O	2.903112	−0.710779	−0.553992
O	−0.036086	1.794887	−0.671277
H	1.068680	1.250021	1.180791
H	2.168886	0.195478	1.125582
H	2.066608	−1.164627	−0.757576
H	3.591155	−1.370852	−0.702001
H	−0.803459	−1.295800	−0.294397
H	0.357360	−0.675195	0.529843
H	0.091065	0.847731	−0.877964
H	0.367416	2.270741	−1.408003
H	−2.166142	1.086437	−0.210158
H	−4.069929	−1.660050	0.350932
RC(A, B, C):	3.0140657	0.9907911	0.9169927

AW_4_m17

O	−0.500802	−1.266787	0.234709
O	0.559904	1.130557	1.334679
O	−1.102303	1.057560	−1.123978
H	−1.451557	−1.365598	0.420251
H	−0.199052	−0.608864	0.893679
H	0.144417	1.538301	0.555571
H	1.479163	0.995789	1.057051
H	−0.945424	1.193683	−2.066825
H	−0.781069	0.148496	−0.927939
O	−3.251369	−0.430672	0.102501
H	−2.833651	0.336673	−0.327204
H	−3.939988	−0.061427	0.668679
C	3.565759	−0.078341	−0.319412
C	2.561103	−0.793198	−0.346380
H	4.456893	0.523640	−0.305307
H	1.665659	−1.396722	−0.356484
RC(A, B, C):	3.4900170	0.9325788	0.8938780

AW_4_sp1[a]

O	−0.566633	−1.326067	0.000000
O	−0.101578	1.334576	0.000000
O	−1.785767	0.187458	1.902544
O	−1.785767	0.187458	−1.902544
H	−1.121765	−1.193358	−0.806688
H	−1.121765	−1.193358	0.806688
H	−1.324603	0.931268	1.453662
H	−2.414893	0.498879	2.573487
H	0.773121	1.763421	0.000000
H	0.000000	0.338403	0.000000
H	−1.324603	0.931268	−1.453662
H	−2.414893	0.498879	−2.573487
C	2.546922	−0.737155	0.000000
C	3.578472	−0.069063	0.000000
H	4.498463	0.471080	0.000000
H	1.616541	−1.276564	0.000000
RC(A, B, C):	2.4431920	1.1114080	0.9769670

AW_4_sp2[a]

C	−3.152385	0.867632	0.000000
C	−4.372965	1.007509	0.000000
O	0.000000	0.466865	0.000000
O	1.307404	−1.860491	0.000000
O	1.899468	0.095329	1.891209
O	1.899468	−0.095329	−1.891209
H	0.514557	0.719194	−0.806207
H	0.514557	0.719194	0.806207
H	2.015397	−0.769476	1.437684
H	2.611060	0.276726	2.526420
H	0.967548	−2.772241	0.000000
H	0.566339	−1.181480	0.000000
H	2.015397	−0.769476	−1.437684
H	2.611060	0.276726	−2.526420

AW_4_m18

C	−2.077778	−0.684880	−0.360999
C	−3.082358	−0.057171	−0.009634
O	0.779859	−1.657166	−0.909189
O	1.507597	−0.723612	1.755768
O	−0.173772	1.473421	0.805075
O	1.570710	1.112118	−1.452643
H	−1.144141	−1.178493	−0.639272
H	−3.997050	0.434191	0.271114
H	1.141433	−0.851602	−1.319144
H	1.117252	−1.589120	0.002635
H	1.409597	1.655460	−2.233885
H	0.940642	1.437501	−0.784736
H	−1.009402	1.013032	0.597845
H	−0.436763	2.245562	1.322657

Table V (Continued)

Atoms	X	Y	Z
H	−5.431566	1.137256	0.000000
H	−2.082972	0.736483	0.000000
RC(A, B, C):	2.6378953	0.7861507	0.7050624

Atoms	X	Y	Z
H	1.032868	0.104956	1.564547
H	2.431219	−0.457265	1.849947
RC(A, B, C):	2.0011713	1.2413144	1.2284133

AW_4_m19[a]

C	−0.548742	2.864238	−0.267836
C	−1.267271	1.917806	0.054025
O	−2.685515	−0.706440	0.689583
O	−0.728372	−2.189341	−0.446414
O	1.051658	−0.238876	−0.802760
O	3.407885	−0.185951	0.648508
H	0.032906	3.720642	−0.526601
H	−1.875758	1.056684	0.313470
H	4.293747	−0.319345	0.267660
H	3.392023	−0.464212	1.581469
H	−2.035073	−1.336639	0.269558
H	−2.885226	−0.991384	1.598415
H	0.592571	0.621179	−0.764445
H	1.908784	−0.205252	−0.316091
H	−0.001431	−1.513207	−0.591588
H	−0.891709	−2.695867	−1.260312
RC(A, B, C):	1.7200434	1.1531126	0.7679001

AW_4_m20

C	1.128142	1.846543	−0.205363
C	−0.098901	1.866902	−0.064904
O	0.689396	−1.105348	0.689428
O	3.384480	−0.360583	−0.214627
O	−2.971871	−0.765209	0.148062
H	2.195728	1.766432	−0.334728
H	−1.175986	1.841131	0.049414
H	2.601401	−0.882258	0.030541
H	4.062900	−1.014433	−0.422235
H	−2.695918	−0.145185	−0.082916
H	−3.887506	0.683986	0.438777
H	0.585990	−0.139529	0.563483
H	0.658704	−1.225370	1.648968
O	−1.835611	−1.743165	−0.465871
H	−0.923643	−1.645614	−0.127207
H	−1.728256	−1.968742	−1.398431
RC(A, B, C):	2.5584913	1.0604451	0.7926346

AW_4_m21

C	0.368277	−1.260795	−0.041435
C	1.541691	−0.874654	−0.016918
O	−2.736755	−1.660956	0.001121
O	−3.021358	1.115189	0.200259
O	−0.353962	1.825829	−0.223718
H	−0.672644	−1.568555	−0.063350
H	2.575909	−0.561526	0.011361
H	−3.391868	−2.014125	−0.612314
H	−2.947837	−0.705632	0.067757
H	−2.103906	1.436864	0.066788
H	−3.289523	1.487227	1.049497
H	0.140568	0.988143	−0.154026
H	−0.141503	2.150894	−1.108413
O	4.617518	−0.142987	0.081121
H	4.962070	0.591088	0.864556
H	5.365386	−0.376072	−0.242005
RC(A, B, C):	2.9925134	0.6821426	0.5618594

AW_4_m22

C	−1.642644	0.772705	−0.231214
C	−0.497134	1.229309	−0.287048
O	2.675711	1.210184	0.148515
O	2.529680	−1.296575	−1.020535
O	1.121460	−0.955925	1.377272
H	−2.654283	0.394298	−0.195020
H	0.519420	1.593659	−0.307635
H	3.532549	1.647837	0.218117
H	2.823913	0.435531	−0.435434
H	1.980096	−1.469939	−1.795175
H	1.934866	−1.438281	−0.252899
H	0.228342	−0.640469	1.167773
H	1.637432	−0.130253	1.397107
O	−4.660577	−0.400194	−0.089773
H	−5.131966	−0.616410	0.725068
H	−5.361896	−0.247982	−0.736164
RC(A, B, C):	3.1441476	0.6555243	0.6183117

AW_4_m23

C	1.544325	−0.881047	−0.055244
C	0.368624	−1.260555	−0.071294

AW_4_m24

C	−1.755372	0.730099	−0.249578
C	−0.613954	1.191006	−0.340312

Table V (Continued)

Atoms	X	Y	Z
O	–2.741693	–1.675138	–0.045632
O	–3.047853	1.104558	0.099582
O	–0.339020	1.844750	0.055475
H	2.580193	–0.572587	–0.042194
H	–0.674350	–1.563431	–0.071310
H	–3.513546	1.535744	–0.627362
H	–2.133551	1.456190	0.054874
H	0.137918	0.994203	0.045898
H	0.057635	2.342476	–0.671110
H	–3.275313	–2.090266	0.642602
H	–2.947447	–0.719106	0.026871
O	4.620311	0.145105	0.016024
H	5.017234	0.400233	0.859094
H	5.339572	–0.288044	–0.461734
RC(A, B, C):	2.9885236	0.6804070	0.5573013

Atoms	X	Y	Z
O	1.087659	–1.002837	1.208516
O	2.822849	–1.185642	–0.956025
O	2.571098	1.311614	0.219274
O	–4.768587	–0.459714	–0.063713
H	–2.764019	0.347579	–0.188383
H	0.400773	1.557030	–0.388534
H	3.318176	1.904301	0.363797
H	2.924949	0.570043	–0.314738
H	3.478840	–1.892357	–0.923835
H	2.183226	–1.394143	–0.240782
H	0.188810	–0.787787	0.913045
H	1.493900	–0.128592	1.306374
H	–5.455149	–0.182548	0.556436
H	–5.257698	–0.832531	–0.808447
RC(A, B, C):	3.3210666	0.6255979	0.5819317

AW_4_m25

C	–1.686909	0.770759	–0.419512
C	–0.555420	1.230533	–0.596964
O	1.012329	–0.717712	1.355876
O	2.621326	1.208611	0.213207
O	2.616977	–1.386746	–0.907259
H	–2.685064	0.380927	–0.280509
H	0.448048	1.605721	–0.720811
H	2.930567	–0.478277	–0.738102
H	3.402122	–1.885120	–1.163313
H	0.155171	–0.459658	0.980178
H	1.399570	–1.295560	0.671981
H	3.225789	1.721867	0.762828
H	2.086876	0.670221	0.841027
O	–4.655879	–0.444801	0.019387
H	–5.184989	–0.428668	0.827136
H	–5.082144	–1.114013	–0.531244
RC(A, B, C):	3.1585170	0.6529019	0.6144885

AW_4_m26[a]

C	1.807332	1.672194	–0.516206
C	1.114358	0.657965	–0.448097
O	–0.057543	–1.482711	0.225517
O	–3.175817	–0.263602	–0.820632
O	–1.805909	1.023597	1.104734
O	4.081765	–0.909725	0.239110
H	2.415291	2.545975	–0.597399
H	0.476693	–0.206783	–0.354948
H	–0.976331	–2.417844	0.478860
H	–1.871415	–1.307011	–0.324461
H	–4.142252	–0.350237	–0.864753
H	–2.894914	0.466010	–0.207322
H	–1.123907	1.706597	0.972813
H	–1.378060	0.135185	1.163397
H	3.329276	–0.290186	0.195245
H	4.295504	–1.203131	–0.665447
RC(A, B, C):	3.0431872	0.7619416	0.6781149

AW_4_m27[a]

Atoms	X	Y	Z
C	–1.791264	–1.470534	–0.675890
C	–1.062541	–0.479759	–0.643229
O	1.229131	1.539318	–0.051790
O	3.319664	0.003696	–0.582760
O	1.613544	–0.851195	1.317502
H	–2.439785	–2.317412	–0.722996
H	–0.387042	0.359010	–0.586564
H	1.322706	2.482287	0.167994
H	2.060331	1.172060	–0.466653
H	3.751908	–0.493030	–1.296151

AW_4_m28

Atoms	X	Y	Z
C	0.445879	–0.427934	0.013871
C	–0.445875	0.427904	–0.015147
O	–3.441718	1.269273	–0.074718
O	–2.939241	–1.535245	0.094044
H	1.293272	–1.102023	0.026565
H	–1.293250	1.102019	–0.027625
H	–4.191755	1.613243	0.424782
H	–3.497751	0.299148	0.020004
H	–1.976808	–1.403425	0.102997
H	–3.095179	–2.084691	–0.685382

Table V (Continued)

Atoms	X	Y	Z
H	2.939281	−0.589688	0.116345
H	0.881650	−1.488256	1.232486
H	1.275731	0.064080	1.164265
O	−4.218297	0.689949	0.380286
H	−3.348974	0.277690	0.218285
H	−4.485308	1.180878	−0.418213
RC(A, B, C):	3.2561618	0.7222321	0.6728818

AW_4_m29

C	0.427108	−0.246168	−0.946060
C	−0.650079	0.346636	−1.061605
O	3.562899	−0.908387	−0.285602
O	2.470009	1.588984	1.001059
H	1.394159	−0.718256	−0.868597
H	−1.621739	0.821304	−1.106880
H	4.288243	−0.717025	−0.895385
H	3.951688	−1.503802	0.369170
H	1.569728	1.615758	0.649040
H	2.845493	0.795160	0.589121
O	−3.659462	0.778916	−0.328936
O	−2.303341	−1.326950	1.050328
H	−4.266644	1.327533	0.181825
H	−3.385961	0.068288	0.281840
H	−1.476999	−1.126081	0.579612
H	−2.520980	−2.226187	0.771449
RC(A, B, C):	2.8947712	0.6643282	0.6286482

AW_4_sp3

C	0.000000	0.000000	0.617644
C	0.000000	0.000000	−0.617644
H	0.000000	0.000000	1.699435
H	0.000000	0.000000	−1.699435
O	0.000000	0.000000	3.803911
H	−0.235333	0.726578	4.394983
H	0.235333	−0.726578	4.394983
O	0.000000	0.000000	−3.803911
H	−0.235333	−0.726578	−4.394983
H	0.235333	−0.726578	−4.394983
H	0.044808	−2.346188	0.000000
O	0.000000	−3.314971	0.000000
H	−0.948670	−3.495207	0.000000
H	−0.044808	2.346188	0.000000
O	0.000000	3.314971	0.000000
H	0.948670	3.495207	0.000000
RC(A, B, C):	1.2911222	0.9062094	0.5346790

Atoms	X	Y	Z
O	3.441700	−1.269289	0.074782
O	2.939274	1.535280	−0.093259
H	4.191937	−1.613072	−0.424546
H	3.497775	−0.299129	−0.019555
H	1.976847	1.403458	−0.102790
H	3.094774	2.084502	0.686412
RC(A, B, C):	3.2873118	0.6716851	0.5598279

AW_4_m30

C	0.000000	0.616733	0.000000
C	0.000000	−0.616733	0.000000
O	3.161931	1.776656	0.000000
O	0.905844	3.770702	0.000000
H	−0.016487	1.695128	0.000000
H	−0.016487	−1.695128	0.000000
H	0.901260	4.363379	0.763529
H	0.901260	4.363379	−0.763529
H	2.657075	0.951820	0.000000
H	2.470357	2.456993	0.000000
O	−3.161931	−1.776656	0.000000
O	−0.905844	−3.770702	0.000000
H	−0.901260	−4.363379	−0.763529
H	−0.901260	−4.363379	0.763529
H	−2.657075	−0.951820	0.000000
H	−2.470357	−2.456993	0.000000
RC(A, B, C):	2.9976560	0.5785855	0.4871759

[a] At the MP2/4–31G level of theory.

TABLE VI: Harmonic Vibrational Frequencies ω (cm^{-1}), Zero Point Energies ZPE (kcal/mol), and IR Intensities IR–I (km/mol) of the m8 and m9 Minima of the $C_2H_2(H_2O)_4$ (AW_4) at the MP2/avdz Level.

AW_4	m8		m9	
	ω	IR–I	ω	IR–I
ω_1	38	1.67	19	0.931
ω_2	56	0.356	37	0.274
ω_3	80	2.16	45	2.27
ω_4	102	2.03	54	2.15
ω_5	124	0.385	124	16.6
ω_6	138	2.39	127	1.86
ω_7	141	3.88	145	4.53
ω_8	148	13.8	162	40.5
ω_9	170	3.91	181	24.1
ω_{10}	192	5.16	195	44.2
ω_{11}	209	7.23	200	21.6
ω_{12}	245	33.6	225	183
ω_{13}	253	58.2	237	20.5
ω_{14}	323	35.5	267	129
ω_{15}	377	13.9	278	11.7
ω_{16}	398	239	298	72.5
ω_{17}	424	95.0	411	44.8
ω_{18}	430	46.1	420	12.6
ω_{19}	477	8.70	444	33.5
ω_{20}	496	42.3	470	11.9
ω_{21}	540	2.15	488	21.9
ω_{22}	545	284	568	36.8
ω_{23}	587	205	749	135
ω_{24}	692	59.1	781	72.6
ω_{25}	814	103	829	105
ω_{26}	830	66.8	854	131
ω_{27}	903	75.8	890	16.6
ω_{28}	1625	102	1633	44.4
ω_{29}	1636	114	1645	48.6
ω_{30}	1653	10.3	1660	59.6
ω_{31}	1676	75.8	1679	16.4
ω_{32}	1923	12.1	1918	26.2
ω_{33}	3300	334	3266	470
ω_{34}	3441	559	3471	592
ω_{35}	3481	2.56	3478	221
ω_{36}	3653	173	3535	1092
ω_{37}	3696	114	3554	203
ω_{38}	3723	152	3684	311
ω_{39}	3799	371	3881	138
ω_{40}	3833	166	3886	86.5
ω_{41}	3888	107	3888	85.2
ω_{42}	3892	102	3890	98.5
ZPE	78.56		78.00	