Partition of the electronic energy of semiempirical methods. Electronic Supporting Information

Hugo Salazar-Lozas[a], José Manuel Guevara-Vela[b], Angel Martín Pendás [c], Evelio Francisco[c] and Tomás Rocha-Rinza*[a]

Partition energy of different semiempirical methods

Partition of the elecronic energy of different Semiempirical Methods (SM)					
System	$\sum_{A} E^{A}_{net}$	$\sum_{A<B} E^{AB}_{int}$	$\sum_{A} E^{A}_{net} + \sum_{A<B} E^{AB}_{int}$	E(SM)	Error (mHa)
			MNDO		
H_2	−17.388552	−10.879203	−28.267755	−28.267756	0.000037
N_2	−378.519364	−36.030637	−414.550001	−414.550001	0.000000
CO	−419.504252	−27.785352	−447.289604	−447.289604	0.000000
NH_3	−211.347405	−38.849854	−250.197259	−250.197259	0.000000
HClO	−666.236800	−23.434724	−689.671524	−689.671523	0.000037
			MNDO−D		
H_2	−17.388552	−10.879034	−28.267586	−28.267585	0.000037
N_2	−378.519618	−36.029319	−414.548937	−414.548937	0.000000
Co	−419.504569	−27.783938	−447.288507	−447.288507	0.000000
NH_3	−211.347637	−38.848902	−250.196539	−250.196539	0.000000
HClO	−572.381843	−27.802618	−600.184461	−600.184459	0.000073
			AM1		
H_2	−16.368854	−11.150883	−27.519737	−27.519738	0.000037
N_2	−378.161946	−35.950918	−414.112864	−414.112864	0.000000
CO	−418.828480	−27.185230	−446.013710	−446.013709	0.000037
NH_3	−209.215236	−39.375591	−248.590827	−248.590829	0.000073
HClO	−684.332305	−22.405675	−706.737980	−706.737978	0.000073
			PM3		
H_2	−18.749538	−12.495110	−31.244648	−31.244647	0.000037
N_2	−292.562330	−31.662567	−324.224897	−324.224898	0.000037
CO	−383.127525	−26.635790	−409.763315	−409.763314	0.000037
NH_3	−171.065026	−37.574889	−208.639915	−208.639913	0.000073
HClO	−601.641752	−23.555368	−625.197120	−625.197119	0.000037

Table S 1: Values of IQA net, $\sum_{A} E^{A}_{net}$, interaction, $\sum_{A<B} E^{AB}_{int}$, and total, $\sum_{A} E^{A}_{net} + \sum_{A<B} E^{AB}_{int}$, electronic energies of the molecules considered herein for different semiempirical methods. The chart also displays the values of the molecular energies E(PM7) computed with Mopac2016. Atomic units are used throughout except for the error in the recovery of the electronic energy by the IQA partition reported in the last column in mHa..

Partition of the elecronic energy of different Semiempirical Methods (SM)					
System	$\sum_{A} E^{A}_{net}$	$\sum_{A<B} E^{AB}_{int}$	$\sum_{A} E^{A}_{net} + \sum_{A<B} E^{AB}_{int}$	E(SM)	Error (mHa)
			PM6		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−534.765672	−23.389459	−558.155131	−558.155128	0.000110
			PM6−D3		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−534.766427	−23.388695	−558.155122	−558.155123	0.000037
			PM6−DH+		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−534.765694	−23.389434	−558.155128	−558.155128	0.000000
			PM6−DH2		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−534.765694	−23.389434	−558.155128	−558.155128	0.000000
			PM6−DH2X		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−536.754491	−17.648688	−554.403179	−554.403179	0.000000
			PM6−D3H4		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−534.765680	−23.389445	−558.155125	−558.155128	0.000110
			PM6−D3H4X		
H_2	−15.269572	−12.769707	−28.039279	−28.039280	0.000037
N_2	−322.971566	−34.971743	−357.943309	−357.943310	0.000037
CO	−385.860602	−25.808080	−411.668682	−411.668682	0.000000
NH_3	−181.104899	−39.396709	−220.501608	−220.501610	0.000073
HClO	−536.757302	−17.626171	−554.383473	−554.383475	0.000073
			RM1		
H_2	−16.929748	−11.592167	−28.521915	−28.521913	0.000073
N_2	−381.275022	−37.315433	−418.590455	−418.590455	0.000000
CO	−412.462697	−26.553402	−439.016099	−439.016100	0.000037
NH_3	−211.262055	−41.680241	−252.942296	−252.942296	0.000000
HClO	−690.400279	−23.077575	−713.477854	−713.477854	0.000000

Table S2: Continuation of Table S8. Values of IQA net, $\sum_{A} E^{A}_{net}$, interaction, $\sum_{A<B} E^{AB}_{int}$, and total, $\sum_{A} E^{A}_{net} + \sum_{A<B} E^{AB}_{int}$, electronic energies of the molecules considered herein for different semiempirical methods. The chart also displays the values of the molecular energies E(PM7) computed with MOPAC2016. Atomic units are used throughout except for the error in the recovery of the electronic energy by the IQA partition reported in the last column in mHa.

Hydrogen bond energies and values of $E_{\text{int}}^{\mathcal{GH}'}$

Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$
3–2	−0.000006	−2.022617
5–3	−0.045612	−3.108423
7–1	−0.137158	−3.451541
9–4	−0.003379	−0.760560
14–7	−1.754451	−3.936458
14–8	−1.812364	−3.324154
16–1	−2.007051	−3.313454
18–14	−0.005424	−2.3577564
21–7	−0.052953	−3.412914
21–8	−1.152567	−2.452696
22–12	−2.880642	−5.347486
23–18	−1.050540	−3.705230
24–11	−0.005485	−3.067998
24–16	−0.530310	−1.852868
26–2	−0.537082	−2.674908
26–9	−0.200164	−0.657087
27-25	−1.913713	−3.813568

Table S 3: Hydrogen bond and interaction energies $E_{\text{int}}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded pairs of water molecules in the cluster $(H_2O)_{30}$. All values are reported in kcal/mol.

[0]*a Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, Ciudad Universitaria, Alcaldía Coyoacán C.P. 04510, Ciudad de México, México. E-mail: tomasrocharinza@gmail.com*

[0]*b MDEA Materials Institute, C/Eric Kandel 2, 28906 - Getafe, Madrid, Spain.*

[0]*c Departamento de Química Física y Analítica, Universidad de Oviedo, Julián Claveria 8, 33006, Oviedo, España.*

Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$
7–3	−0.000002	−2.816891
14–8	−0.083461	−2.478293
17–13	−0.716981	−1.286778
19–12	−0.000030	−1.434458
22–19	−0.083297	−2.100631
23–10	−1.419183	−3.466622
28–5	−0.079743	−2.620000
30–29	−0.108119	−0.013583
33–13	−0.003693	−0.308389
37–6	−0.264614	−3.694253
37–25	−0.006063	−1.626079
38–13	−0.905103	−1.755668
39–1	−0.005728	−2.263369
39–24	−0.609248	−1.877705
40–33	−0.015430	−1.677585
41–29	−0.007598	−1.724375
42–32	−0.001348	−2.491161
44–2	−0.117848	−2.580083
45-23	−0.085679	−2.501700
45–43	−0.001506	−2.430397
46–18	−0.243271	0.284060
46–28	−0.630453	−2.674954
46–33	−1.758792	−2.281656
47–6	−0.894470	−0.943453
47–25	−0.000044	−1.584974
47-41	−0.000046	−2.642623
48–12	−0.022346	−1.545840
49–16	−2.269660	−2.934846
49–25	−0.013517	−1.874960
50–12	−0.007181	−1.754815
50–26	−1.256747	−2.289151

Table S 4: Hydrogen bond and interaction energies $E_{\text{int}}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded pairs of water molecules in the cluster $(H_2O)_{50}$. All values are reported in kcal/mol.

Water molecule pairs	EHB	$E_{\rm int}^{\mathcal{GH}'}$	Water molecule pairs	EHB	$E_{\rm int}^{\mathcal{GH}'}$
19 – 16	−0.000197	−2.227487	65 – 53	−0.002837	−1.491717
21 – 4	−0.039860	−1.540237	67 – 47	−0.001689	−3.432769
22 – 6	−0.024179	−0.737361	68 – 29	−1.211491	−1.745130
29 – 5	−0.000003	−2.914345	69 – 23	−1.054229	−1.679638
29 – 14	−0.008592	−1.015817	69 – 63	−0.007605	−2.701773
33 – 16	−3.608194	−3.581717	70 – 34	−0.006189	−3.163030
34 – 17	−0.000043	−2.067908	71 – 25	−0.000005	−2.567492
34 – 33	−0.311582	−0.721979	72 – 3	−0.003322	−2.210883
35 – 5	−0.454819	−2.551557	73 – 24	−0.000198	−3.261891
36 – 15	−0.000049	−1.496883	73 – 52	−0.060175	−1.218565
37 – 35	−0.091170	−3.674075	74 – 9	−0.023018	−1.694143
39 – 6	−1.266469	−4.344998	74 – 27	−1.624030	−3.859366
39 – 13	−0.206905	−0.393482	77 – 56	−0.970392	−1.997227
41 – 5	−2.094915	−3.415520	78 – 58	−0.001317	−1.426733
41 – 19	−0.169654	−3.599243	78 – 69	−2.396407	−3.046390
42 – 36	−0.001601	−1.526285	80 – 24	−0.975322	−1.360918
46 – 26	−0.237506	−2.583288	83 – 49	−1.738256	−3.971994
47 – 18	−0.441031	−2.201844	83 – 73	−0.003874	−2.860038
48 – 46	−0.435624	−2.430351	84 – 5	−0.007066	−2.340645
50 – 44	−0.028699	−0.670278	85 – 37	−1.404687	−3.137917
51 – 30	−0.000168	−2.606625	86 – 14	−0.025901	−2.525844
53 – 7	−0.131073	−1.768744	87 – 15	−1.247557	−2.119264
55 – 39	−0.017713	−0.420209	87 – 24	−0.708668	−2.138381
55 – 53	−0.479326	−2.087141	88 – 9	−0.012759	−2.119541
56 – 8	−0.516350	−3.497938	88 – 33	−3.300223	−3.004281
56 – 14	−0.000271	−1.002396	88 – 48	−0.202718	−2.229124
56 – 41	−0.000915	−0.835391	88 – 81	−2.657339	−4.950591
57 – 15	−0.174266	−1.161813	89 – 7	−1.493204	−1.726543
57 – 32	−0.000125	−0.530047	93 – 76	−0.056556	−1.813504
57 – 36	−0.236586	−0.517479	93 – 81	−2.337041	−2.287675
57 – 52	−0.002807	−0.711648	94 – 54	−0.004423	−0.002675
58 – 23	−0.000047	−2.742360	97 – 65	−0.687034	−1.293973
59 – 30	−0.000667	−1.160222	97 – 86	−0.000001	−3.201449
60 – 7	−0.000263	−1.117537	98 – 27	−0.242693	−3.247155
63 – 59	−0.073083	−1.675095	99 – 20	−1.630887	−1.371134

Table S 5: Hydrogen bond and interaction energies $E_{\rm int}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded pairs of water molecules in the cluster $(H_2O)_{100}$. All values are reported in kcal/mol.

Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$	Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$
12 – 9	−0.691822	−1.042909	108 – 90	−0.341994	−0.452344
27 – 6	−0.159476	−0.456971	109 – 25	−1.080919	−2.475322
29 – 9	−0.270858	−1.511565	109 – 74	−2.226470	−2.614476
33 – 30	−0.008643	−1.055631	110 – 37	−0.296594	−0.905019
39 – 22	−3.450598	−5.330012	111 – 6	−0.014099	−0.016604
39 – 24	−2.015294	−1.199764	111 – 48	−1.856550	−2.134269
40 – 20	−4.456852	−0.650586	112 – 104	−1.065536	3.389285
40 – 23	−0.056055	0.182803	115 – 4	−0.081380	−1.475122
41 – 36	−2.426032	−3.970086	116 – 77	−3.900760	−1.846719
44 – 5	−0.157814	0.359113	117 – 84	−1.201139	−2.546104
47 – 32	−2.276941	−0.136133	119 – 2	−0.160606	−0.947191
50 – 48	−0.491112	−1.573069	119 – 43	−0.150313	−1.300087
54 – 4	−0.297458	2.813982	119 – 62	−0.316561	−1.108872
55 – 21	−0.300600	−1.263516	120 – 104	−0.272533	−0.338370
56 – 9	−0.523780	−1.214881	120 – 117	−3.277148	−2.730544
56 – 12	−0.000134	−0.026585	124 – 53	−0.668437	−0.883009
57 – 15	−2.158796	−1.279434	124 – 100	−0.090731	−0.913204
58 – 11	−0.007037	−0.481295	125 – 27	−0.553055	−0.532715
60 – 49	−0.124048	−1.425608	128 – 16	−1.034524	−1.663777
61 – 54	−0.164395	1.355321	128 – 59	−2.008916	−1.630087
64 – 42	−0.084702	−0.515365	128 – 91	−0.285734	−1.100884
66 – 35	−1.012397	−1.506313	130 – 32	−0.792058	0.438343
67 – 48	−0.122567	−1.538335	131 – 68	−0.773734	−2.221431
74 – 53	−4.237664	−2.748248	133 – 39	−0.574475	−0.927391
75 – 11	−0.267101	−0.184855	133 – 77	−0.000006	0.015705
78 – 50	−0.636840	0.001759	135 – 93	−0.004696	−1.028272
80 – 51	−1.128976	−2.401244	137 – 4	−2.617869	−0.960854
83 – 37	−0.780777	−0.341542	137 – 46	−0.566781	−0.293062
87 – 74	−0.051249	−1.720266	137 – 64	−2.739930	−1.222303
90 – 8	−1.623701	−1.391799	143 – 34	−2.759779	−1.751643
90 – 31	−2.823889	−3.046743	143 – 53	−3.677431	−3.229644
95 – 81	−1.551309	3.454529	145 – 73	0.000000	0.015019
96 – 32	−0.904875	−1.085118	145 – 86	−1.538323	1.123850
99 – 2	−1.673398	−2.330216	145 – 90	−1.092117	−0.489550
99 – 66	−0.747178	−1.708197	145 – 103	−0.337408	0.178756
100 – 8	−1.795912	−1.019869	145 – 138	−0.457938	0.164905
100 – 74	−0.627167	−1.474435	146 – 123	−2.203967	0.722382
101 – 5	−1.399095	−0.411546	147 – 19	−0.994542	−0.414175
103 – 73	−1.288773	−1.209797	147 – 26	−0.406203	0.407905
104 – 9	−0.558664	−0.964844	147 – 40	−1.538132	0.459628
107 – 62	−0.664067	−1.028774	149 – 62	−0.000006	0.221997
108 – 34	−0.332425	−0.113812	149 – 68	−0.809266	−2.032109
108 – 73	−0.460509	0.048539	149 – 119	−0.232606	−0.710792

Table S6: Hydrogen bond and interaction energies $E_{\text{int}}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded species in the solvatation of the caprylate anion. The caprylate anion is labelled with the number 201. All values are reported in kcal/mol.

Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$	Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$
150 – 111	−0.503210	2.150317	179 – 52	−2.245503	0.123698
152 – 86	−0.571686	1.602647	179 – 169	−1.583256	−0.954971
153 – 22	−2.331732	−2.108603	180 – 59	−0.117616	−1.318904
153 – 67	−0.606239	−1.502194	180 – 84	−0.807232	−1.819573
153 – 133	−1.397548	−1.178762	180 – 128	−0.000134	−0.244620
154 – 56	−1.903782	0.438601	181 – 123	−0.010739	−0.898790
155 – 22	−0.666496	0.041335	181 – 141	−2.330332	−0.961872
155 – 70	−0.103171	0.228416	182 – 64	−4.707212	−1.225399
156 – 94	−0.034885	1.216250	182 – 76	−0.726549	−0.781385
156 – 136	−0.658021	0.194469	184 – 110	−1.208386	−1.327679
157 – 50	−0.422286	−0.880633	184 – 118	−0.019733	−0.136962
157 – 129	−2.210934	0.373945	184 – 137	−0.168867	−0.829375
158 – 136	−2.046035	−2.981389	184 – 152	−0.107590	−0.293602
159 – 15	−1.797378	−0.349957	186 – 172	−4.676661	−3.328032
159 – 150	−0.239251	1.744264	187 – 89	−0.814012	2.867015
160 – 100	−1.806660	0.082844	188 – 22	−1.842196	−2.309634
161 – 43	−0.458240	0.983344	188 – 51	−2.396630	−2.624057
162 – 75	−0.186386	−1.176214	189 – 28	−0.796857	−0.075292
162 – 135	−2.281445	−2.426044	190 – 140	−1.081099	−0.553703
163 – 37	−0.432633	−0.925902	191 – 182	−2.928615	0.456710
163 – 83	−0.000632	0.046139	192 – 62	−1.946318	−2.086933
163 – 118	−0.493443	0.064172	192 – 139	−0.686582	−1.128650
165 – 33	−0.151079	0.479834	193 – 60	−3.389027	−2.352357
166 – 28	−0.585122	−0.293584	194 – 48	−3.351003	−2.032998
166 – 39	−2.121141	−1.228001	194 – 71	−0.365920	−0.505322
166 – 77	−2.313801	−0.653621	194 – 77	−2.348553	−1.054344
166 – 93	−2.349592	−0.210243	194 – 85	−2.036958	−0.217829
166 – 133	−0.316515	−0.044354	195 – 71	−0.840335	−1.700635
168 – 27	−0.084676	0.015194	195 – 162	−1.918579	−3.270078
168 – 45	−0.281990	−0.006094	196 – 129	−0.999535	2.117401
170 – 141	−0.971627	−1.781690	197 – 122	−1.557282	1.621049
171 – 43	−0.309928	−0.951689	198 – 188	−2.008342	1.143232
171 – 107	−0.730844	−0.352110	199 – 35	−2.081518	0.252122
171 – 116	−0.050243	−0.588908	199 – 119	−1.026023	0.022229
172 – 71	−3.523410	−3.181378	199 – 192	−2.641307	0.215857
174 – 16	−3.433334	−2.270959	200 – 115	−0.340023	−1.634607
175 – 79	−1.175608	1.455556	201 – 12	−1.513619	−1.399018
175 – 80	−1.711963	−0.497978	201 – 69	−0.016202	1.273797
176 – 127	−0.671013	−1.058121	201 – 89	−2.086218	−0.483670
177 – 78	−1.610634	0.403106	201 – 92	−2.305526	−3.393633
177 – 107	−3.434137	−0.736354	201 – 117	−0.261533	−2.052919
179 – 36	−0.070650	−1.724097	201 – 162	−0.809776	−1.993736

Table S7: Continuation of Table S4. Hydrogen bond and interaction energies $E_{\text{int}}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded species in the solvatation of the caprylate anion. The caprylate anion is labelled with the number 201. All values are reported in kcal/mol.

Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$	Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$
208 – 92	−2.305526	−9.763073	200 – 115	−0.340023	−1.634607
208 – 180	−2.452700	−8.456566	128 – 59	−2.008916	−1.630087
208 – 12	−1.513619	−6.255936	50 – 48	−0.491112	−1.573069
208 – 89	−2.086218	−6.228136	67 – 48	−0.122567	−1.538335
208 – 117	−0.261533	−5.830420	29 – 9	−0.270858	−1.511565
39 – 22	−3.450598	−5.330012	66 – 35	−1.012397	−1.506313
41 – 36	−2.426032	−3.970086	153 – 67	−0.606239	−1.502194
186 – 172	−4.676661	−3.328032	115 – 4	−0.081380	−1.475122
208 – 162	−0.809776	−3.301172	100 – 74	−0.627167	−1.474435
195 – 162	−1.918579	−3.270078	60 – 49	−0.124048	−1.425608
143 – 53	−3.677431	−3.229644	90 – 8	−1.623701	−1.391799
172 – 71	−3.523410	−3.181378	184 – 110	−1.208386	−1.327679
90 – 31	−2.823889	−3.046743	180 – 59	−0.117616	−1.318904
158 – 136	−2.046035	−2.981389	119 – 43	−0.150313	−1.300087
74 – 53	−4.237664	−2.748248	57 – 15	−2.158796	−1.279434
120 – 117	−3.277148	−2.730544	55 – 21	−0.300600	−1.263516
188 – 51	−2.396630	−2.624057	166 – 39	−2.121141	−1.228001
109 – 74	−2.226470	−2.614476	182 – 64	−4.707212	−1.225399
117 – 84	−1.201139	−2.546104	137 – 64	−2.739930	−1.222303
109 – 25	−1.080919	−2.475322	56 – 9	−0.523780	−1.214881
162 – 135	−2.281445	−2.426044	103 – 73	−1.288773	−1.209797
80 – 51	−1.128976	−2.401244	39 – 24	−2.015294	−1.199764
193 – 60	−3.389027	−2.352357	153 – 133	−1.397548	−1.178762
99 – 2	−1.673398	−2.330216	162 – 75	−0.186386	−1.176214
188 – 22	−1.842196	−2.309634	192 – 139	−0.686582	−1.128650
174 – 16	−3.433334	−2.270959	119 – 62	−0.316561	−1.108872
131 – 68	−0.773734	−2.221431	128 – 91	−0.285734	−1.100884
111 – 48	−1.856550	−2.134269	96 – 32	−0.904875	−1.085118
153 – 22	−2.331732	−2.108603	176 – 127	−0.671013	−1.058121
192 – 62	−1.946318	−2.086933	33 – 30	−0.008643	−1.055631
194 – 48	−3.351003	−2.032998	194 – 77	−2.348553	−1.054344
149 – 68	−0.809266	−2.032109	12 – 9	−0.691822	−1.042909
208 – 69	−0.016202	−1.918657	107 – 62	−0.664067	−1.028774
116 – 77	−3.900760	−1.846719	135 – 93	−0.004696	−1.028272
180 – 84	−0.807232	−1.819573	100 – 8	−1.795912	−1.019869
170 – 141	−0.971627	−1.781690	104 – 9	−0.558664	−0.964844
143 – 34	−2.759779	−1.751643	181 – 141	−2.330332	−0.961872
179 – 36	−0.070650	−1.724097	137 – 4	−2.617869	−0.960854
87 – 74	−0.051249	−1.720266	179 – 169	−1.583256	−0.954971
99 – 66	−0.747178	−1.708197	171 – 43	−0.309928	−0.951689
195 – 71	−0.840335	−1.700635	119 – 2	−0.160606	−0.947191
128 – 16	−1.034524	−1.663777	133 – 39	−0.574475	−0.927391

Table S8: Hydrogen bond and interaction energies $E_{\text{int}}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded species in the solvatation of the caprylate anion. The caprylate anion was further partitioned into fragments. The number of each fragment within the caprylate anion is as follows: methylene ($-CH_2$, 201-206), methyl ($-CH_3$, 207) and carboxylate ($-COO-$, 208). All values are reported in kcal/mol.

Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$	Water molecule pairs	EHB	$E_{\text{int}}^{\mathcal{GH}'}$
163 – 37	−0.432633	−0.925902	78 – 50	−0.636840	0.001759
124 – 100	−0.090731	−0.913204	168 – 27	−0.084676	0.015194
110 – 37	−0.296594	−0.905019	133 – 77	−0.000006	0.015705
181 – 123	−0.010739	−0.898790	199 – 119	−1.026023	0.022229
124 – 53	−0.668437	−0.883009	155 – 22	−0.666496	0.041335
157 – 50	−0.422286	−0.880633	108 – 73	−0.460509	0.048539
184 – 137	−0.168867	−0.829375	163 – 118	−0.493443	0.064172
182 – 76	−0.726549	−0.781385	160 – 100	−1.806660	0.082844
177 – 107	−3.434137	−0.736354	179 – 52	−2.245503	0.123698
149 – 119	−0.232606	−0.710792	145 – 138	−0.457938	0.164905
166 – 77	−2.313801	−0.653621	145 – 103	−0.337408	0.178756
40 – 20	−4.456852	−0.650586	40 – 23	−0.056055	0.182803
171 – 116	−0.050243	−0.588908	156 – 136	−0.658021	0.194469
190 – 140	−1.081099	−0.553703	199 – 192	−2.641307	0.215857
125 – 27	−0.553055	−0.532715	149 – 62	−0.000006	0.221997
64 – 42	−0.084702	−0.515365	155 – 70	−0.103171	0.228416
194 – 71	−0.365920	−0.505322	199 – 35	−2.081518	0.252122
175 – 80	−1.711963	−0.497978	44 – 5	−0.157814	0.359113
145 – 90	−1.092117	−0.489550	157 – 129	−2.210934	0.373945
58 – 11	−0.007037	−0.481295	177 – 78	−1.610634	0.403106
27 – 6	−0.159476	−0.456971	147 – 26	−0.406203	0.407905
108 – 90	−0.341994	−0.452344	130 – 32	−0.792058	0.438343
147 – 19	−0.994542	−0.414175	154 – 56	−1.903782	0.438601
101 – 5	−1.399095	−0.411546	191 – 182	−2.928615	0.456710
171 – 107	−0.730844	−0.352110	147 – 40	−1.538132	0.459628
159 – 15	−1.797378	−0.349957	165 – 33	−0.151079	0.479834
83 – 37	−0.780777	−0.341542	146 – 123	−2.203967	0.722382
120 – 104	−0.272533	−0.338370	161 – 43	−0.458240	0.983344
184 – 152	−0.107590	−0.293602	145 – 86	−1.538323	1.123850
166 – 28	−0.585122	−0.293584	198 – 188	−2.008342	1.143232
137 – 46	−0.566781	−0.293062	156 – 94	−0.034885	1.216250
180 – 128	−0.000134	−0.244620	61 – 54	−0.164395	1.355321
194 – 85	−2.036958	−0.217829	175 – 79	−1.175608	1.455556
166 – 93	−2.349592	−0.210243	152 – 86	−0.571686	1.602647
75 – 11	−0.267101	−0.184855	197 – 122	−1.557282	1.621049
184 – 118	−0.019733	−0.136962	159 – 150	−0.239251	1.744264
47 – 32	−2.276941	−0.136133	196 – 129	−0.999535	2.117401
108 – 34	−0.332425	−0.113812	150 – 111	−0.503210	2.150317
189 – 28	−0.796857	−0.075292	54 – 4	−0.297458	2.813982
166 – 133	−0.316515	−0.044354	187 – 89	−0.814012	2.867015
56 – 12	−0.000134	−0.026585	112 – 104	−1.065536	3.389285
111 – 6	−0.014099	−0.016604	95 – 81	−1.551309	3.454529
168 – 45	−0.281990	−0.006094			

Table S9: Continuation of Table S6. Hydrogen bond and interaction energies $E_{\text{int}}^{\mathcal{GH}'}$ (Equation (24) in the main body of the paper) among H-bonded species in the solvatation of the caprylate anion. The caprylate anion was further partitioned into fragments. The number of each fragment within the caprylate anion is as follows: methylene ($-CH_2$, 201-206), methyl ($-CH_3$, 207) and carboxylate ($-COO-$, 208). All values are reported in kcal/mol.