Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

Dimers of Acetic Acid in Helium Nanodroplets

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Selected results from calculations at the MP2/6-311(2+,2+)G(2d,2p) level of theory are presented in Figure S1 and in Tables S1 and S2 for the *trans* acetic acid (AA) monomer and the six lowest energy *trans-trans* dimers, D1 to D6. Those dimers prepared inside helium nanodroplets are D3 and D6.

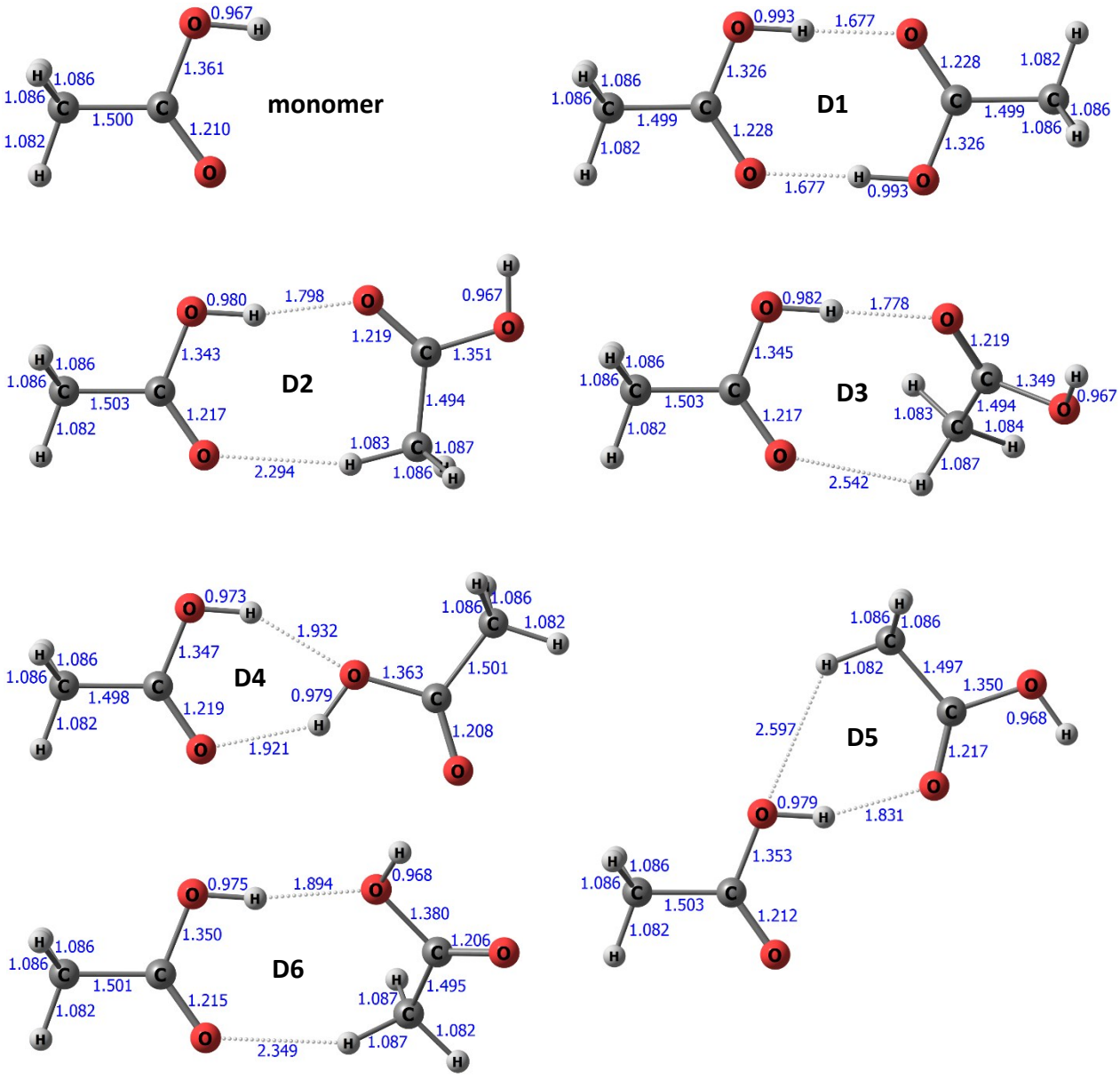

Figure S1. Inter- and intra-molecular bond lengths (in Å) are indicated on the calculated structures for the acetic acid monomer and the six lowest energy dimers, D1 to D6.

Table S1. Cartesian coordinates (in Å) for the structures of the acetic acid monomer and the six lowest energy dimers, D1 to D6, calculated at the MP2/6-311(2+,2+)G(2d,2p) level of theory.

mono	*X*	*Y*	*Z*
H	-1.6603	-0.7072	-0.8810
C	-1.3908	-0.1321	-0.0001
H	-1.9210	0.8108	0.0070
H	-1.6593	-0.7206	0.8722
C	0.0870	0.1250	0.0004
O	0.6243	1.2093	0.0006
O	0.7905	-1.0404	-0.0007
H	1.7234	-0.7869	-0.0014

D1	*X*	*Y*	*Z*
H	-3.7968	-0.4328	-0.8737
C	-3.4262	0.0950	0.0002
H	-3.7754	1.1188	-0.0037
H	-3.7961	-0.4255	0.8788
C	-1.9274	0.0673	0.0002
O	-1.2352	1.0821	-0.0004
O	-1.4340	-1.1632	0.0002
H	-0.4417	-1.1183	0.0003
H	3.7961	0.4257	-0.8787
C	3.4262	-0.0949	-0.0002
H	3.7754	-1.1188	0.0035
H	3.7967	0.4326	0.8739
C	1.9274	-0.0673	-0.0001
O	1.2352	-1.0821	0.0004
O	1.4340	1.1632	-0.0002
H	0.4417	1.1183	-0.0003

D2	*X*	*Y*	*Z*
H	-3.9121	-0.6420	-0.8473
C	-3.5938	-0.0683	0.0185
H	-4.0630	0.9067	0.0115
H	-3.8894	-0.6217	0.9050
C	-2.0995	0.0882	-0.0054
O	-1.5141	1.1542	-0.0563
O	-1.4750	-1.1001	0.0343
H	-0.5071	-0.9458	0.0125
H	2.2181	1.7753	0.9932
C	1.8165	1.3756	0.0657
H	0.7470	1.5369	0.0172
H	2.3224	1.8791	-0.7528
C	2.1097	-0.0885	0.0044
O	1.2897	-0.9900	-0.0063
O	3.4351	-0.3467	-0.0338
H	3.5250	-1.3094	-0.0636

D3	*X*	*Y*	*Z*
H	-3.8405	-0.7027	-0.5385
C	-3.3937	0.1555	-0.0443
H	-3.7285	1.0702	-0.5155
H	-3.7030	0.1314	0.9965
C	-1.8969	0.0583	-0.1332
O	-1.1802	0.8585	-0.7052
O	-1.4308	-1.0327	0.5003
H	-0.4568	-1.0593	0.3818
H	2.5007	1.6795	1.0951
C	1.6036	1.1607	0.7777
H	0.9614	0.9441	1.6223
H	1.0517	1.7864	0.0814
C	1.9506	-0.1110	0.0737
O	1.2942	-1.1380	0.0853
O	3.1004	-0.0176	-0.6251
H	3.2138	-0.8653	-1.0773

D4	*X*	*Y*	*Z*
H	-3.9985	-0.4325	-0.9325
C	-3.6533	0.0643	-0.0306
H	-4.0128	1.0841	-0.0033
H	-4.0363	-0.4929	0.8192
C	-2.1552	0.0576	0.0013
O	-1.4567	1.0557	0.0493
O	-1.6588	-1.1946	-0.0296
H	-0.6878	-1.1334	-0.0061
H	3.0215	-1.5904	0.8972
C	3.1852	-1.0104	-0.0065
H	4.2182	-0.6943	-0.0638
H	2.9409	-1.6431	-0.8550
C	2.2926	0.1962	-0.0014
O	2.6523	1.3484	-0.0534
O	0.9791	-0.1591	0.0728
H	0.4199	0.6446	0.0696

D5	*X*	*Y*	*Z*
H	-3.4622	-1.3818	-0.8771
C	-3.4995	-0.7398	-0.0017
H	-4.4139	-0.1613	-0.0031
H	-3.4628	-1.3784	0.8763
C	-2.3163	0.1874	-0.0031
O	-2.3746	1.3982	-0.0060
O	-1.1515	-0.5002	-0.0010
H	-0.4128	0.1428	-0.0025
H	2.6780	-1.8248	-0.8514
C	2.1581	-1.4317	0.0174
H	1.1241	-1.7509	0.0122
H	2.6636	-1.8084	0.9018
C	2.2312	0.0638	0.0043
O	1.2846	0.8290	-0.0051
O	3.5057	0.5093	0.0051
H	3.4576	1.4756	-0.0028

D6	*X*	*Y*	*Z*
H	-3.8831	-0.7845	-0.6675
C	-3.5349	0.0448	-0.0586
H	-3.9461	0.9757	-0.4259
H	-3.8647	-0.1355	0.9604
C	-2.0357	0.1042	-0.1000
O	-1.3812	1.0484	-0.4957
O	-1.4798	-1.0351	0.3635
H	-0.5117	-0.9409	0.2980
H	0.8347	1.5162	0.1293
C	1.7900	1.2546	0.5774
H	2.5234	2.0310	0.4053
H	1.6303	1.1207	1.6440
C	2.2795	-0.0264	-0.0168
O	3.3163	-0.2160	-0.6032
O	1.3752	-1.0500	0.1809
H	1.7689	-1.8325	-0.2301

Table S2. Calculated unscaled harmonic vibrational frequencies (ν in cm^{-1}) and IR intensities (I in km mol^{-1}) for the acetic acid monomer and selected dimers at the MP2/6-311(2+,2+)G(2d,2p) level of theory.

AA monomer	
ν	I
3786.4	77.2
3228.4	2.6
3187.4	1.9
3107.3	1.2
1799.8	290.5
1504.4	8.4
1500.0	16.3
1432.7	48.7
1350.3	39.1
1208.5	213.3
1082.4	5.1
1009.3	81.8
867.7	7.8
660.5	91.0
584.6	36.1
549.6	30.4
425.0	4.1
64.7	0.2

AA dimer D1	
ν	I
3301.0	2969.5
3228.6	0.0
3227.8	13.0
3202.6	0.0
3186.6	0.0
3186.6	3.0
3106.4	2.0
3106.3	0.0
1759.5	716.9
1719.6	0.0
1510.4	0.0
1504.0	0.0
1504.0	16.9
1499.6	60.4
1485.6	0.0
1478.9	125.0
1420.9	0.0
1415.3	40.7
1335.5	391.8
1318.0	0.0
1087.3	6.8
1086.1	0.0
1042.3	41.2
1038.7	0.0
1027.5	172.6
983.5	0.0
910.7	0.0
909.7	7.0
635.0	43.7
627.2	0.0
609.9	0.0
604.0	0.5
483.3	45.9
443.7	0.0
179.8	0.0
177.3	29.5
155.4	0.0
121.6	0.0
73.7	0.2
57.5	1.8
33.9	0.1
33.0	3.0

AA dimer D2	
ν	I
3779.0	83.2
3514.7	1013.0
3223.8	5.4
3222.5	15.0
3184.5	2.9
3182.7	1.5
3104.4	2.2
3100.0	13.4
1783.1	617.9
1762.0	75.8
1517.4	7.8
1504.7	7.7
1500.5	26.8
1498.8	1.0
1448.3	39.0
1442.4	60.9
1398.1	16.9
1367.9	91.8
1270.2	270.1
1227.1	220.4
1093.5	6.0
1082.7	4.3
1029.8	49.5
1028.0	73.5
898.2	86.9
890.3	4.4
881.7	6.5
673.2	93.2
610.2	32.9
600.4	38.5
599.2	1.0
556.9	25.9
447.5	16.2
433.8	3.2
145.5	12.9
109.7	0.4
106.4	0.1
99.6	3.4
93.5	0.9
56.4	0.0
33.1	3.2
-	-

AA dimer D3	
ν	I
3777.5	85.4
3486.4	946.9
3223.5	4.7
3222.9	4.2
3197.3	2.5
3184.0	2.9
3109.4	2.9
3104.0	2.2
1781.2	597.5
1762.2	43.1
1509.1	12.4
1505.5	7.6
1500.0	18.2
1491.3	23.5
1447.9	37.4
1436.2	93.8
1398.5	6.1
1368.4	71.1
1272.7	247.2
1224.3	235.8
1086.6	7.7
1082.8	4.4
1029.7	56.8
1027.2	47.0
912.3	82.9
887.0	5.3
882.4	4.4
686.1	94.9
610.9	8.7
601.6	35.4
597.4	24.9
550.1	22.3
444.4	12.2
434.8	0.9
165.1	17.5
122.2	1.8
120.8	0.4
85.7	1.6
64.4	0.2
58.0	0.5
28.7	3.0
24.5	1.3

AA dimer D4	
ν	I
3665.2	657.7
3559.6	312.3
3229.0	2.2
3226.3	3.9
3187.3	1.3
3184.3	2.4
3106.9	0.8
3104.2	1.6
1803.4	153.2
1769.3	473.9
1505.6	8.8
1504.0	8.6
1499.8	25.5
1498.9	9.3
1445.6	44.2
1429.9	42.2
1396.9	11.2
1347.8	10.8
1271.5	381.1
1204.3	473.4
1085.2	5.1
1081.6	3.9
1027.4	54.9
1014.7	135.1
887.5	4.8
869.6	4.1
855.4	164.7
741.1	15.6
620.5	55.3
603.0	18.1
591.4	0.4
588.2	1.9
453.2	4.4
435.9	13.0
186.1	22.3
117.5	0.2
97.4	0.0
77.2	0.1
57.9	0.2
53.6	1.6
49.4	2.0
21.3	0.0

AA dimer D5	
ν	I
3777.0	87.9
3538.0	871.0
3226.6	0.4
3223.4	5.5
3187.3	0.7
3183.5	3.7
3105.9	1.4
3103.7	2.8
1791.1	126.6
1772.6	572.5
1505.4	0.1
1505.0	15.8
1500.8	26.1
1500.0	7.2
1442.6	71.3
1437.0	28.4
1388.1	1.0
1368.4	43.3
1251.5	282.4
1219.2	452.5
1086.9	6.5
1081.1	4.2
1024.7	70.6
1020.8	95.2
881.8	7.3
876.7	5.1
874.2	81.5
671.1	93.5
611.5	7.5
598.3	86.5
595.8	0.8
555.4	26.5
441.1	0.5
434.0	6.2
165.7	16.5
95.3	0.4
92.2	0.4
59.1	0.4
53.9	0.5
35.0	0.1
28.8	1.4
-21.7	0.5

AA dimer D6	
ν	I
3775.2	81.5
3625.8	632.7
3227.0	2.2
3225.8	3.3
3185.0	2.2
3179.0	11.0
3105.1	1.6
3097.9	11.1
1816.7	313.2
1780.1	282.3
1508.6	24.4
1505.1	7.9
1502.6	8.7
1499.5	22.5
1441.9	58.4
1435.5	36.3
1388.0	3.3
1328.6	23.5
1261.7	270.6
1199.5	207.0
1089.4	5.5
1083.4	4.5
1025.3	56.5
1004.9	81.3
883.1	11.1
850.7	33.1
825.4	91.1
645.0	66.4
605.5	34.4
594.8	2.6
585.7	19.7
542.6	38.1
441.2	7.7
428.3	1.6
142.2	0.7
131.9	8.1
110.9	3.3
94.0	3.5
75.2	0.5
59.9	1.1
20.5	0.8
17.6	0.9