Supplementary information

Insight in supramolecular self-assembly directed by weak interactions in acetophenone derivatives: Crystal structures and Hirshfeld surface analyses

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Table S1. Selected bond-lengths (Å) and bond-angles (º) for **1**.

	X-ray	DFT	MOGUL(mean)	XRD-DFT	XRD-MOGUL
O1-C1	1.357(2)	1.382	1.361	-0.025	-0.004
O2-C8	1.232(2)	1.235	1.223	-0.003	0.009
C2-C7	1.499(2)	1.514	1.506	-0.015	-0.007
C4-C8	1.472(2)	1.498	1.492	-0.026	-0.020
C8-C9	1.505(2)	1.528	1.491	-0.023	0.014
O2-C8-C9	120.22(11)	119.99	119.943	0.230	0.277
C1-C2-C3	117.71(11)	117.41	117.435	0.300	0.275
C2-C3-C4	122.41(11)	122.56	122.000	-0.150	0.410
C3-C4-C5	118.37(11)	118.30	119.228	0.070	-0.858
C4-C5-C6	120.43(11)	120.50	120.822	-0.070	-0.392
C5-C6-C1	120.06(11)	120.04	120.512	0.020	-0.452
C6-C1-C2	120.89(11)	121.18	120.791	-0.290	0.099

Table S2. Selected bond-lengths (Å) and and bond-angles (º) for **2**.

	X-ray	DFT	MOGUL(mean)	XRD-DFT	XRD-MOGUL
O1-C8	1.218(2)	1.235	1.223	-0.017	-0.005
O2-C1	1.363(2)	1.377	1.370	-0.017	-0.014
O2-C10	1.430(2)	1.461	1.432	-0.031	-0.002
C2-C7	1.502(2)	1.513	1.506	-0.011	-0.004
C4-C8	1.485(2)	1.497	1.492	-0.012	-0.007
C8-C9	1.505(2)	1.528	1.491	-0.023	0.014
C10-C11	1.498(2)	1.510	1.500	-0.012	-0.002
C1-O2-C10	117.66(10)	118.67	117.664	-1.010	-0.004
C1-C2-C3	117.87(11)	119.90	117.768	-2.030	0.102
C2-C3-C4	122.33(11)	120.86	122.000	1.470	0.330
C3-C4-C5	118.26(11)	118.10	119.228	0.160	-0.968
C4-C5-C6	120.97(11)	122.62	120.822	-1.650	0.148
C5-C6-C1	119.36(11)	117.88	119.478	1.480	-0.118
C6-C1-C2	121.13(11)	120.64	121.536	0.490	-0.406
O1-C8-C9	120.10(12)	119.99	119.943	0.110	0.157
O2-C10-C11	108.45(10)	108.39	109.267	0.060	-0.817

Table S3. Selected bond-lengths (Å) and and bond-angles (º) for **3**.

	X-ray	DFT	MOGUL(mean)	XRD-DFT	XRD-MOGUL
O1-C8	1.212(2)	1.225	1.223	-0.013	-0.011
O2-C3	1.367(2)	1.381	1.370	-0.014	-0.003
O2-C10	1.444(2)	1.455	1.432	-0.011	0.012
O3-C5	1.376(2)	1.389	1.370	-0.013	0.006
O3-C17	1.439(2)	1.452	1.432	-0.013	0.007
C1-C7	1.504(2)	1.516	1.510	-0.012	-0.006
C4-C8	1.512(2)	1.524	1.486	-0.012	0.026
C8-C9	1.496(2)	1.517	1.491	-0.021	0.005
C10-C11	1.500(2)	1.513	1.500	-0.013	0.000
O1-C8-C9	122.63(14)	122.38	119.943	0.250	2.687
O2-C10-C11	108.16(12)	108.39	109.267	-0.230	-1.107
O3-C17-C18	112.99(12)	114.73	109.267	-1.740	3.723
C3-O2-C10	117.52(12)	118.67	117.664	-1.150	-0.144
C5-O3-C17	118.32(12)	119.37	117.664	-1.050	0.656
C1-C2-C3	119.88(14)	120.10	119.945	-0.220	-0.065
C2-C3-C4	120.51(14)	120.82	122.083	-0.310	-1.573
C3-C4-C5	118.79(14)	118.43	117.647	0.360	1.143
C4-C5-C6	121.18(14)	121.06	122.083	0.120	-0.903
C5-C6-C1	119.47(14)	119.94	119.945	-0.470	-0.475
C6-C1-C2	120.12(14)	119.65	117.960	0.470	2.160

Table S4. Selected bond-lengths (Å) and and bond-angles (º) for **4**.

	X-ray	DFT	MOGUL(mean)	XRD-DFT	XRD-MOGUL
O1-C8	1.189(3)	1.231	1.223	-0.042	-0.034
O2-C10	1.197(3)	1.226	1.223	-0.029	-0.189
O3-C3	1.391(2)	1.398	1.386	-0.007	-0.005
O3-C12	1.439(2)	1.465	1.432	-0.026	0.007
O4-C5	1.360(2)	1.380	1.370	-0.020	-0.010
O4-C19	1.442(3)	1.467	1.432	-0.025	0.010
C1-C7	1.524(3)	1.518	1.506	0.006	0.018
C4-C10	1.502(3)	1.525	1.486	-0.023	0.016
C10-C11	1.477(3)	1.516	1.491	-0.039	-0.014
C2-C8	1.494(3)	1.517	1.486	-0.023	0.008
C8-C9	1.476(3)	1.521	1.491	-0.045	-0.015
C12-C13	1.496(3)	1.516	1.500	-0.020	-0.004
C19-C20	1.496(3)	1.509	1.500	-0.013	-0.004
O1-C8-C9	119.7(2)	121.10	119.94	1.400	-0.243
O2-C10-C11	122.2(2)	122.46	119.94	-0.260	2.257
O3-C12-C13	110.22(16)	109.97	109.26	0.250	0.953
O4-C19-C20	107.42(18)	108.22	109.26	-0.800	-1.847
C3-O3-C12	113.71(15)	114.88	114.80	-1.170	-1.094
C5-O4-C19	118.03(17)	118.65	117.66	-0.620	0.366
C1-C2-C3	118.7(2)	118.54	119.60	0.160	-0.904
C2-C3-C4	122.49(19)	122.21	121.59	0.280	0.891
C3-C4-C5	117.76(19)	118.43	117.19	-0.670	0.569
C4-C5-C6	120.5(2)	120.05	122.08	0.450	-1.583
C5-C6-C1	120.8(2)	121.39	121.12	-0.590	-0.319
C6-C1-C2	119.7(2)	119.25	118.61	0.450	1.086

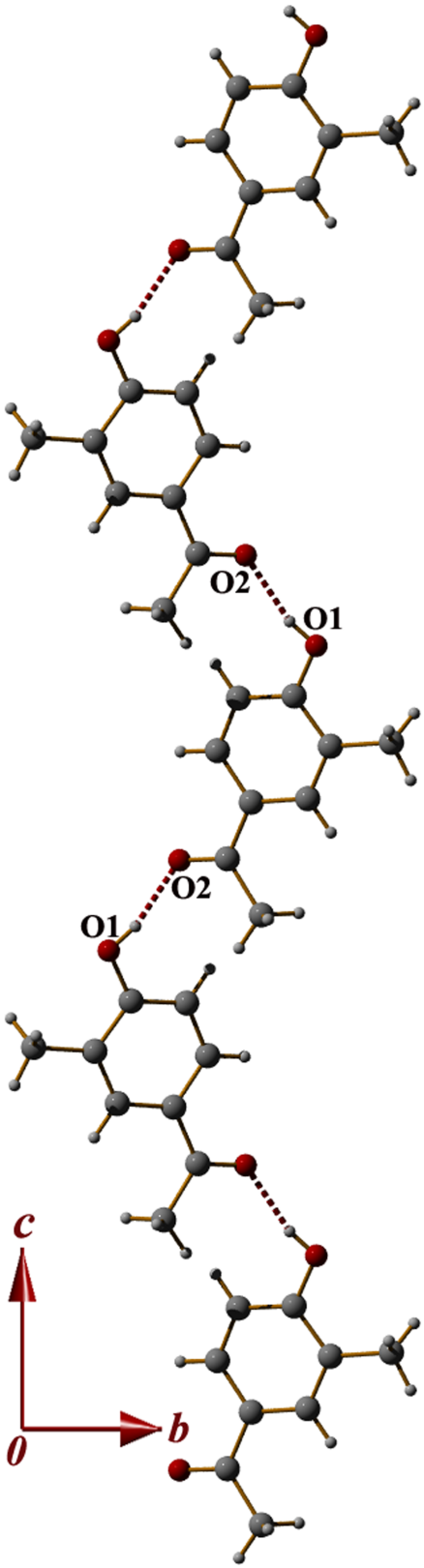

Figure S1. Formation of 1D chain in (**1**) propagating along (0 0 1) direction.

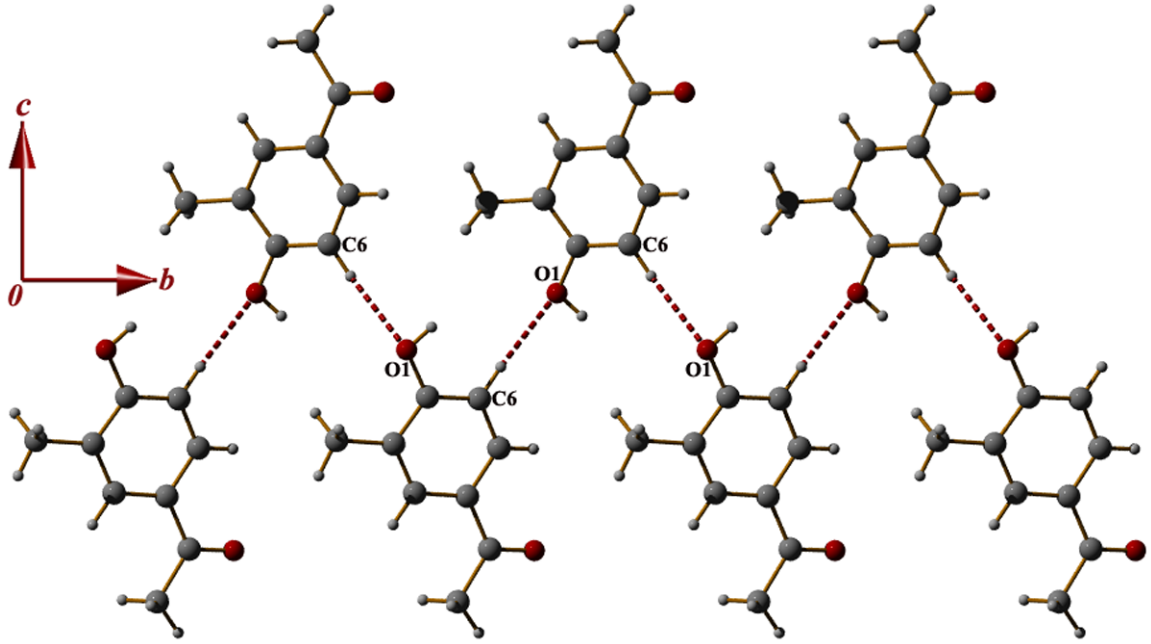

Figure S2. Formation of 1D zigzag chain in (1) propagating parallel to (0 1 0) direction.