

Electronic Supplementary Information for

Vibrational Stark Fields in Carboxylic Acid Dimers

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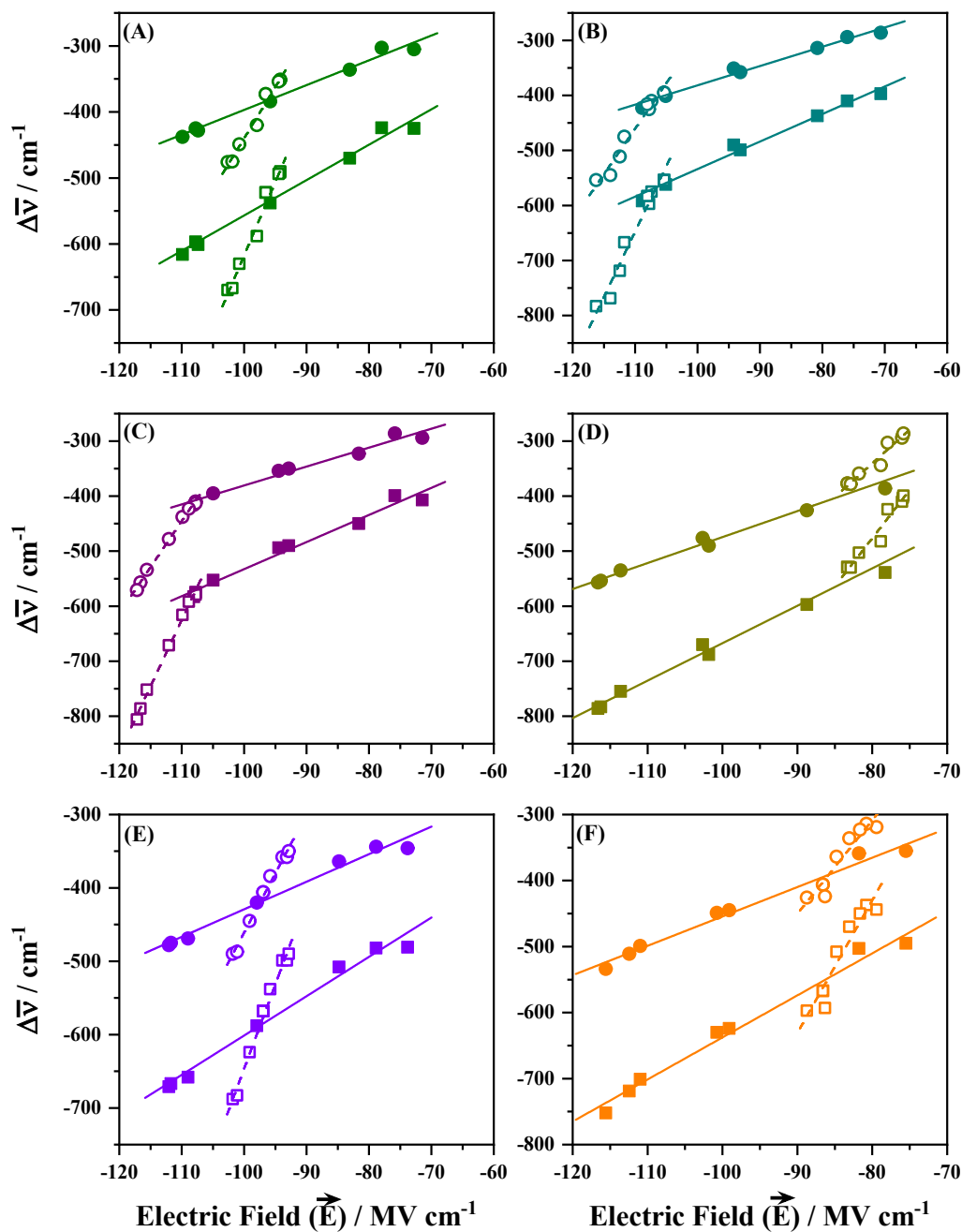


Fig. S1 Plots of the red-shifts in the O–H (squares) and O–D (circles) stretching frequencies against the corresponding Stark fields in the dimers of (A) formic acid, (B) propanoic acid, (C) methylpropanoic acid, (D) fluoroformic acid, (E) fluoroacetic acid, and (F) difluoroacetic acid calculated at MP2/aug-cc-pVDZ level of theory. The solid symbols represent the shifts in the O–H/O–D stretching frequencies of acetic acid/trifluoroacetic acid due to change in the substituent on the dimerizing partner, while open symbols represent the shifts in the O–H/O–D stretching frequencies of the other carboxylic acids due to their dimerization with acetic acid/trifluoroacetic acid. The straight-lines are linear least-square fits to the data points and the slopes of these straight lines are called Stark tuning rates ($\Delta\vec{\mu}$).

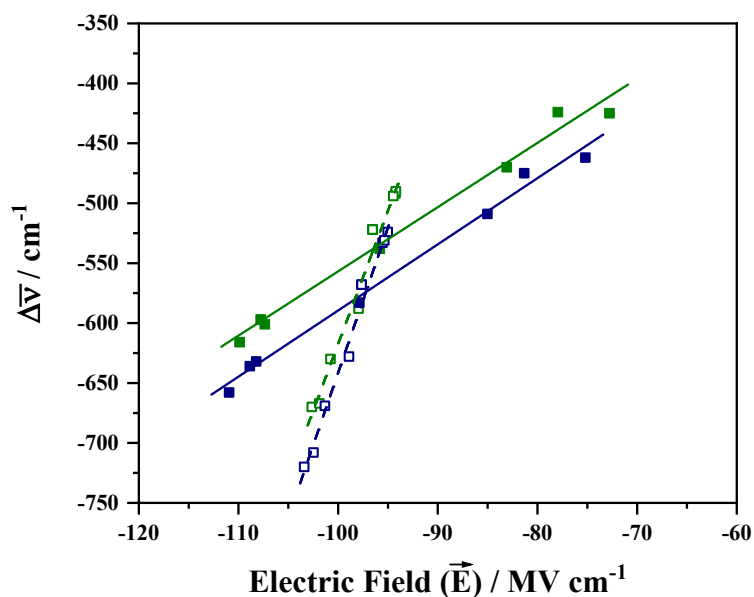


Fig. S2 Plots of the red-shifts in the harmonic O–H stretching frequencies against the corresponding Stark fields in various formic acid dimers calculated at MP2 level of theory using aug-cc-pVDZ (filled and open green squares) and aug-cc-pVTZ (filled and open blue squares) basis sets. The solid symbols represent the shifts in the O–H stretching frequencies of formic acid dimer due change in the substituent on the dimerizing partner, while open symbols represent the shifts in the O–H stretching frequencies of the other carboxylic acids due to dimerization with formic acid. The straight-lines are linear least-square fits to the data points and the slopes of these straight lines are called Stark tuning rates ($\Delta\vec{\mu}$). The Stark tuning rates ($\Delta\vec{\mu}$) are comparable (5.4 vs 5.5 and 22.3 vs 24.2) and are very weakly dependent on the basis set (aug-cc-pVDZ vs. aug-cc-pVTZ).

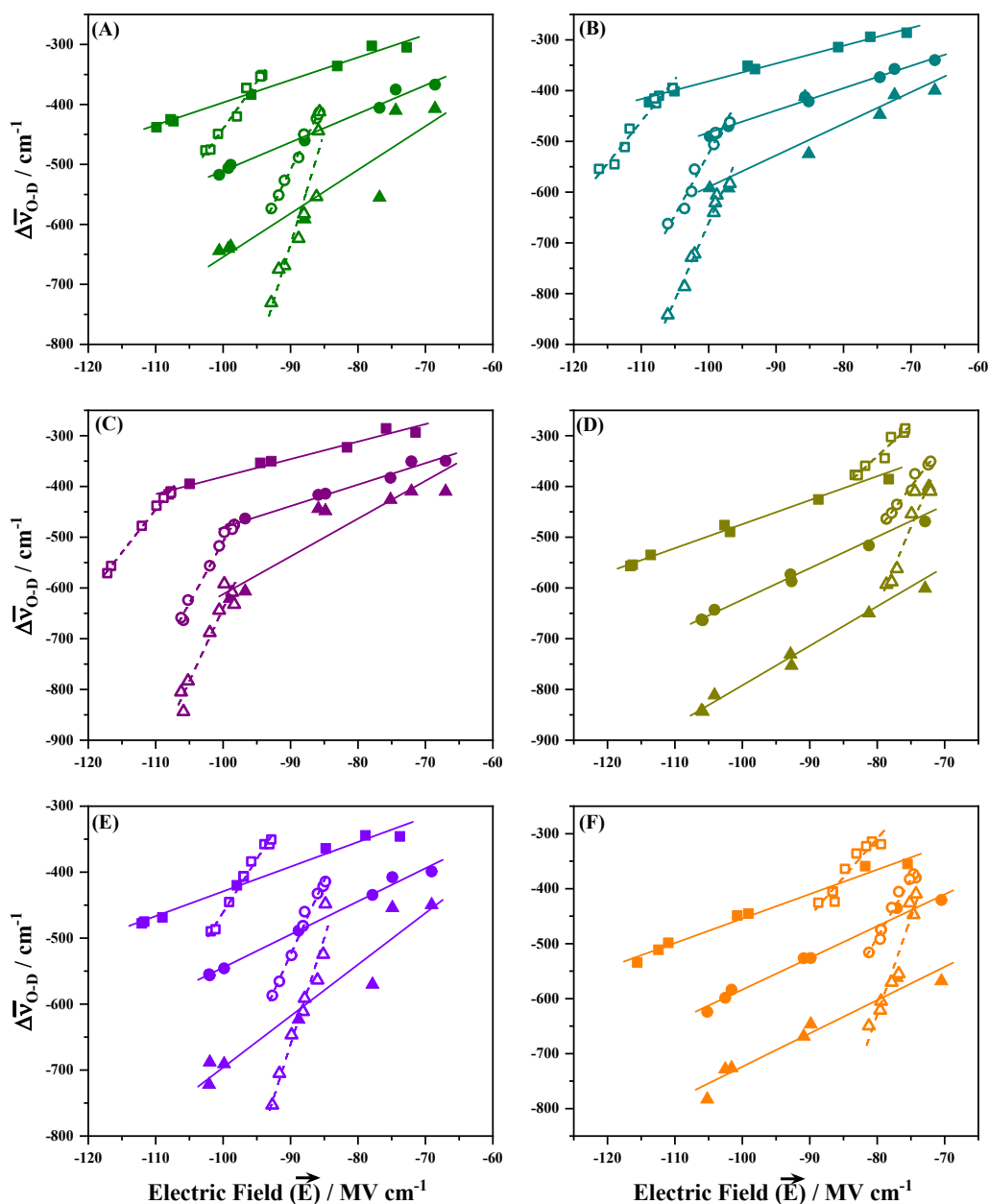


Fig. S3 Plots of the red-shifts in the O–D stretching frequencies against the corresponding Stark fields in the dimers of (A) formic acid, (B) propanoic acid, (C) methylpropanoic acid, (D) fluoroformic acid, (E) fluoroacetic acid, and (F) difluoroacetic acid. In each case the squares, circles and triangles represent harmonic MP2, harmonic B3LYP-D3, and anharmonic B3LYP-D3 frequency shifts calculated with aug/cc-pVDZ basis set, respectively. . The solid symbols represent the shifts in the O–H/O–D stretching frequencies of acetic acid/trifluoroacetic acid due change in the substituent on the dimerizing partner, while open symbols represent the shifts in the O–H/O–D stretching frequencies of the other carboxylic acids due to their dimerization with acetic acid/trifluoroacetic acid. The straight-lines are linear least-square fits to the data points and the slopes of these straight lines are called Stark tuning rates ($\Delta\bar{\mu}$).

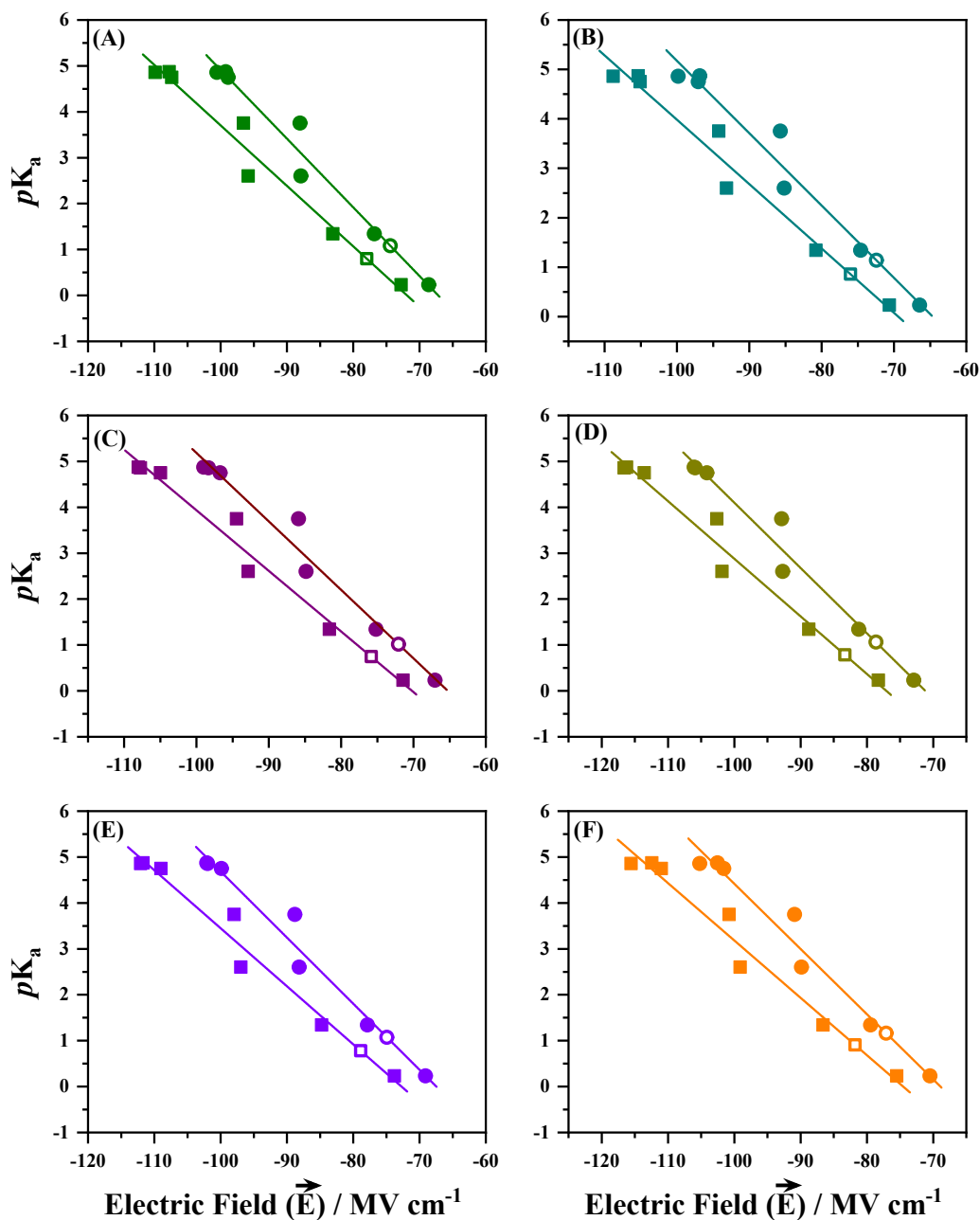


Fig. S4 Plots of pK_a of the carboxylic acid against the electric field along the O–H group (A) formic acid, (B) propanoic acid, (C) methylpropanoic acid, (D) fluoroformic acid, (E) fluoroacetic acid, and (F) difluoroacetic acid. In each case the squares, and circles represent the electric field values calculated using MP2 and B3LYP-D3 levels, respectively. The straight-lines are linear least-square fits to the data points. In each case the data point representing open square / open circle is due to fluoroformic acid, whose pK_a is unknown and is estimated using the linear correlation.

Table S1. ZPE corrected dimerization energies (kJ mol⁻¹) and total electric field (MV cm⁻¹) (*red italics*) for various carboxylic acid dimers calculated at MP2/aug-cc-pVDZ level of theory.

	FA	AA	PA	MPA	FFA	FAA	DFAA	TFAA
FA	-60.2 <i>-193.1</i>	-63.1 <i>-201.6</i>	-63.3 <i>-202.0</i>	-64.4 <i>-204.4</i>	-65.1 <i>-180.6</i>	-62.1 <i>-193.8</i>	-63.5 <i>-183.8</i>	-62.9 <i>-174.7</i>
AA		-65.4 <i>-209.9</i>	-62.4 <i>-212.4</i>	-66.6 <i>-212.7</i>	-69.7 <i>-189.5</i>	-65.4 <i>-202.9</i>	-68.3 <i>-190.4</i>	-67.8 <i>-183.8</i>
PA			-65.8 <i>-210.7</i>	-62.1 <i>-216.0</i>	-67.1 <i>-192.3</i>	-64.3 <i>-204.8</i>	-68.0 <i>-193.2</i>	-68.4 <i>-184.6</i>
MPA				-68.0 <i>-215.5</i>	-71.5 <i>-192.5</i>	-68.6 <i>-204.9</i>	-67.7 <i>-197.2</i>	-68.0 <i>-188.6</i>
FFA					-66.2 <i>-166.6</i>	-66.8 <i>-180.7</i>	-66.3 <i>-170.5</i>	-64.4 <i>-161.1</i>
FAA						-67.8 <i>-193.9</i>	-67.1 <i>-183.9</i>	-64.7 <i>-174.9</i>
DFAA							-65.4 <i>-173.2</i>	-64.7 <i>-161.8</i>
TFAA								-62.1 <i>-154.9</i>

Table S2. ZPE corrected dimerization energies (kJ mol⁻¹) and total electric field (MV cm⁻¹) (*in italics*) for various carboxylic acid dimers calculated at B3LYP-D3/aug-cc-pVDZ level of theory.

	FA	AA	PA	MPA	FFA	FAA	DFAA	TFAA
FA	-58.9 <i>-176.0</i>	-61.6 <i>-185.0</i>	-61.4 <i>-184.9</i>	-62.2 <i>-186.4</i>	-64.5 <i>-167.2</i>	-61.1 <i>-176.7</i>	-61.7 <i>-167.7</i>	-60.9 <i>-160.3</i>
AA		-63.1 <i>-194.0</i>	-59.1 <i>-195.8</i>	-64.0 <i>-195.4</i>	-69.1 <i>-176.4</i>	-64.1 <i>-185.9</i>	-66.4 <i>-175.8</i>	-65.5 <i>-170.0</i>
PA			-63.2 <i>-193.7</i>	-58.2 <i>-198.8</i>	-64.9 <i>-178.5</i>	-61.1 <i>-187.2</i>	-65.7 <i>-177.1</i>	-65.9 <i>-170.0</i>
MPA				-64.8 <i>-196.7</i>	-70.0 <i>-177.9</i>	-66.0 <i>-186.8</i>	-65.0 <i>-180.4</i>	-65.3 <i>-173.2</i>
FFA					-65.6 <i>-157.3</i>	-66.5 <i>-167.6</i>	-65.0 <i>-158.3</i>	-62.8 <i>-150.8</i>
FAA						-65.9 <i>-176.3</i>	-65.1 <i>-167.7</i>	-63.0 <i>-160.7</i>
DFAA							-63.2 <i>-158.8</i>	-62.2 <i>-150.0</i>
TFAA								-59.4 <i>-143.6</i>

Table S3. Harmonic frequencies (cm^{-1}) of the O–H stretching vibration and their shifts (cm^{-1}) calculated at MP2/aug-cc-pVDZ level for various carboxylic acid dimer and the corresponding electric field along the O–H bond (MV cm^{-1}). For each set of carboxylic acid dimer two cases **R** and **R'** arise, (i) frequency shift in a particular carboxylic acid (**R**) when the interaction partner is changed (**R'**), (ii) frequency shifts of the partners (**R'**) when paired with a particular carboxylic acid (**R**). The pK_a values of the varying partner (**R'**) are also listed.

Dimer	$\nu_{\text{O-H}}$	$\Delta\nu_{\text{O-H}}$	Field	$\nu_{\text{O-H}}$	$\Delta\nu_{\text{O-H}}$	Field	pK_a (R')
	R			R'			
FA-FA	3202	-522	-96.54	3202	-522	-96.54	3.75
FA-AA	3124	-601	-107.36	3250	-492	-94.24	4.75
FA-PA	3128	-597	-107.77	3248	-490	-94.20	4.87
FA-MPA	3109	-616	-109.88	3236	-494	-94.46	4.86
FA-FFA	3301	-424	-77.95	3108	-670	-102.64	-
FA-FAA	3187	-538	-95.82	3156	-588	-97.95	2.60
FA-DFAA	3255	-470	-83.07	3108	-630	-100.76	1.34
FA-TFAA	3300	-425	-72.77	3070	-667	-101.88	0.23
	R			R'			
AA-AA	3184	-558	-104.95	3184	-558	-104.95	4.75
AA-FA	3250	-492	-94.24	3124	-601	-107.36	3.75
AA-PA	3166	-575	-107.35	3177	-562	-105.09	4.87
AA-MPA	3162	-579	-107.76	3177	-553	-104.96	4.86
AA-FFA	3338	-403	-75.91	3023	-755	-113.58	-
AA-FAA	3242	-499	-93.86	3086	-658	-108.99	2.60
AA-DFAA	3297	-444	-79.42	3037	-701	-110.98	1.34
AA-TFAA	3337	-404	-70.80	2979	-758	-112.97	0.23
	R			R'			
PA-PA	3185	-554	-105.35	3185	-554	-105.35	4.87
PA-FA	3248	-490	-94.20	3128	-597	-107.77	3.75
PA-AA	3177	-562	-105.09	3166	-575	-107.35	4.75
PA-MPA	3147	-592	-108.83	3147	-583	-108.04	4.86
PA-FFA	3329	-410	-76.02	2995	-783	-116.24	-
PA-FAA	3239	-499	-93.13	3077	-667	-111.71	2.60
PA-DFAA	3302	-437	-80.78	3019	-719	-112.43	1.34
PA-TFAA	3342	-397	-70.62	2968	-769	-113.96	0.23
	R			R'			
MPA-MPA	3155	-575	-107.74	3155	-575	-107.74	4.86
MPA-FA	3236	-494	-94.46	3109	-616	-109.88	3.75
MPA-AA	3177	-553	-104.96	3162	-579	-107.76	4.75
MPA-PA	3147	-583	-108.04	3147	-592	-108.83	4.87
MPA-FFA	3332	-399	-75.84	2992	-786	-116.61	-
MPA-FAA	3241	-490	-92.84	3073	-671	-112.05	2.60
MPA-DFAA	3281	-450	-81.62	2986	-752	-115.57	1.34
MPA-TFAA	3323	-407	-71.44	2931	-806	-117.17	0.23

	R			R'			
FFA-FFA	3248	-529	-83.31	3248	-529	-83.31	-
FFA-FA	3108	-670	-102.64	3301	-424	-77.95	3.75
FFA-AA	3023	-755	-113.58	3338	-403	-75.91	4.75
FFA-PA	2995	-783	-116.24	3329	-410	-76.02	4.87
FFA-MPA	2992	-786	-116.61	3332	-399	-75.84	4.86
FFA-FAA	3090	-688	-101.83	3262	-482	-78.86	2.60
FFA-DFAA	3181	-597	-88.73	3234	-503	-81.78	1.34
FFA-TFAA	3239	-539	-78.27	3207	-530	-82.87	0.23
	R			R'			
FAA-FAA	3175	-568	-96.94	3175	-568	-96.94	2.60
FAA-FA	3156	-588	-97.95	3187	-538	-95.82	3.75
FAA-AA	3086	-658	-108.99	3242	-499	-93.86	4.75
FAA-PA	3077	-667	-111.71	3239	-499	-93.13	4.87
FAA-MPA	3073	-671	-112.05	3241	-490	-92.84	4.86
FAA-FFA	3262	-482	-78.86	3090	-688	-101.83	-
FAA-DFAA	3236	-508	-84.77	3114	-624	-99.11	1.34
FAA-TFAA	3263	-481	-73.78	3054	-683	-101.13	0.23
	R			R'			
DFAA-DFAA	3171	-567	-86.59	3171	-567	-86.59	1.34
DFAA-FA	3108	-630	-100.76	3255	-470	-83.07	3.75
DFAA-AA	3037	-701	-110.98	3297	-444	-79.42	4.75
DFAA-PA	3019	-719	-112.43	3302	-437	-80.78	4.87
DFAA-MPA	2986	-752	-115.57	3281	-450	-81.62	4.86
DFAA-FFA	3234	-503	-81.78	3181	-597	-88.73	-
DFAA-FAA	3114	-624	-99.11	3236	-508	-84.77	2.60
DFAA-TFAA	3243	-495	-75.50	3144	-593	-86.30	0.23
	R			R'			
TFAA-TFAA	3204	-534	-77.44	3204	-534	-77.44	0.23
TFAA-FA	3070	-667	-101.88	3300	-425	-72.77	3.75
TFAA-AA	2979	-758	-112.97	3337	-404	-70.80	4.75
TFAA-PA	2968	-769	-113.96	3342	-397	-70.62	4.87
TFAA-MPA	2931	-806	-117.17	3323	-407	-71.44	4.86
TFAA-FFA	3207	-530	-82.87	3239	-539	-78.27	-
TFAA-FAA	3054	-683	-101.13	3263	-481	-73.78	2.60
TFAA-DFAA	3144	-593	-86.30	3243	-495	-75.50	1.34

Table S4. Harmonic frequencies (cm^{-1}) of the O–D stretching vibration and their shifts (cm^{-1}) calculated at MP2/aug-cc-pVDZ level for various carboxylic acid dimer and the corresponding electric field along the O–D bond (MV cm^{-1}). For each set of carboxylic acid dimer two cases arise, (i) frequency shift in a particular carboxylic acid (R) when the interaction partner is changed (R'), (ii) frequency shifts of the partners (R') when paired with a particular carboxylic acid (R). The pK_a values of the varying partner (R') are also listed.

Dimer	$\nu_{\text{O-D}}$	$\Delta\nu_{\text{O-D}}$	Field	$\nu_{\text{O-D}}$	$\Delta\nu_{\text{O-D}}$	Field	pK_a (R')
	R			R'			
FA-FA	2336	-373	-96.54	2336	-373	-96.54	3.75
FA-AA	2281	-428	-107.36	2370	-352	-94.24	4.75
FA-PA	2284	-425	-107.77	2369	-351	-94.20	4.87
FA-MPA	2271	-438	-109.88	2360	-354	-94.46	4.86
FA-FFA	2406	-303	-77.95	2273	-476	-102.64	
FA-FAA	2325	-384	-95.82	2303	-420	-97.95	2.60
FA-DFAA	2373	-336	-83.07	2270	-449	-100.76	1.34
FA-TFAA	2404	-305	-72.77	2244	-475	-101.88	0.23
	R			R'			
AA-AA	2323	-398	-104.95	2323	-398	-104.95	4.75
AA-FA	2370	-352	-94.24	2281	-428	-107.36	3.75
AA-PA	2311	-410	-107.35	2318	-401	-105.09	4.87
AA-MPA	2309	-413	-107.76	2318	-395	-104.96	4.86
AA-FFA	2432	-289	-75.91	2214	-535	-113.58	
AA-FAA	2364	-358	-93.86	2255	-469	-108.99	2.60
AA-DFAA	2402	-319	-79.42	2221	-499	-110.98	1.34
AA-TFAA	2431	-291	-70.80	2181	-538	-112.97	0.23
	R			R'			
PA-PA	2325	-395	-105.35	2325	-395	-105.35	4.87
PA-FA	2369	-351	-94.20	2284	-425	-107.77	3.75
PA-AA	2318	-401	-105.09	2311	-410	-107.35	4.75
PA-MPA	2297	-423	-108.83	2298	-416	-108.04	4.86
PA-FFA	2426	-294	-76.02	2195	-554	-116.24	
PA-FAA	2362	-358	-93.13	2248	-475	-111.71	2.60
PA-DFAA	2405	-314	-80.78	2208	-511	-112.43	1.34
PA-TFAA	2434	-286	-70.62	2174	-545	-113.96	0.23
	R			R'			
MPA-MPA	2303	-410	-107.74	2303	-410	-107.74	4.86
MPA-FA	2360	-354	-94.46	2271	-438	-109.88	3.75
MPA-AA	2318	-395	-104.96	2309	-413	-107.76	4.75
MPA-PA	2298	-416	-108.04	2297	-423	-108.83	4.87
MPA-FFA	2428	-286	-75.84	2193	-557	-116.61	
MPA-FAA	2363	-350	-92.84	2246	-478	-112.05	2.60
MPA-DFAA	2390	-323	-81.62	2185	-534	-115.57	1.34
MPA-TFAA	2420	-294	-71.44	2148	-571	-117.17	0.23

	R			R'			
FFA-FFA	2372	-377	-83.31	2372	-377	-83.31	
FFA-FA	2273	-476	-102.64	2406	-303	-77.95	3.75
FFA-AA	2214	-535	-113.58	2432	-289	-75.91	4.75
FFA-PA	2195	-554	-116.24	2426	-294	-76.02	4.87
FFA-MPA	2193	-557	-116.61	2428	-286	-75.84	4.86
FFA-FAA	2260	-490	-101.83	2379	-344	-78.86	2.60
FFA-DFAA	2323	-426	-88.73	2360	-359	-81.78	1.34
FFA-TFAA	2364	-386	-78.27	2341	-378	-82.87	0.23
	R			R'			
FAA-FAA	2317	-406	-96.94	2317	-406	-96.94	2.60
FAA-FA	2303	-420	-97.95	2325	-384	-95.82	3.75
FAA-AA	2255	-469	-108.99	2364	-358	-93.86	4.75
FAA-PA	2248	-475	-111.71	2362	-358	-93.13	4.87
FAA-MPA	2246	-478	-112.05	2363	-350	-92.84	4.86
FAA-FFA	2379	-344	-78.86	2260	-490	-101.83	
FAA-DFAA	2359	-364	-84.77	2274	-445	-99.11	1.34
FAA-TFAA	2378	-346	-73.78	2232	-487	-101.13	0.23
	R			R'			
DFAA-DFAA	2314	-406	-86.59	2314	-406	-86.59	1.34
DFAA-FA	2270	-449	-100.76	2373	-336	-83.07	3.75
DFAA-AA	2221	-499	-110.98	2402	-319	-79.42	4.75
DFAA-PA	2208	-511	-112.43	2405	-314	-80.78	4.87
DFAA-MPA	2185	-534	-115.57	2390	-323	-81.62	4.86
DFAA-FFA	2360	-359	-81.78	2323	-426	-88.73	
DFAA-FAA	2274	-445	-99.11	2359	-364	-84.77	2.60
DFAA-TFAA	2364	-355	-75.50	2295	-424	-86.30	0.23
	R			R'			
TFAA-TFAA	2337	-382	-77.44	2337	-382	-77.44	0.23
TFAA-FA	2244	-475	-101.88	2404	-305	-72.77	3.75
TFAA-AA	2181	-538	-112.97	2431	-291	-70.80	4.75
TFAA-PA	2174	-545	-113.96	2434	-286	-70.62	4.87
TFAA-MPA	2148	-571	-117.17	2420	-294	-71.44	4.86
TFAA-FFA	2341	-378	-82.87	2364	-386	-78.27	
TFAA-FAA	2232	-487	-101.13	2378	-346	-73.78	2.60
TFAA-DFAA	2295	-424	-86.30	2364	-355	-75.50	1.34

Table S5. Harmonic frequencies (cm^{-1}) of the O–D stretching vibration and their shifts (cm^{-1}) calculated at B3LYP-D3/aug-cc-pVDZ level using VPT2 method for various carboxylic acid dimer and the corresponding electric field along the O–D bond (MV cm^{-1}). For each set of carboxylic acid dimer two cases arise, (i) frequency shift in a particular carboxylic acid (R) when the interaction partner is changed (R'), (ii) frequency shifts of the partners (R') when paired with a particular carboxylic acid (R). The pK_a values of the varying partner (R') are also listed.

Dimer	$\nu_{\text{O-D}}$	$\Delta\nu_{\text{O-D}}$	Field	$\nu_{\text{O-D}}$	$\Delta\nu_{\text{O-D}}$	Field	pK_a
	R			R'			
FA-FA	2252	-450	-88.00	2252	-450	-88.00	3.75
FA-AA	2201	-501	-98.87	2299	-423	-86.16	4.75
FA-PA	2196	-506	-99.21	2310	-413	-85.71	4.87
FA-MPA	2185	-517	-100.57	2305	-417	-85.88	4.86
FA-FFA	2327	-375	-74.39	2172	-573	-92.85	
FA-FAA	2242	-460	-87.89	2235	-489	-88.80	2.60
FA-DFAA	2297	-406	-76.80	2193	-527	-90.91	1.34
FA-TFAA	2335	-367	-68.58	2163	-551	-91.74	0.23
	R			R'			
AA-AA	2252	-471	-96.99	2252	-471	-96.99	4.75
AA-FA	2299	-423	-86.16	2201	-501	-98.87	3.75
AA-PA	2239	-484	-98.78	2253	-470	-97.05	4.87
AA-MPA	2238	-484	-98.64	2258	-463	-96.72	4.86
AA-FFA	2368	-355	-72.33	2103	-643	-104.12	
AA-FAA	2290	-433	-86.00	2178	-546	-99.85	2.60
AA-DFAA	2343	-380	-74.24	2135	-584	-101.60	1.34
AA-TFAA	2374	-349	-66.81	2089	-626	-103.18	0.23
	R			R'			
PA-PA	2260	-463	-96.86	2260	-463	-96.86	4.87
PA-FA	2310	-413	-85.71	2196	-506	-99.21	3.75
PA-AA	2253	-470	-97.05	2239	-484	-98.78	4.75
PA-MPA	2232	-490	-99.82	2239	-483	-98.99	4.86
PA-FFA	2366	-357	-72.43	2084	-662	-106.04	
PA-FAA	2302	-421	-85.16	2169	-555	-102.08	2.60
PA-DFAA	2349	-374	-74.60	2120	-599	-102.53	1.34
PA-TFAA	2383	-340	-66.45	2082	-632	-103.58	0.23
	R			R'			
MPA-MPA	2246	-476	-98.34	2246	-476	-98.34	4.86
MPA-FA	2305	-417	-85.88	2185	-517	-100.57	3.75
MPA-AA	2258	-463	-96.72	2238	-484	-98.64	4.75
MPA-PA	2239	-483	-98.99	2232	-490	-99.82	4.87
MPA-FFA	2371	-351	-72.07	2082	-664	-105.87	
MPA-FAA	2307	-414	-84.84	2168	-556	-101.96	2.60
MPA-DFAA	2339	-383	-75.17	2095	-624	-105.20	1.34
MPA-TFAA	2372	-350	-67.01	2056	-659	-106.23	0.23

	R			R'			
FFA-FFA	2282	-464	-78.63	2282	-464	-78.63	
FFA-FA	2172	-573	-92.85	2327	-375	-74.39	3.75
FFA-AA	2103	-643	-104.12	2368	-355	-72.33	4.75
FFA-PA	2084	-662	-106.04	2366	-357	-72.43	4.87
FFA-MPA	2082	-664	-105.87	2371	-351	-72.07	4.86
FFA-FAA	2159	-587	-92.70	2316	-408	-74.91	2.60
FFA-DFAA	2230	-516	-81.22	2283	-436	-77.08	1.34
FFA-TFAA	2277	-469	-72.91	2262	-452	-77.84	0.23
	R			R'			
FAA-FAA	2242	-482	-88.15	2242	-482	-88.15	2.60
FAA-FA	2235	-489	-88.80	2242	-460	-87.89	3.75
FAA-AA	2178	-546	-99.85	2290	-433	-86.00	4.75
FAA-PA	2169	-555	-102.08	2302	-421	-85.16	4.87
FAA-MPA	2168	-556	-101.96	2307	-414	-84.84	4.86
FAA-FFA	2316	-408	-74.91	2159	-587	-92.70	
FAA-DFAA	2289	-435	-77.86	2193	-526	-89.84	1.34
FAA-TFAA	2325	-399	-69.08	2149	-566	-91.66	0.23
	R			R'			
DFAA-DFAA	2245	-475	-79.42	2245	-475	-79.42	1.34
DFAA-FA	2193	-527	-90.91	2297	-406	-76.80	3.75
DFAA-AA	2135	-584	-101.60	2343	-380	-74.24	4.75
DFAA-PA	2120	-599	-102.53	2349	-374	-74.60	4.87
DFAA-MPA	2095	-624	-105.20	2339	-383	-75.17	4.86
DFAA-FFA	2283	-436	-77.08	2230	-516	-81.22	
DFAA-FAA	2193	-526	-89.84	2289	-435	-77.86	2.60
DFAA-TFAA	2298	-421	-70.47	2223	-492	-79.54	0.23
	R			R'			
TFAA-TFAA	2267	-447	-71.79	2267	-447	-71.79	0.23
TFAA-FA	2163	-551	-91.74	2335	-367	-68.58	3.75
TFAA-AA	2089	-626	-103.18	2374	-349	-66.81	4.75
TFAA-PA	2082	-632	-103.58	2383	-340	-66.45	4.87
TFAA-MPA	2056	-659	-106.23	2372	-350	-67.01	4.86
TFAA-FFA	2262	-452	-77.84	2277	-469	-72.91	
TFAA-FAA	2149	-566	-91.66	2325	-399	-69.08	2.60
TFAA-DFAA	2223	-492	-79.54	2298	-421	-70.47	1.34

Table S6. Anharmonic frequencies (cm^{-1}) of the O–D stretching vibration and their shifts (cm^{-1}) calculated at B3LYP-D3/aug-cc-pVDZ level using VPT2 method for various carboxylic acid dimer and the corresponding electric field along the O–D bond (MV cm^{-1}). For each set of carboxylic acid dimer two cases arise, (i) frequency shift in a particular carboxylic acid (R) when the interaction partner is changed (R'), (ii) frequency shifts of the partners (R') when paired with a particular carboxylic acid (R). The pK_a values of the varying partner (R') are also listed.

Dimer	$\nu_{\text{O-D}}$	$\Delta\nu_{\text{O-D}}$	Field	$\nu_{\text{O-D}}$	$\Delta\nu_{\text{O-D}}$	Field	pK_a (R')
	R			R'			
FA-FA	2013	-582	-88.00	2013	-582	-88.00	3.75
FA-AA	1959	-637	-98.87	2067	-554	-86.16	4.75
FA-PA	1955	-640	-99.21	2205	-412	-85.71	4.87
FA-MPA	1951	-644	-100.57	2174	-444	-85.88	4.86
FA-FFA	2185	-410	-74.39	1917	-731	-92.85	
FA-FAA	2004	-591	-87.89	2003	-623	-88.80	2.60
FA-DFAA	2040	-555	-76.80	1947	-669	-90.91	1.34
FA-TFAA	2188	-407	-68.58	1935	-675	-91.74	0.23
	R			R'			
AA-AA	2022	-600	-96.99	2022	-600	-96.99	4.75
AA-FA	2067	-554	-86.16	1959	-637	-98.87	3.75
AA-PA	2015	-606	-98.78	2024	-592	-97.05	4.87
AA-MPA	2012	-609	-98.64	2011	-607	-96.72	4.86
AA-FFA	2221	-400	-72.33	1836	-811	-104.12	
AA-FAA	2058	-564	-86.00	1935	-691	-99.85	2.60
AA-DFAA	2211	-410	-74.24	1890	-726	-101.60	1.34
AA-TFAA	2225	-396	-66.81	1832	-778	-103.18	0.23
	R			R'			
PA-PA	2034	-583	-96.86	2034	-583	-96.86	4.87
PA-FA	2205	-412	-85.71	1955	-640	-99.21	3.75
PA-AA	2024	-592	-97.05	2015	-606	-98.78	4.75
PA-MPA	2025	-592	-99.82	1997	-621	-98.99	4.86
PA-FFA	2208	-409	-72.43	1806	-842	-106.04	
PA-FAA	2092	-525	-85.16	1904	-722	-102.08	2.60
PA-DFAA	2170	-447	-74.60	1887	-729	-102.53	1.34
PA-TFAA	2217	-400	-66.45	1823	-786	-103.58	0.23
	R			R'			
MPA-MPA	1986	-632	-98.34	1986	-632	-98.34	4.86
MPA-FA	2174	-444	-85.88	1951	-644	-100.57	3.75
MPA-AA	2011	-607	-96.72	2012	-609	-98.64	4.75
MPA-PA	1997	-621	-98.99	2025	-592	-99.82	4.87
MPA-FFA	2208	-410	-72.07	1804	-844	-105.87	
MPA-FAA	2170	-448	-84.84	1938	-688	-101.96	2.60
MPA-DFAA	2192	-426	-75.17	1833	-783	-105.20	1.34
MPA-TFAA	2208	-410	-67.01	1805	-805	-106.23	0.23

	R			R'			
FFA-FFA	2055	-593	-78.63	2055	-593	-78.63	
FFA-FA	1917	-731	-92.85	2185	-410	-74.39	3.75
FFA-AA	1836	-811	-104.12	2221	-400	-72.33	4.75
FFA-PA	1806	-842	-106.04	2208	-409	-72.43	4.87
FFA-MPA	1804	-844	-105.87	2208	-410	-72.07	4.86
FFA-FAA	1895	-753	-92.70	2172	-454	-74.91	2.60
FFA-DFAA	1998	-650	-81.22	2054	-562	-77.08	1.34
FFA-TFAA	2047	-601	-72.91	2022	-588	-77.84	0.23
	R			R'			
FAA-FAA	2015	-611	-88.15	2015	-611	-88.15	2.60
FAA-FA	2003	-623	-88.80	2004	-591	-87.89	3.75
FAA-AA	1935	-691	-99.85	2058	-564	-86.00	4.75
FAA-PA	1904	-722	-102.08	2092	-525	-85.16	4.87
FAA-MPA	1938	-688	-101.96	2170	-448	-84.84	4.86
FAA-FFA	2172	-454	-74.91	1895	-753	-92.70	
FAA-DFAA	2056	-570	-77.86	1969	-647	-89.84	1.34
FAA-TFAA	2176	-450	-69.08	1905	-705	-91.66	0.23
	R			R'			
DFAA-DFAA	2011	-605	-79.42	2011	-605	-79.42	1.34
DFAA-FA	1947	-669	-90.91	2040	-555	-76.80	3.75
DFAA-AA	1890	-726	-101.60	2211	-410	-74.24	4.75
DFAA-PA	1887	-729	-102.53	2170	-447	-74.60	4.87
DFAA-MPA	1833	-783	-105.20	2192	-426	-75.17	4.86
DFAA-FFA	2054	-562	-77.08	1998	-650	-81.22	
DFAA-FAA	1969	-647	-89.84	2056	-570	-77.86	2.60
DFAA-TFAA	2048	-568	-70.47	1989	-621	-79.54	0.23
	R			R'			
TFAA-TFAA	2019	-591	-71.79	2019	-591	-71.79	0.23
TFAA-FA	1935	-675	-91.74	2188	-407	-68.58	3.75
TFAA-AA	1832	-778	-103.18	2225	-396	-66.81	4.75
TFAA-PA	1823	-786	-103.58	2217	-400	-66.45	4.87
TFAA-MPA	1805	-805	-106.23	2208	-410	-67.01	4.86
TFAA-FFA	2022	-588	-77.84	2047	-601	-72.91	
TFAA-FAA	1905	-705	-91.66	2176	-450	-69.08	2.60
TFAA-DFAA	1989	-621	-79.54	2048	-568	-70.47	1.34

Table S7. Fitting parameters for linear least-square fits for the dimers of formic acid (FA) from the plots shown in Figures 3, 4, S1 and S2 for the O–H and O–D shifts corresponding to of R'.

	MP2 (Harmonic)			MP2 (Harmonic)			B3LYP-D3 (Harmonic)			B3LYP-D3 (Anharmonic)		
	O–H			O–D			O–D			O–D		
	Slope	Residual	R ²	Slope	Residual	R ²	Slope	Residual	R ²	Slope	Residual	R ²
FA	5.36	16.3	0.979	3.76	11.3	0.978	4.76	13.5	0.984	7.27	69.3	0.829
AA	4.86	14.6	0.976	3.40	10.7	0.974	4.37	12.2	0.985	7.42	38.8	0.928
PA	5.00	14.9	0.982	3.50	10.3	0.981	4.39	8.3	0.988	6.23	88.7	0.783
MPA	4.92	14.9	0.973	3.45	11.5	0.970	4.23	12.2	0.80	7.44	63.1	0.833
FFA	6.81	24.7	0.978	4.73	18.2	0.977	6.20	26.9	0.971	7.78	32.7	0.968
FAA	5.36	20.3	0.976	3.75	15.0	0.975	5.02	11.1	0.991	7.80	46.8	0.919
DFAA	6.37	18.6	0.978	4.45	14.0	0.976	5.78	15.7	0.982	6.05	27.9	0.941
TFAA	6.90	24.3	0.976	4.80	18.4	0.974	6.23	20.6	0.979	6.66	25.7	0.963
Average	5.70 ($\sigma=0.86$)			3.98 ($\sigma=0.59$)			5.12 ($\sigma=0.83$)			7.08 ($\sigma=0.68$)		

Table S8. Fitting parameters for linear least-square fits for the plots shown in Figures 3, 4, S1 and S2 for the O–H and O–D shifts of R' due to R.

	MP2 (Harmonic)			MP2 (Harmonic)			B3LYP-D3 (Harmonic)			B3LYP-D3 (Anharmonic)		
	O–H			O–D			O–D			O–D		
	Slope	Residual	R ²	Slope	Residual	R ²	Slope	Residual	R ²	Slope	Residual	R ²
FA	22.28	18.3	0.981	15.62	13.4	0.979	22.72	13.2	0.990	37.37	64.5	0.849
AA	24.14	11.8	0.992	16.85	8.9	0.991	24.90	14.1	0.991	29.02	16.7	0.983
PA	23.78	27.4	0.956	16.59	18.9	0.956	24.33	21.8	0.951	30.28	17.7	0.979
MPA	24.10	8.1	0.995	16.78	5.9	0.995	24.15	13.8	0.984	28.67	42.9	0.909
FFA	17.53	25.6	0.948	12.32	18.2	0.945	17.47	14.4	0.977	31.76	50.0	0.905
FAA	22.96	12.4	0.986	16.13	9.6	0.986	22.52	17.3	0.985	32.26	46.1	0.933
DFAA	20.13	36.7	0.889	14.10	26.2	0.885	21.24	14.9	0.964	35.42	39.3	0.929
TFAA	19.48	22.0	0.960	13.74	16.1	0.956	20.21	14.5	0.981	36.27	50.7	0.883
Average	21.80 ($\sigma=2.48$)			15.29 ($\sigma=1.70$)			22.19 ($\sigma=2.49$)			32.63 ($\sigma=3.35$)		

Table S9. Harmonic frequencies (cm^{-1}) of the O–H stretching vibration and their shifts (cm^{-1}) calculated at MP2/aug-cc-pVTZ level for various formic acid dimers and the corresponding electric field along the O–H bond (MV cm^{-1}). For each set of carboxylic acid dimer two cases arise, (i) frequency shift in a particular carboxylic acid (R) when the interaction partner is changed (R'), (ii) frequency shifts of the partners (R') when paired with a particular carboxylic acid (R). The pK_a values of the varying partner (R') are also listed.

Dimer	$\nu_{\text{O-H}}$	$\Delta\nu_{\text{O-H}}$	Field	$\nu_{\text{O-H}}$	$\Delta\nu_{\text{O-H}}$	Field	pK_a (R')
	Effect of R' on FA			Effect on R' due to FA			
FA-FA	3202	-522	-96.54	3202	-522	-96.54	3.75
FA-AA	3124	-601	-107.36	3250	-492	-94.24	4.75
FA-PA	3128	-597	-107.77	3248	-490	-94.20	4.87
FA-MPA	3109	-616	-109.88	3236	-494	-94.46	4.86
FA-FFA	3301	-424	-77.95	3108	-670	-102.64	-
FA-FAA	3187	-538	-95.82	3156	-588	-97.95	2.60
FA-DFAA	3255	-470	-83.07	3108	-630	-100.76	1.34
FA-TFAA	3300	-425	-72.77	3070	-667	-101.88	0.23

Cartesian coordinates of various hydrogen bonded carboxylic acid dimers considered in the present investigation at MP2/aug-cc-pVDZ level of theory.

FA-FA		FA-AA
C -1.90542500 -0.16761700 -0.00010000		C -1.41235000 -0.06944500 0.00025900
H -3.00449800 -0.24009600 -0.00065300		O -0.70120300 -1.08335800 -0.00010200
O -1.18317100 -1.16724800 -0.00023200		O -0.93293800 1.17618000 -0.00011100
O -1.50008600 1.09414700 0.00016900		H 0.06445900 1.14517400 -0.00037800
H -0.49948600 1.11799300 0.00046100		C 2.43088100 0.09796000 0.00045600
C 1.90549100 0.16745700 -0.00014500		H 3.53243700 0.11109400 0.00038000
H 3.00458100 0.23959000 -0.00079300		O 1.76330100 1.13499800 -0.00016600
O 1.18356000 1.16732800 0.00010400		O 1.95639100 -1.13914700 -0.00021100
O 1.49969500 -1.09411700 0.00026800		H 0.95174900 -1.10541400 -0.00000100
H 0.49902700 -1.11740900 -0.00001900		C -2.91636200 -0.11613300 0.00009300
		H -3.29563900 0.41251400 0.88685600
		H -3.29523100 0.41052100 -0.88805500
		H -3.25520200 -1.15756400 0.00107100
FA-PA		FA-MPA
C -2.88634400 -0.18709200 0.00027100		C -3.20813200 0.05750000 0.10728500
H -3.97387600 -0.36348800 0.00098400		H -4.30156100 0.14089900 0.21397900
O -2.40690900 0.94917800 -0.00073700		O -2.66373000 -0.98785100 -0.25668800
O -2.20653600 -1.32441200 0.00064300		O -2.59854800 1.19281700 0.41388900
H -1.22311000 -1.11814300 -0.00008000		H -1.60604900 1.07260400 0.30371300
C 0.92861600 0.30852600 -0.00010000		C 0.61786800 -0.11760900 -0.22181300
O 0.40259300 -0.81303700 -0.00090600		O 0.02482900 0.90914300 0.14036200
O 0.24204000 1.45314300 0.00029200		O 0.00184600 -1.25440900 -0.55384100
H -0.73524100 1.25087700 -0.00022100		H -0.98388500 -1.13930200 -0.44136600
C 2.42363300 0.52224900 0.00056200		C 2.12599700 -0.22176400 -0.27653200
H 2.65917600 1.14476200 -0.87834800		H 2.37127200 -0.94252000 -1.07317500
H 2.65856400 1.14343700 0.88057700		C 2.60198300 -0.79747700 1.07352300
C 3.21821600 -0.78294000 -0.00012500		C 2.76715400 1.13857700 -0.56298600
H 2.98194600 -1.38530000 -0.88907200		H 3.86286300 1.03432400 -0.59400100
H 4.29721300 -0.56883900 0.00055600		H 2.42990000 1.54695600 -1.52789100
H 2.98108200 -1.38673900 0.88761300		H 2.50295900 1.85965600 0.22474000
		H 3.69655900 -0.91475200 1.06232700
		H 2.33506700 -0.11066200 1.89284600
		H 2.14847600 -1.78017800 1.27218800
FA-FFA		FA-FAA
C 2.35703000 0.13475100 0.00018600		C 2.85345200 0.27587700 0.00018700
H 3.45534000 0.20303100 0.00012600		H 3.94510100 0.42075600 0.00076500
O 1.63987900 1.13872000 -0.00003900		O 2.06713200 1.22637000 -0.00070000
O 1.94577200 -1.12462700 0.00001600		O 2.53026000 -1.00911700 0.00056000
H 0.94981100 -1.14433600 -0.00017100		H 1.53234500 -1.09581400 0.00002300
C -1.40605200 -0.08163900 -0.00005100		C -0.92355200 -0.28081200 -0.00013300
O -0.76508800 -1.11755400 0.00016000		O -0.13769000 -1.23774600 -0.00040600
O -0.99361700 1.16150500 -0.00032000		O -0.59146900 0.99598100 0.00026700
H 0.01213800 1.15391000 -0.00038600		H 0.40921400 1.06986200 -0.00002900
F -2.74874700 -0.11062500 0.00012000		C -2.41519000 -0.55776800 -0.00032500
		H -2.65941000 -1.14384400 -0.89867300
		H -2.65942100 -1.14516600 0.89715800
		F -3.17799400 0.60739000 0.00051300
FA-DFAA		FA-TFAA
C 3.17590400 -0.00429000 0.08936100		C 0.35508400 0.04095300 -0.00001200
H 4.27285200 -0.03595300 0.17577200		O -0.28236500 1.09137400 -0.00002100

O	2.56891300	1.04236800	-0.15236400	O	-0.11319100	-1.18946200	-0.00020200
O	2.63628700	-1.19987100	0.27571300	H	-1.12080200	-1.15835000	-0.00051800
H	1.64420300	-1.13015100	0.19022700	C	-3.44450900	-0.09978300	0.00013100
C	-0.62259000	0.07941700	-0.18414700	H	-4.54424400	-0.14154600	0.00035100
O	-0.04776100	-0.98295700	0.04388800	O	-2.75094500	-1.11998700	0.00013000
O	-0.06128700	1.26132900	-0.38883500	O	-3.00294700	1.15001400	-0.00011100
H	0.93665600	1.17459300	-0.29767900	H	-2.00704700	1.14586200	-0.00023000
C	-2.15129800	0.19458100	-0.24172800	C	1.89889500	0.04016900	0.00005200
H	-2.49787900	0.89853300	-1.01050200	F	2.36497600	-0.60025800	-1.09624900
F	-2.57792000	0.64309300	0.99007700	F	2.38235000	1.29153900	0.00061000
F	-2.70398500	-1.03111700	-0.46407200	F	2.36499200	-0.60122700	1.09575100
AA-AA				AA-PA			
C	-1.93270300	-0.06117900	-0.00015300	C	2.37484300	-0.06841600	0.07796100
O	-1.24272800	-1.08973500	-0.00005700	O	1.68509100	-1.09210000	-0.02595000
O	-1.42724000	1.17321400	-0.00008600	O	1.87917700	1.16898200	0.04326400
H	-0.42739400	1.11821200	-0.00011700	H	0.88550400	1.12188600	-0.07862000
C	1.93269300	0.06119900	0.00038200	C	3.86947600	-0.09562800	0.25718800
O	1.24290700	1.08988800	0.00028900	H	4.22154500	-1.13241300	0.28499600
O	1.42712500	-1.17310900	-0.00010000	H	4.34374300	0.44858200	-0.57272500
H	0.42726600	-1.11786000	0.00008100	H	4.13286600	0.42503500	1.18951400
C	-3.43810100	-0.07730800	-0.00014000	C	-1.46022800	0.08803400	-0.37550700
H	-3.80656700	0.45763700	0.88744800	O	-0.76712300	1.11095200	-0.27411700
H	-3.80659400	0.45800800	-0.88748900	O	-0.96483800	-1.15067800	-0.35739900
H	-3.79838700	-1.11162900	-0.00033800	H	0.02836400	-1.10475800	-0.23494900
C	3.43806900	0.07704400	-0.00002900	C	-2.96438500	0.12428300	-0.47098100
H	3.80666200	-0.45803000	0.88742800	H	-3.25350100	1.09929900	-0.88635100
H	3.80627000	-0.45825300	-0.88751500	H	-3.29922400	-0.67799800	-1.14482600
H	3.79848500	1.11131600	-0.00022400	C	-3.57453000	-0.06950000	0.93090900
AA-MPA				AA-FFA			
C	2.73885200	0.00060800	0.02995200	C	1.87001100	-0.05817900	-0.00051700
O	2.13672600	-1.02378800	-0.31998100	O	1.14831100	-1.06597300	-0.00183000
O	2.13492700	1.14690000	0.34550000	O	1.40340000	1.19126300	-0.00224100
H	1.14350700	1.03225100	0.25199300	H	0.40994300	1.17107700	-0.00446300
C	4.23827100	0.07815100	0.14268500	C	3.37187000	-0.12240000	0.00318300
H	4.68123000	-0.88785200	-0.12240200	H	3.69881100	-1.16753000	0.00469600
H	4.61150400	0.86783700	-0.52584500	H	3.75822900	0.40066500	-0.88380500
H	4.51112200	0.35688300	1.17105700	H	3.75395200	0.40192300	0.89128100
C	-1.11530000	-0.11750200	-0.22597100	C	-1.91655000	0.06119000	0.00017700
O	-0.50781900	0.90506400	0.12385300	O	-1.31378400	1.11990100	-0.00017600
O	-0.51416000	-1.25949400	-0.56459800	O	-1.45927400	-1.16483100	-0.00129200
C	-2.62562000	-0.20840700	-0.25608400	H	-0.45004700	-1.11799600	-0.00269500
H	0.47681600	-1.14887500	-0.46780600	F	-3.26134300	0.04281200	0.00247100
H	-2.89049700	-0.92815000	-1.04741200				
C	-3.08534500	-0.77716700	1.10223600				
C	-3.25909500	1.15713500	-0.53480800				
H	-4.18107100	-0.88410600	1.10975400				
H	-2.63773000	-1.76373700	1.29515200				
H	-2.79815900	-0.09173600	1.91589200				
H	-4.35619200	1.06358700	-0.54664700				
H	-2.97405100	1.87745400	0.24634000				
H	-2.93446100	1.56008600	-1.50633300				
AA-FAA				AA-DFAA			
C	-2.37274600	-0.12760500	-0.00040100	C	2.70823500	-0.10799200	-0.00023200
O	-1.59005500	-1.08779300	-0.00405900	O	1.93744300	-1.07804500	-0.00036000
O	-1.98622200	1.14920600	-0.00128000	O	2.30284300	1.16371800	0.00085800

H	-0.98895600	1.19463700	-0.00500700	H	1.30778700	1.19059800	0.00141900
C	-3.86914000	-0.28486700	0.00532500	C	4.20569500	-0.24523900	-0.00091000
H	-4.13057500	-1.34839200	0.00651500	H	4.48102500	-1.30517100	-0.00359800
H	-4.28241300	0.21382600	0.89423400	H	4.61519600	0.26117600	-0.88717700
H	-4.28904600	0.21328200	-0.88079800	H	4.61531600	0.25645000	0.88801700
C	1.44310300	0.28046700	-0.00110200	C	-1.10829700	0.23705800	0.00096600
O	0.70267500	1.27293500	-0.00224700	O	-0.40954300	1.25636300	0.00231500
O	1.05101000	-0.97831900	-0.00282900	O	-0.68973600	-1.00993200	-0.00052200
H	0.04417600	-0.99998400	-0.00479000	H	0.31989700	-1.02047300	-0.00055000
C	2.94619900	0.48872500	0.00255600	C	-2.63482800	0.35710600	0.00068400
H	3.21534400	1.06272400	0.90158700	H	-2.95497800	1.40665500	0.00314600
H	3.21950800	1.06448000	-0.89408300	F	-3.14159700	-0.27458400	1.10920100
F	3.65646700	-0.70990400	0.00304400	F	-3.14030600	-0.26893500	-1.11171600
AA-TFAA				PA-PA			
C	0.82411100	0.05369900	0.00001400	C	-1.90661500	0.32323600	0.00025200
O	0.20743400	1.11682300	0.00020500	O	-1.43446900	-0.82193800	0.00045400
O	0.33142100	-1.16592400	-0.00034800	O	-1.16618500	1.43315100	-0.00032900
H	-0.68012600	-1.11215500	-0.00055700	C	-3.39052400	0.60765000	0.00084000
C	-2.99568700	-0.05338500	-0.00012300	H	-3.59646700	1.23813900	0.88150700
O	-2.27997300	-1.06531600	-0.00015900	H	-3.59683100	1.24119700	-0.87750700
O	-2.52066200	1.19370400	-0.00011500	C	-4.24586100	-0.65861400	-0.00102200
H	-1.52760900	1.16718000	-0.00003600	H	-4.03776700	-1.27077700	-0.89034900
C	2.36762600	0.02374300	0.00011100	H	-4.03718100	-1.27377700	0.88608000
C	-4.49782400	-0.10765800	0.00009300	H	-5.31377300	-0.39442400	-0.00025600
H	-4.87831800	0.41850600	0.88779000	H	-0.19736600	1.18068400	-0.00028200
H	-4.87858800	0.41870700	-0.88736600	C	1.90663100	-0.32324700	0.00004200
H	-4.83145000	-1.15065200	0.00004000	O	1.43444500	0.82190900	-0.00009700
F	2.82304000	-0.62518000	-1.09623400	O	1.16618300	-1.43315100	0.00027900
F	2.82297800	-0.62644200	1.09570800	H	0.19736600	-1.18055300	0.00035100
F	2.87631300	1.26559200	0.00084800	C	3.39053800	-0.60764900	-0.00005200
PA-MPA				PA-FFA			
C	-2.28419900	0.30178500	-0.25968600	C	2.35080000	-0.05979800	0.09089500
O	-1.53236900	1.07722000	0.34984600	O	1.75631100	-1.12136800	0.02455500
O	-1.85782600	-0.74444500	-0.96808900	O	1.89383600	1.16383800	0.02184800
H	-0.85782400	-0.79822600	-0.90730500	H	0.89126500	1.11407000	-0.10539400
C	-3.78682800	0.41927300	-0.21930100	F	3.68504900	-0.03661200	0.26101600
H	-4.03860400	1.46471200	0.00519100	C	-1.40340600	0.05307100	-0.38124100
H	-4.19317200	0.14500100	-1.20395900	O	-0.68759900	1.06337100	-0.29882600
C	-4.34817300	-0.51843400	0.86728600	O	-0.93628900	-1.19553000	-0.33166100
H	-3.93397000	-0.25837700	1.85344000	H	0.04960100	-1.17215000	-0.20547400
H	-5.44324600	-0.42807900	0.91813000	C	-2.90348200	0.12357300	-0.48528100
H	-4.09575100	-1.56564000	0.64418700	H	-3.25661800	-0.69998000	-1.12261100
C	1.54616200	-0.17884600	-0.21824100	H	-3.16563900	1.08592700	-0.94530700
O	0.79354500	-0.94861400	-0.83477000	C	-3.52055000	0.01090100	0.92314800
O	1.11914100	0.88098000	0.46955800	H	-4.61633400	0.07888300	0.86054000
H	0.11954000	0.93517600	0.40534400	H	-3.25815300	-0.95142100	1.38697400
C	3.04576000	-0.37201500	-0.15496500	H	-3.15980900	0.82521700	1.56967800
H	3.26916800	-1.19393300	-0.85236000				
C	3.44263800	-0.78877100	1.27326700				
C	3.78690500	0.90241600	-0.58814100				
H	4.87273400	0.71820500	-0.58401900				
H	3.49509700	1.21260300	-1.60379700				

H	3.56782200	1.72819800	0.10500900			
H	4.52467400	-0.98951300	1.31412400			
H	3.20864200	0.01741500	1.98526500			
H	2.91137400	-1.70111200	1.58707000			
PA-FAA				PA-DFAA		
C	1.90487000	0.21403100	0.02443300	C	-1.56175200	-0.07266800 -0.18646700
O	1.33299300	-0.86689300	-0.11507500	O	-1.08404100	1.04187100 0.01615100
O	1.31890100	1.40798900	0.05650900	O	-0.89668800	-1.20119100 -0.37586100
H	0.32473400	1.29092300	-0.05327200	H	0.09409600	-1.01850600 -0.29709900
C	3.40744700	0.35615900	0.18579100	C	-3.07411800	-0.32705600 -0.22497500
H	3.80316100	0.97447200	-0.63395800	H	-3.36211900	-1.07876200 -0.97218000
H	3.62436400	0.84336900	1.14830500	F	-3.73929300	0.83706600 -0.47159700
F	4.02696300	-0.88807600	0.15641000	F	-3.44971700	-0.78114800 1.02203800
C	-1.91123200	0.07950900	-0.36837600	C	2.24022100	0.31944600 0.04688200
O	-1.29121700	1.14419000	-0.22408100	O	1.68204000	-0.76440600 -0.17816800
O	-1.32969700	-1.12004800	-0.41662200	O	1.58835100	1.47056400 0.22028600
H	-0.34331400	-1.01390400	-0.30335700	H	0.60928200	1.31044900 0.14152800
C	-3.41450600	0.01357000	-0.44571600	C	3.73797400	0.47092800 0.15339500
H	-3.77721500	0.98368100	-0.81169000	H	4.03637600	1.23155600 -0.58676300
H	-3.70105900	-0.77881500	-1.15257500	H	3.94483500	0.91537100 1.14090500
C	-3.98898000	-0.28744000	0.95261700	C	4.49233900	-0.84274000 -0.04676200
H	-5.08751700	-0.32080100	0.91110700	H	5.57539200	-0.67295100 0.04211800
H	-3.62546300	-1.25806900	1.32108200	H	4.19233400	-1.58599200 0.70578600
H	-3.69380400	0.49495900	1.66833000	H	4.28561800	-1.26658000 -1.03996600
PA-TFAA				MPA-MPA		
C	-1.26377200	0.08477900	-0.00046800	C	-1.91581300	-0.05299400 -0.23535900
O	-0.74648800	1.19959900	-0.00155100	O	-1.35739600	0.84165300 0.41663200
O	-0.66225100	-1.08504600	-0.00015800	O	-1.26446700	-1.04372800 -0.84682100
H	0.34073600	-0.93973300	-0.00143800	H	-0.28171200	-0.94695600 -0.67168300
C	-2.79821000	-0.08560800	0.00057100	C	-3.41976500	-0.15821600 -0.36804500
F	-3.41811000	1.10473400	0.00178500	H	-3.62622400	-0.63321000 -1.34075100
F	-3.19208100	-0.77482200	1.09610700	C	-3.92191600	-1.09120300 0.75324900
F	-3.19335000	-0.77319100	-1.09577200	C	-4.08245400	1.21952300 -0.28896800
C	2.54954700	0.31850000	-0.00070700	H	-3.72789600	1.88288300 -1.09264900
O	1.92558700	-0.75277500	-0.00320900	H	-5.17453400	1.11383400 -0.38225700
O	1.96624600	1.51914200	0.00030700	H	-3.85466000	1.69858000 0.67483800
H	0.97965800	1.40548600	-0.00099600	H	-3.69305000	-0.65488400 1.73893800
C	4.05602500	0.39709900	0.00130400	H	-5.01298700	-1.21545400 0.67413200
H	4.34590700	0.99653700	-0.87741600	H	-3.45246700	-2.08427900 0.68752500
H	4.34366000	0.99564700	0.88135100	C	1.91570300	0.05395900 0.23472900
C	4.73100900	-0.97379500	0.00134000	O	1.35721600	-0.84006200 -0.41807400
H	5.82439400	-0.85508100	0.00234900	O	1.26446500	1.04474100 0.84619200
H	4.44184900	-1.55365000	0.88953300	H	0.28178200	0.94835500 0.67062000
H	4.44333900	-1.55289600	-0.88781600	C	3.41965700	0.15827300 0.36829100
				H	3.62581500	0.63460800 1.34039100
				C	4.08120300	-1.22024600 0.29199900
				C	3.92347500	1.08886100 -0.75416400
				H	5.17334200	-1.11535900 0.38554500
				H	3.72573800	-1.88178700 1.09678100
				H	3.85334100	-1.70081500 -0.67103000
				H	5.01456700	1.21243600 -0.67430900
				H	3.69508900	0.65102300 -1.73928300
				H	3.45477300	2.08245000 -0.69062800
MPA-FFA				MPA-FAA		
C	2.70633500	0.01186200	0.03970400	C	2.26418600	0.22954800 0.05651700
O	2.20594600	-1.04630300	-0.29838400	O	1.76460700	-0.84676300 -0.27010700
O	2.13796700	1.15047000	0.34248400	O	1.59699700	1.34635500 0.33545800
H	1.13707500	1.03060300	0.25311300	H	0.60950900	1.17357400 0.23819500

F	4.04233700	0.12915300	0.14817700	C	3.75869100	0.45572400	0.19575900
C	-1.06668600	-0.14333800	-0.22860200	H	4.07192700	1.24796800	-0.50074900
O	-0.43754400	0.86949800	0.11499800	H	3.98402900	0.76605600	1.22715400
O	-0.48995000	-1.29999500	-0.55976100	F	4.46308200	-0.70766400	-0.09284300
H	0.49599700	-1.21403900	-0.46622000	C	-1.54774800	-0.12725000	-0.22389300
C	-2.57639100	-0.20079000	-0.25737100	O	-0.99579200	0.93530300	0.10025800
H	-2.85657400	-0.92591600	-1.03820100	O	-0.88721000	-1.24554200	-0.52859600
C	-3.04583800	-0.74104900	1.11000500	H	0.09367100	-1.08562000	-0.43222300
C	-3.17972400	1.17454100	-0.55461200	C	-3.05033900	-0.29600400	-0.25719900
H	-4.14339100	-0.82420100	1.11745300	H	-3.27311100	-1.05330300	-1.02600500
H	-2.62018300	-1.73444700	1.31676800	C	-3.48711900	-0.84448400	1.11725900
H	-2.74470900	-0.05027500	1.91385600	C	-3.75131900	1.02577600	-0.58187900
H	-4.27817200	1.10221400	-0.56816600	H	-4.57581000	-1.00746600	1.12312300
H	-2.88322000	1.89847700	0.21878900	H	-2.99076100	-1.80017600	1.34336100
H	-2.84538400	1.55850100	-1.53043000	H	-3.24057500	-0.11958200	1.90968600
				H	-4.84181500	0.87456600	-0.59614600
				H	-3.50971200	1.78385900	0.17784400
				H	-3.44202500	1.41442400	-1.56414500
MPA-DFAA				MPA-TFAA			
C	-1.92575000	-0.01417800	-0.21591000	C	-1.61125900	0.04017000	-0.00446400
O	-1.28518500	0.90794100	0.28614700	O	-0.94773600	1.05416500	0.20327100
O	-1.43837700	-1.09384000	-0.80429900	O	-1.17449500	-1.17013400	-0.27326100
H	-0.42742500	-1.07048600	-0.75680700	H	-0.15915700	-1.15975500	-0.28798900
C	-3.45935300	-0.05213000	-0.20496200	C	-3.15441700	0.07460700	0.02951000
H	-3.88271300	-0.48685000	-1.12038900	F	-3.62055500	-0.77127900	0.97718400
F	-3.95842400	1.20383600	-0.02519000	F	-3.60617100	1.30868000	0.30253700
F	-3.84687700	-0.82636600	0.86874600	F	-3.65801800	-0.31104600	-1.16556200
C	1.89509700	-0.18918300	-0.19873100	C	2.19319700	-0.23040200	-0.11676300
O	1.17621900	-1.06610400	-0.70420600	O	1.42754500	-1.18690700	-0.31714300
O	1.42011300	0.91548300	0.37903300	O	1.77544400	1.00821100	0.15278900
H	0.42462000	0.90626100	0.34223100	H	0.78173100	1.02496200	0.17126100
C	3.40233800	-0.29236800	-0.15295000	C	3.69755100	-0.37006600	-0.12623000
H	3.66022400	-1.15298400	-0.78890100	H	3.89836700	-1.38653900	-0.49756700
C	3.83837200	-0.57851500	1.29676600	C	4.34793100	0.66975600	-1.05183900
C	4.06705200	0.98307800	-0.69313700	C	4.22105400	-0.23894200	1.31687100
H	5.16068300	0.85488300	-0.69546700	H	5.43655100	0.50691800	-1.07892700
H	3.74472700	1.20093100	-1.72334600	H	3.96340100	0.59107700	-2.08068900
H	3.81603900	1.84620300	-0.05902800	H	4.15440200	1.68801100	-0.68326800
H	4.93002300	-0.71716300	1.33311300	H	5.30993900	-0.40108800	1.32967100
H	3.57069500	0.26576300	1.95034800	H	4.01242200	0.76784700	1.70979700
H	3.36213900	-1.49185600	1.68638100	H	3.75465600	-0.98204100	1.98252500
FFA-FFA				FFA-FAA			
C	1.85860400	-0.06451700	-0.00010700	C	-1.38663200	0.26811700	-0.00415800
O	1.20986400	-1.09637100	-0.00161600	O	-0.61574200	1.23829300	-0.00716200
O	1.45307600	1.18195600	0.00025700	O	-1.03211700	-1.00243600	-0.00934400
H	0.45446600	1.17925600	-0.00108200	H	-0.03544200	-1.05542900	-0.01623300
F	3.19664600	-0.10235000	0.00156400	C	-2.88159600	0.51983900	0.00661000
C	-1.85861600	0.06451100	-0.00021700	H	-3.12919200	1.09966700	0.90817600
O	-1.20935700	1.09603400	-0.00191400	H	-3.14106500	1.10547900	-0.88783200
O	-1.45361200	-1.18215700	0.00003500	F	-3.62052800	-0.65899400	0.00766400
H	-0.45504500	-1.17997700	-0.00135900	C	2.35391700	-0.13503000	0.00076400
F	-3.19654800	0.10291300	0.00180100	O	1.65743400	-1.13517500	-0.00434600
				O	2.00836500	1.12798800	-0.00159500
				H	1.00274700	1.17300800	-0.00746800
				F	3.69222800	-0.23763300	0.01051700
FFA-DFAA				FFA-TFAA			
C	-1.06706900	-0.10092300	-0.19037600	C	-0.78141400	0.02268000	-0.00177100
O	-0.46308200	0.94862100	0.02399300	O	-0.13156200	1.06588300	-0.00392000

O	-0.53753700	-1.29761300	-0.39313600	O	-0.32685200	-1.21321100	-0.00017500
H	0.45708600	-1.23470100	-0.31719900	H	0.67407500	-1.19312900	-0.00219300
C	-2.59861600	-0.17635200	-0.22910000	C	-2.32491200	0.04032200	0.00030900
H	-2.97205600	-0.87110700	-0.99344000	F	-2.79081700	1.29741700	-0.00489100
F	-3.11924300	1.06314200	-0.44435500	F	-2.79333400	-0.58982600	1.10048900
F	-3.01748500	-0.61423600	1.00825100	F	-2.79743800	-0.60054500	-1.09161200
C	2.67991100	-0.00639800	0.03461800	C	2.96620300	-0.05134600	0.00008100
O	2.12272400	-1.06733600	-0.18843200	O	2.33787500	-1.09570100	-0.00222600
O	2.17077200	1.18603400	0.22231700	O	2.53573300	1.18712900	0.00094000
H	1.17415800	1.11058200	0.15392800	H	1.53722300	1.16566800	0.00071000
F	4.01588800	0.05549700	0.11920700	F	4.30468800	-0.06207600	0.00188200
FAA-FAA				FAA-DFAA			
C	1.89197500	-0.24883900	-0.00057600	C	2.24097800	0.24286200	0.03696700
O	1.39720600	0.87818900	-0.00882000	O	1.69827400	-0.83909500	-0.18786500
O	1.21850500	-1.39715200	0.00024700	O	1.61860000	1.40626200	0.21444800
H	0.23550900	-1.20310300	-0.00463000	H	0.63251200	1.26766200	0.13851300
C	3.38641600	-0.51066600	0.00890900	C	3.74311300	0.42123400	0.14975300
H	3.64835900	-1.07810700	0.91470700	H	4.08066600	1.13915000	-0.61284100
H	3.65781000	-1.09722800	-0.88165800	H	3.98692600	0.80902100	1.15032800
F	4.09460000	0.68542200	0.00007400	F	4.39574300	-0.78962200	-0.04227200
C	-1.89155800	0.24782300	-0.00282100	C	-1.54299000	-0.08608500	-0.18795200
O	-1.39935100	-0.88036800	-0.01275400	O	-1.03158700	1.01374500	0.01472200
O	-1.21644700	1.39507300	0.00254900	O	-0.91332300	-1.23408200	-0.38198000
H	-0.23286900	1.20125300	-0.00409400	H	0.07843100	-1.08510100	-0.30913700
C	-3.38561700	0.51244000	0.00494000	C	-3.06257000	-0.29368300	-0.21840600
H	-3.64748900	1.08805000	0.90545400	H	-3.37641400	-1.04720000	-0.95314700
H	-3.65517300	1.09179100	-0.89101800	F	-3.44499600	-0.71620100	1.03694700
F	-4.09601700	-0.68243700	0.00534300	F	-3.68952700	0.88758500	-0.48028500
FAA-TFAA				DFAA-DFAA			
C	1.24808400	0.02548800	-0.00100500	C	1.89335800	0.12866200	-0.19042100
O	0.56350900	1.04635300	-0.00033300	O	1.34176100	-0.97050600	-0.21162800
O	0.83552700	-1.22434700	-0.00184100	O	1.30466800	1.31475500	-0.20679500
H	-0.17321000	-1.23793200	-0.00146000	H	0.31014700	1.18889300	-0.21089800
C	2.79030300	0.09554100	0.00042200	C	3.41741300	0.28327200	-0.11084200
F	3.28669800	-0.52822500	-1.09186200	H	3.79013000	1.14144900	-0.68602100
F	3.21580500	1.36757400	-0.00422000	F	4.02335100	-0.85641900	-0.54638100
F	3.28281000	-0.51890800	1.10016700	C	-1.89272300	-0.12779500	-0.18694600
C	-2.53533800	-0.26486300	-0.00122700	O	-1.34094300	0.97137300	-0.20245500
O	-1.79646700	-1.25932600	-0.00219000	O	-1.30390800	-1.31380400	-0.20531100
O	-2.13889400	0.99407500	-0.00354200	H	-0.30949500	-1.18737700	-0.20219300
H	-1.14133700	1.01476400	-0.00603800	C	-3.41701600	-0.28272500	-0.11338600
C	-4.03809400	-0.46640700	0.00339600	H	-3.78757100	-1.13837000	-0.69373900
H	-4.30836800	-1.03757400	0.90404500	F	-4.02151800	0.85882700	-0.54592000
H	-4.31321300	-1.04346400	-0.89196000	F	3.74163700	0.46639600	1.21574500
F	-4.73675800	0.73640500	0.00137500	F	-3.74591800	-0.47187200	1.21121500
DFAA-TFAA				TFAA-TFAA			
C	-1.59082900	0.02027000	-0.00296100	C	-1.89006800	-0.02837200	0.00038300
O	-0.91030900	1.04337000	-0.00536200	O	-1.24956400	-1.07715300	0.00079200
O	-1.17126300	-1.22859300	-0.00349400	O	-1.42338200	1.20381600	0.00032800
H	-0.16734700	-1.23461300	-0.00677800	H	-0.42291800	1.17435700	0.00080100
C	-3.13329600	0.08228400	0.00148100	C	1.89005800	0.02864700	0.00049100
F	-3.56379800	1.35210600	0.00188300	O	1.24986900	1.07762400	0.00098900
F	-3.61967400	-0.53883400	1.09939300	O	1.42303600	-1.20340000	0.00048200
F	-3.62614500	-0.54033200	-1.09266100	H	0.42251800	-1.17365400	0.00088800
C	2.19317100	-0.22094800	-0.00169000	C	-3.43382100	-0.03123100	-0.00031900
O	1.48755200	-1.23543300	-0.00154600	C	3.43381800	0.03105800	-0.00020100
O	1.78217800	1.03057500	-0.00500800	F	-3.89753700	0.60901300	-1.09646800
H	0.78359900	1.05045000	-0.00631800	F	-3.89845400	0.60864300	1.09567200

C	3.71918900	-0.34762300	0.00246200	F	-3.91134400	-1.28386700	-0.00072800
H	4.03444600	-1.39862200	0.00440100	F	3.91174200	1.28354500	-0.00024400
F	4.21924400	0.28126900	1.11374300	F	3.89736300	-0.60899200	-1.09653900
F	4.22533000	0.27907400	-1.10722100	F	3.89831900	-0.60927800	1.09558000

Cartesian coordinates of various hydrogen bonded carboxylic acid dimers considered in the present investigation at B3LYP-D3/aug-cc-pVDZ level of theory.

FA-FA				FA-AA			
C	-1.88953600	-0.16900800	-0.00019000	C	-1.40080900	-0.06932400	-0.00003800
H	-2.98919500	-0.24375200	0.00004900	O	-0.69941000	-1.08259600	0.00000700
O	-1.17584700	-1.16591100	-0.00014200	O	-0.91715100	1.16279000	-0.00014200
O	-1.48107100	1.08030700	-0.00004100	H	0.08379500	1.15039700	-0.00036700
H	-0.47644300	1.12392000	-0.00004100	C	2.41122300	0.09935000	0.00010900
C	1.88941600	0.16907200	-0.00009500	H	3.51383700	0.11470300	0.00040900
H	2.98907900	0.24390900	-0.00000400	O	1.75247100	1.13354900	-0.00015400
O	1.17566100	1.16592800	0.00007900	O	1.93494000	-1.12478100	0.00024600
O	1.48108800	-1.08028800	-0.00028600	H	0.92548900	-1.11027900	-0.00000500
H	0.47653700	-1.12414900	-0.00026900	C	-2.90290900	-0.11817400	0.00003900
FA-PA				FA-MPA			
C	-2.87077300	-0.18012400	0.00010800	C	-3.19654100	0.05584500	0.09611400
H	-3.95953300	-0.35459100	0.00021000	H	-4.29185300	0.13890000	0.19277600
O	-2.39937700	0.95154000	0.00013100	O	-2.65399100	-1.00510100	-0.19239500
O	-2.19108900	-1.30453100	-0.00008000	O	-2.59299800	1.20009400	0.32363000
H	-1.19873500	-1.11666600	-0.00018800	H	-1.59191600	1.09644700	0.22943200
C	0.91676600	0.30122600	0.00018200	C	0.60453600	-0.10818600	-0.20686300
O	0.39501000	-0.81514900	-0.00028800	O	0.01022000	0.93196800	0.08462400
O	0.23154400	1.43473700	0.00047400	O	-0.00571700	-1.25678100	-0.45767900
H	-0.75212400	1.25450400	0.00030700	H	-0.99665700	-1.16192800	-0.35837500
C	2.41089700	0.51279000	0.00040800	C	2.11472800	-0.20573100	-0.26793000
H	2.64401200	1.13806000	-0.87444000	H	2.34907300	-0.90799000	-1.08054600
H	2.64383400	1.13725500	0.87587800	C	2.61227700	-0.82269500	1.05650500
C	3.21855900	-0.78222800	-0.00010100	C	2.75916700	1.15423800	-0.54379300
H	2.98960500	-1.38815500	-0.88577600	H	3.85081700	1.04585300	-0.59317200
H	4.29301100	-0.55754100	0.00009000	H	2.40995100	1.57743600	-1.49457900
H	2.98945500	-1.38894500	0.88499400	H	2.51305300	1.86754100	0.25280000
FA-FFA				FA-FAA			
C	2.33944400	0.13655800	-0.00004700	C	2.83522100	0.27328200	0.00029300
H	3.43833700	0.20646800	0.00024200	H	3.92786600	0.41670100	0.00049000
O	1.63171800	1.13898000	-0.00012400	O	2.06092500	1.22431700	0.00030500
O	1.92413500	-1.10956900	0.00003900	O	2.50385000	-0.99827800	0.00001200
H	0.92476900	-1.14855400	-0.00011000	H	1.50291200	-1.10124800	-0.00017700
C	-1.39144800	-0.08272700	0.00017200	C	-0.91308700	-0.27637600	-0.00025200
O	-0.75636800	-1.11645500	0.00012300	O	-0.13575100	-1.23204500	-0.00046600
O	-0.97389600	1.14768100	-0.00021900	O	-0.57416300	0.98800000	0.00008100
H	0.03831700	1.15925300	-0.00034800	H	0.42791600	1.08222200	0.00014700
F	-2.72854300	-0.11849900	-0.00008700	C	-2.40346600	-0.55526000	-0.00030600
				H	-2.64343700	-1.14686400	-0.89551900
				H	-2.64343700	-1.14720300	0.89468500

	F	-3.17257300	0.59872300	-0.00008500			
FA-DFAA	FA-TFAA						
C	3.15911400	-0.00249400	0.08464800	C	0.34154800	0.03852200	-0.00020600
H	4.25688500	-0.03372900	0.16998400	O	-0.28825300	1.08377000	0.00004800
O	2.56294900	1.03789700	-0.17437800	O	-0.13111100	-1.17873300	-0.00027500
O	2.61462100	-1.18048500	0.29040600	H	-1.14366900	-1.16556800	-0.00024200
H	1.61731800	-1.12803600	0.20851700	C	-3.42836900	-0.09997000	0.00008600
C	-0.61048500	0.07991200	-0.17889200	H	-4.52883300	-0.14171700	0.00014400
O	-0.04301600	-0.97423200	0.06399700	O	-2.74496100	-1.11849500	-0.00006200
O	-0.04543300	1.24452400	-0.40148600	O	-2.98186300	1.13651400	0.00012500
H	0.95851900	1.17543500	-0.31474900	H	-1.98290400	1.14973000	0.00005200
C	-2.14448800	0.19168300	-0.23727000	C	1.89392300	0.04246200	-0.00002900
H	-2.48392600	0.91938100	-0.98691700	F	2.36156900	-0.59474600	-1.09442700
F	-2.57693100	0.60266800	1.00127100	F	2.37182100	1.29294600	0.00039200
F	-2.69303300	-1.02294700	-0.49942100	F	2.36134900	-0.59541500	1.09407700
AA-AA	AA-PA						
C	-1.91779900	-0.06095600	-0.00019700	C	2.36866300	-0.06694900	0.07647000
O	-1.23750200	-1.08836200	-0.00030200	O	1.67676300	-1.08571000	0.03449800
O	-1.40828200	1.15990800	-0.00038500	O	1.88130600	1.15907500	-0.01929500
H	-0.40428500	1.12305200	-0.00070700	H	0.88204600	1.13537000	-0.13037600
C	1.91772300	0.06088200	-0.00015200	C	3.86259800	-0.10301900	0.24266100
O	1.23739400	1.08826500	-0.00020400	H	4.20420300	-1.13815800	0.32278400
O	1.40833100	-1.16003300	-0.00044200	H	4.33623600	0.39056500	-0.61652000
H	0.40436500	-1.12347600	-0.00067900	H	4.14366900	0.46397400	1.14013800
C	-3.42131100	-0.07914900	0.00017500	C	-1.44042700	0.10940000	-0.34875200
H	-3.79209200	0.45595600	0.88468800	O	-0.74480700	1.12663200	-0.30784800
H	-3.79255400	0.45615000	-0.88402400	O	-0.95278800	-1.11838400	-0.26777800
H	-3.78174100	-1.11103400	0.00016900	H	0.04514800	-1.09673700	-0.15494800
C	3.42125800	0.07916900	0.00027500	C	-2.94353000	0.15490000	-0.45410600
H	3.79203900	-0.45600400	0.88474400	H	-3.22212700	1.14485900	-0.83179800
H	3.79256300	-0.45602300	-0.88396100	H	-3.26604900	-0.61069000	-1.17238700
H	3.78165600	1.11107000	0.00038200	C	-3.59535900	-0.10699500	0.91637100
				H	-4.68833800	-0.05931000	0.82768700
				H	-3.32116000	-1.09966900	1.29525700
				H	-3.27807600	0.64689200	1.64950400
AA-MPA	AA-FFA						
C	2.72921000	0.00021100	0.02973300	C	1.85742600	-0.05803500	0.00103500
O	2.12989900	-1.03799500	-0.25448200	O	1.14458000	-1.06506300	0.00116400
O	2.12942200	1.15403500	0.27331300	O	1.38643700	1.17811000	0.00019000
H	1.13156800	1.05756400	0.19373600	H	0.39040200	1.17783100	-0.00049600
C	4.22747100	0.07438000	0.13292000	C	3.35680000	-0.12543500	0.00188500
H	4.66470500	-0.90573500	-0.07394200	H	3.68330800	-1.16830100	0.00240700
H	4.60501700	0.81978500	-0.57978100	H	3.74450800	0.39784400	-0.88235200
H	4.50744900	0.41417000	1.13896400	H	3.74350800	0.39838300	0.88624400
C	-1.09999400	-0.10503600	-0.21116500	C	-1.89910500	0.06128300	-0.00122000
O	-0.49400300	0.92911100	0.07674400	O	-1.30483300	1.11899300	-0.00174200
O	-0.50172600	-1.25569800	-0.47673800	O	-1.43418600	-1.15043600	-0.00022800
C	-2.61228900	-0.19102100	-0.25001900	H	-0.41645700	-1.11990300	0.00029200
H	0.49446300	-1.16478100	-0.39074900	F	-3.23885900	0.04665000	-0.00239300
H	-2.86458800	-0.88876700	-1.06116000				
C	-3.09501800	-0.80780300	1.07971900				
C	-3.25029400	1.17470100	-0.51206300				
H	-4.18727100	-0.91816600	1.06164700				
H	-2.64868200	-1.79605900	1.24571100				
H	-2.83066000	-0.15498800	1.92338500				
H	-4.34355900	1.07584000	-0.54394600				
H	-2.98486300	1.88391700	0.28200500				
H	-2.91280200	1.59747900	-1.46730300				

AA-FAA				AA-DFAA			
C	-2.35889500	-0.12984800	0.00171500	C	2.69543800	-0.10706500	-0.00016000
O	-1.58927000	-1.09274700	0.00061100	O	1.93482600	-1.07725400	-0.00136900
O	-1.95983100	1.13202000	0.00210900	O	2.28329000	1.15147200	0.00108700
H	-0.95973200	1.18634400	0.00135000	H	1.28675000	1.19577300	0.00119800
C	-3.85349300	-0.28251000	0.00249200	C	4.19059800	-0.24455900	-0.00055000
H	-4.12001600	-1.34239800	0.00207200	H	4.46751300	-1.30171800	-0.00308300
H	-4.26987500	0.21711700	0.88737600	H	4.60227500	0.26215700	-0.88361600
H	-4.27092000	0.21807400	-0.88136000	H	4.60208200	0.25770700	0.88516000
C	1.42881900	0.27956800	0.00002300	C	-1.09360400	0.23066500	0.00058100
O	0.69864500	1.27175400	0.00024200	O	-0.40530200	1.24749100	0.00196700
O	1.02883000	-0.96576100	0.00002100	O	-0.66746600	-1.00268100	-0.00123400
H	0.01872900	-1.00905300	0.00016100	H	0.34692400	-1.02964300	-0.00143500
C	2.93110900	0.48771900	-0.00001900	C	-2.62526500	0.35591600	0.00087800
H	3.19936600	1.06709400	0.89508200	H	-2.93159300	1.40957900	0.00309200
H	3.19926500	1.06726200	-0.89504100	F	-3.13622300	-0.26690300	1.10753000
F	3.64659800	-0.70121700	-0.00017000	F	-3.13609200	-0.26218200	-1.10850400
AA-TFAA				MPA-MPA			
C	0.80783000	0.05222400	-0.00001000	C	-1.90622800	-0.04989500	-0.21901800
O	0.20016200	1.11087000	0.00025600	O	-1.34349300	0.88555600	0.35334500
O	0.30961400	-1.15329500	-0.00034100	O	-1.26411300	-1.08269700	-0.74171200
H	-0.70864000	-1.11623000	-0.00039100	H	-0.27462800	-0.99958500	-0.58751600
C	-2.98313700	-0.05305000	0.00022200	C	-3.41248300	-0.14906300	-0.35214400
O	-2.27626600	-1.06386200	-0.00018100	H	-3.60963300	-0.61160600	-1.32976700
O	-2.50347900	1.18101200	0.00028100	C	-3.93243900	-1.10420400	0.74283800
H	-1.50831200	1.17302100	0.00018400	C	-4.07931700	1.22576400	-0.27562700
C	2.35995200	0.02497600	-0.00000300	H	-3.71447600	1.89226800	-1.06794200
C	-4.48290800	-0.10956700	-0.00000600	H	-5.16682400	1.11972300	-0.38548500
H	-4.86640500	0.41646900	0.88446000	H	-3.86890300	1.70406400	0.68923100
H	-4.86623900	0.41707100	-0.88419000	H	-3.72276200	-0.69387600	1.74059600
H	-4.81671400	-1.15012000	-0.00039300	H	-5.01929400	-1.22443600	0.64385000
F	2.81623000	-0.62153700	-1.09443400	H	-3.46463800	-2.09324000	0.66342600
F	2.81621600	-0.62217500	1.09405500	C	1.90631300	0.04928900	0.21951800
F	2.86478200	1.26543500	0.00036200	O	1.34355300	-0.88613200	-0.35286800
				O	1.26418500	1.08209100	0.74221400
				H	0.27467900	0.99893700	0.58804800
				C	3.41256200	0.14849400	0.35255400
				H	3.60974800	0.61103500	1.33017100
				C	4.07941200	-1.22632600	0.27600300
				C	3.93244600	1.10364700	-0.74244700
				H	5.16692500	-1.12026300	0.38578000
				H	3.71463800	-1.89282400	1.06835300
				H	3.86893300	-1.70463600	-0.68883600
				H	5.01930200	1.22390900	-0.64350800
				H	3.72273500	0.69331800	-1.74019800
				H	3.46462600	2.09267300	-0.66301600
MPA-FFA				MPA-FAA			
C	2.69534200	0.00871600	0.03234900	C	2.25577100	0.22685000	0.05524300
O	2.19605100	-1.06276000	-0.24019700	O	1.75689700	-0.86055100	-0.20187200
O	2.12883700	1.15392100	0.25894900	O	1.59286400	1.34920700	0.26064200
H	1.11725300	1.05199500	0.17783100	H	0.59692700	1.19344300	0.17788000
F	4.02730000	0.11874600	0.13581200	C	3.75140000	0.45146100	0.17981600
C	-1.05255600	-0.13180200	-0.21662100	H	4.06698200	1.20085800	-0.56081500
O	-0.42401500	0.89429000	0.05960400	H	3.97739200	0.82805900	1.18818600
O	-0.47860900	-1.29703100	-0.47164200	F	4.45274200	-0.72280700	-0.03450700
H	0.51157600	-1.23115000	-0.39096700	C	-1.53352300	-0.11412900	-0.20736000
C	-2.56396900	-0.18472900	-0.24941800	O	-0.98240800	0.95790500	0.05492500
H	-2.83352700	-0.89348200	-1.04506300	O	-0.87638500	-1.24000300	-0.43725900

C	-3.05311800	-0.76473900	1.09539200	H	0.11018800	-1.10082800	-0.34968200
C	-3.17312000	1.18925000	-0.53659500	C	-3.03834000	-0.27692700	-0.25166900
H	-4.14725800	-0.85198100	1.08101500	H	-3.24919600	-1.01009300	-1.04307800
H	-2.62823200	-1.75903000	1.28024000	C	-3.49762600	-0.87860500	1.09354300
H	-2.77311100	-0.10036000	1.92461600	C	-3.74242300	1.04665000	-0.55729800
H	-4.26783000	1.11064600	-0.56600600	H	-4.58269300	-1.04414700	1.07228600
H	-2.89414200	1.90754600	0.24441000	H	-3.00377100	-1.83806100	1.29069800
H	-2.82898100	1.58691900	-1.50010800	H	-3.27243500	-0.18906900	1.91908700
MPA-DFAA				MPA-TFAA			
C	-1.91270800	-0.01397300	-0.21228300	C	-1.59809400	0.03981100	-0.00453500
O	-1.28442700	0.89841800	0.30355200	O	-0.94664300	1.04890300	0.21440100
O	-1.41570800	-1.06963200	-0.81134400	O	-1.15133500	-1.15373000	-0.27922600
H	-0.39854100	-1.05882800	-0.76972100	H	-0.12972600	-1.15815500	-0.29368600
C	-3.45109800	-0.05495700	-0.20492900	C	-3.14942400	0.07361000	0.02379500
H	-3.86360600	-0.51988200	-1.11054600	F	-3.61854900	-0.77724100	0.96218700
F	-3.95478300	1.20016000	-0.06811500	F	-3.60152100	1.30303000	0.30358800
F	-3.84235200	-0.79649000	0.88552800	F	-3.64779300	-0.30185300	-1.17410400
C	1.88236300	-0.18212500	-0.19113700	C	2.18213300	-0.22350700	-0.10684900
O	1.17456000	-1.05039200	-0.71070300	O	1.42727400	-1.17798300	-0.31675300
O	1.39863600	0.90258100	0.39294700	O	1.75465300	0.99925500	0.16860300
H	0.40167200	0.91098400	0.36078300	H	0.76045400	1.03275200	0.18770400
C	3.39111800	-0.28638500	-0.14612100	C	3.68796000	-0.36254700	-0.11875500
H	3.64207000	-1.14381800	-0.78292800	H	3.88259500	-1.37730100	-0.48741400
C	3.83862700	-0.58480800	1.29781000	C	4.33920200	0.66403800	-1.05904600
C	4.06023700	0.98217400	-0.69777900	C	4.22435900	-0.23837300	1.32043900
H	5.15038600	0.85020700	-0.70306300	H	5.42421200	0.49798400	-1.08840200
H	3.73654400	1.19152800	-1.72625600	H	3.95194100	0.57284700	-2.08274900
H	3.81698900	1.85184800	-0.07481900	H	4.15214600	1.68637000	-0.70771400
H	4.92751500	-0.72389000	1.32359700	H	5.30999700	-0.40234800	1.32236700
H	3.57895800	0.24909500	1.96267600	H	4.02342900	0.76290300	1.72273300
H	3.36778200	-1.49945900	1.68229300	H	3.76511300	-0.98226200	1.98513000
FFA-FFA				FFA-FAA			
C	1.84397400	-0.06594600	-0.00007100	C	-1.37526400	0.26242900	0.00091300
O	1.20130800	-1.09596800	-0.00075000	O	-0.61210400	1.23086300	0.00188100
O	1.43243300	1.16775400	0.00002100	O	-1.01626800	-0.99611900	-0.00229000
H	0.42882700	1.18329000	-0.00031500	H	-0.01881300	-1.07491000	-0.00380000
F	3.17602300	-0.10959000	-0.00011600	C	-2.86847200	0.51796700	0.00292300
C	-1.84404000	0.06584500	-0.00009800	H	-3.11623200	1.10383800	0.89987400
O	-1.20149600	1.09594700	-0.00068500	H	-3.11792200	1.10860400	-0.89042500
O	-1.43251500	-1.16784800	-0.00008200	F	-3.61586400	-0.64850300	0.00054500
H	-0.42891100	-1.18362900	-0.00040300	C	2.33774500	-0.13047500	-0.00378600
F	-3.17612400	0.10944400	-0.00013900	O	1.65011700	-1.13022300	-0.00647600
FFA-DFAA				FFA-TFAA			
C	-1.05446400	-0.10029100	-0.18604400	C	-0.76775700	0.02186500	-0.00033200
O	-0.45866200	0.94164100	0.04570900	O	-0.12639600	1.06097100	-0.00208300
O	-0.51944300	-1.27840900	-0.41109200	O	-0.30682400	-1.20025300	0.00098900
H	0.48023200	-1.23256600	-0.33957200	H	0.69833200	-1.19688800	0.00057700
C	-2.59102000	-0.17428000	-0.22330900	C	-2.31940700	0.04250600	0.00017700
H	-2.95775400	-0.89581900	-0.96600100	F	-2.78133900	1.29798500	-0.00284000
F	-3.11010100	1.05274400	-0.48199000	F	-2.78981300	-0.58736400	1.09641200
F	-3.01258600	-0.57059600	1.02253300	F	-2.79089200	-0.59303300	-1.09229500
C	2.66464200	-0.00827300	0.03190000	C	2.95240800	-0.05197600	-0.00045800

O	2.11551700	-1.06299600	-0.21211100	O	2.33192500	-1.09524300	0.00013000
O	2.14865800	1.16698500	0.23806000	O	2.51384500	1.17311600	-0.00141700
H	1.14524000	1.10933500	0.16875500	H	1.51020100	1.16748000	-0.00181100
F	3.99519200	0.04773500	0.11943700	F	4.28518600	-0.06590000	0.00057500
FAA-FAA				FAA-DFAA			
C	1.87953000	-0.24211400	0.00254900	C	2.22881500	0.23820800	0.03666100
O	1.39315000	0.88158200	-0.00168200	O	1.69332900	-0.83782700	-0.19784900
O	1.20226600	-1.37510600	0.00519900	O	1.60253000	1.38493200	0.22798200
H	0.21254100	-1.19750600	0.00333000	H	0.61068000	1.26311400	0.15691400
C	3.37362000	-0.50387500	0.00502300	C	3.73071000	0.41567400	0.14464700
H	3.63649400	-1.08403400	0.90179800	H	4.06239100	1.14636200	-0.60768000
H	3.63869900	-1.08778600	-0.88868500	H	3.97684900	0.79739400	1.14649700
F	4.08655400	0.68154700	0.00337700	F	4.38798500	-0.78316700	-0.06177700
C	-1.87872200	0.24254300	0.00045600	C	-1.52876200	-0.08473200	-0.18137300
O	-1.39197700	-0.88100000	0.00109200	O	-1.02453800	1.00734700	0.03437700
O	-1.20180400	1.37576000	-0.00078900	O	-0.89566300	-1.21605700	-0.38803400
H	-0.21217400	1.19839500	-0.00122900	H	0.10303100	-1.08382800	-0.31575900
C	-3.37287400	0.50386200	0.00116200	C	-3.05346600	-0.28987100	-0.21670400
H	-3.63649500	1.08597900	0.89647000	H	-3.35649200	-1.06707200	-0.93126000
H	-3.63753400	1.08567400	-0.89402000	F	-3.44787900	-0.67262300	1.04329700
F	-4.08541500	-0.68177900	0.00180300	F	-3.67568400	0.87859700	-0.52214600
FAA-TFAA				DFAA-DFAA			
C	1.23368500	0.02255400	-0.00041700	C	1.87931100	0.13000100	-0.18249300
O	0.55914800	1.03982200	-0.00324100	O	1.33389900	-0.96356000	-0.19870800
O	0.81267400	-1.21314100	0.00238800	O	1.28897000	1.30317600	-0.19973500
H	-0.20058900	-1.24025400	0.00206500	H	0.28872400	1.19748300	-0.19796800
C	2.78415400	0.09388800	-0.00059800	C	3.40906100	0.28096700	-0.11157200
F	3.27822500	-0.52561100	-1.09364600	H	3.76857700	1.17056900	-0.64617200
F	3.20731100	1.36370600	-0.00348800	F	4.01025300	-0.82840800	-0.61381100
F	3.27831800	-0.52063900	1.09517800	C	-1.87886800	-0.12927100	-0.18370100
C	-2.52436400	-0.25984700	0.00075600	O	-1.33344000	0.96430900	-0.19795300
O	-1.79292800	-1.25187300	0.00271400	O	-1.28851600	-1.30241700	-0.20269100
O	-2.12357400	0.98707200	-0.00239100	H	-0.28826700	-1.19672700	-0.20022900
H	-1.12518500	1.03190400	-0.00304000	C	-3.40864300	-0.28036900	-0.11363500
C	-4.02565700	-0.46491400	0.00177100	H	-3.76796800	-1.16888800	-0.65016300
H	-4.29335100	-1.04247600	0.89845100	F	-4.00967600	0.83001200	-0.61382100
H	-4.29397700	-1.04702600	-0.89177100	F	3.74955900	0.39565500	1.21454500
F	-4.73283200	0.72598800	-0.00100400	F	-3.74960300	-0.39777100	1.21213000
DFAA-TFAA				TFAA-TFAA			
C	-1.57709500	0.01770700	-0.00079600	C	-1.87761200	-0.02702900	-0.00020400
O	-0.90551600	1.03661700	-0.00170700	O	-1.24546500	-1.07124700	-0.00008400
O	-1.15080500	-1.21779300	-0.00005400	O	-1.40455300	1.19152500	-0.00002200
H	-0.14347700	-1.24153800	-0.00023700	H	-0.40044900	1.17781500	0.00001200
C	-3.12762700	0.08225500	-0.00096300	C	1.87751300	0.02711800	0.00017500
F	-3.55463100	1.35020800	-0.00280600	O	1.24533900	1.07132300	0.00032800
F	-3.61725900	-0.53544600	1.09442100	O	1.40463400	-1.19149500	-0.00010900
F	-3.61733000	-0.53866800	-1.09447600	H	0.40057300	-1.17807900	-0.00018700
C	2.18137200	-0.21447700	-0.00035100	C	-3.42968200	-0.03224100	0.00013000
O	1.48551800	-1.22622400	-0.00004800	C	3.42959700	0.03242400	0.00028800
O	1.76199700	1.02363400	-0.00130400	F	-3.89442000	0.60497300	-1.09427700
H	0.76099500	1.05851700	-0.00164100	F	-3.89399300	0.60545300	1.09444500
C	3.71235500	-0.34604400	-0.00000300	F	-3.90363100	-1.28311600	0.00048400
H	4.01392800	-1.40106500	0.00036800	F	3.90346300	1.28333100	0.00073100
F	4.21953500	0.27365500	1.10798700	F	3.89422200	-0.60463600	-1.09426300
F	4.22008900	0.27306400	-1.10806400	F	3.89409700	-0.60536300	1.09446100