Supporting Information for the Article "Synthesis, Crystal Structure and Intermolecular Interactions of 2-(1-Hydroxy-2,2,2-trifluoroethyl)estrone Derivatives

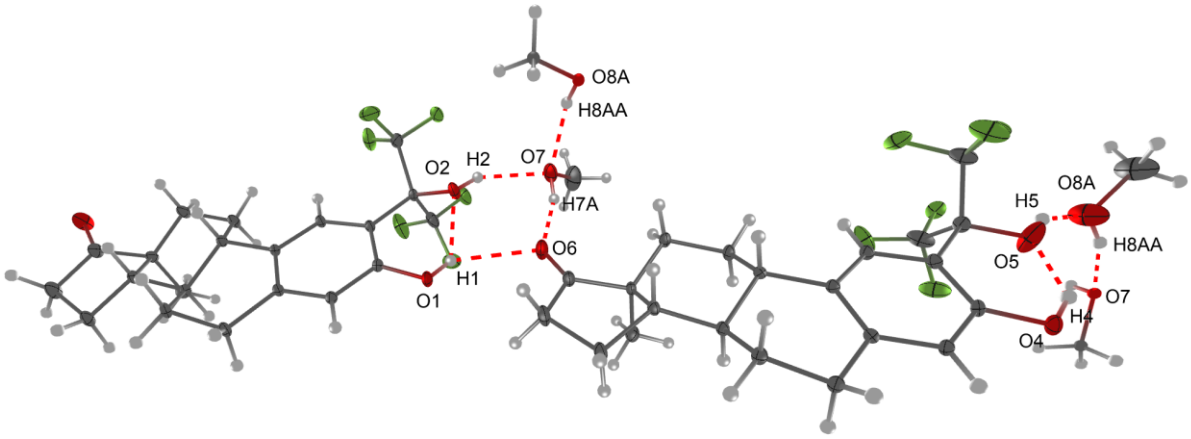

Figure 1S. Hydrogen bonding diagram in the crystal of compound **3**, part 1.

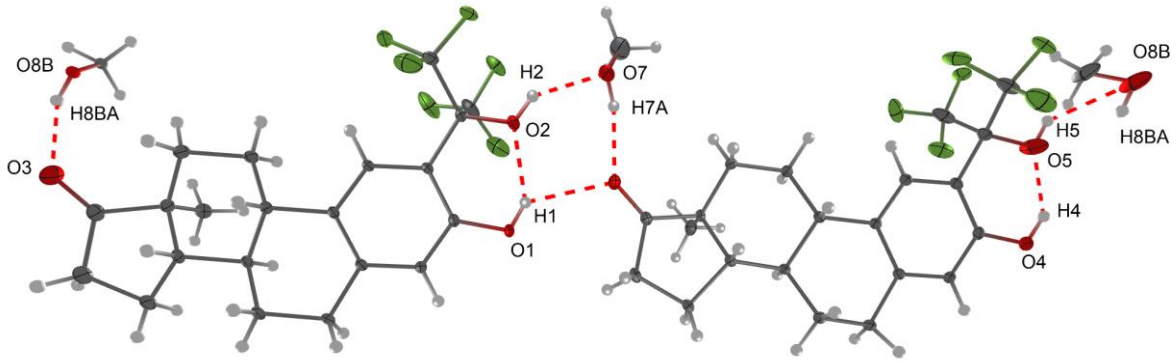

Figure 2S. Hydrogen bonding diagram in the crystal of compound **3**, part 2.

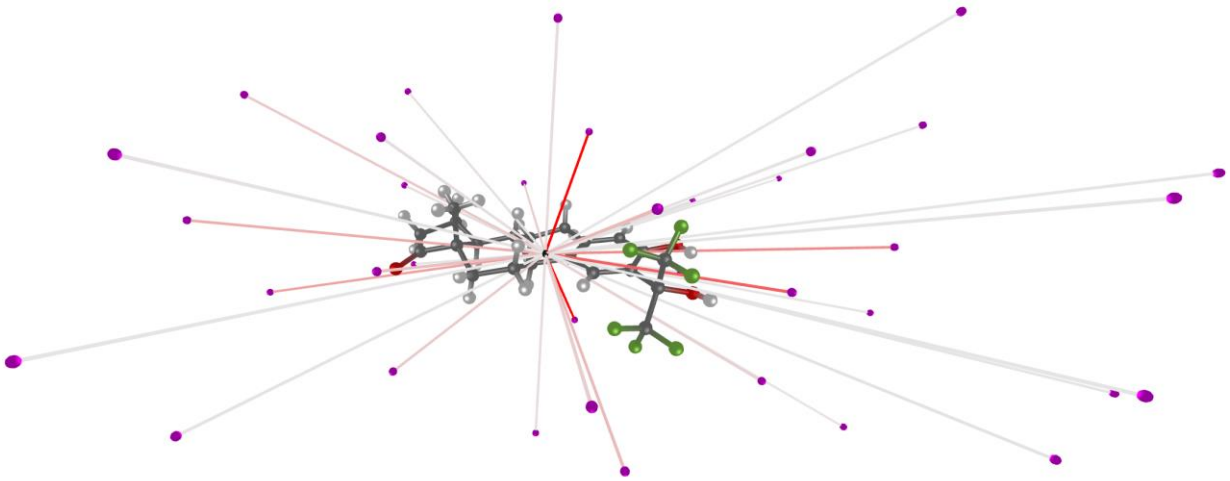

Figure 3S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of compound **3**.

Table 1S. Pair interaction energy and distance in the molecular cluster of compound **3**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
1	x, y, z	13.4	-21.27	-26.35	-20.63	-22.53	-28.40
2	x, y, z	8.9	-38.22	-41.07	-31.02	-33.25	-37.88
3	x, y, z	6.8	-5.86	-11.99	-8.78	-10.52	-12.34
4	-x, y-1/2, -z	8.6	-23.54	-18.05	-10.04	-12.41	-17.73
5	-x, y-1/2, -z	13.4	0.00	-0.50	-0.53	-0.53	-0.47
6	-x, y-1/2, -z	7.1	-3.89	-7.40	-5.90	-7.00	-8.20
7	-x, y-1/2, 1-z	17.6	0.00	0.24	0.66	0.61	0.42
8	-x, y-1/2, 1-z	21.8	0.00	-0.36	0.11	0.10	0.06
9	x-1, y, z-1	15.8	0.00	-0.40	-0.31	-0.37	-0.40
10	-x, y+1/2, -z	8.6	-23.54	-18.13	-10.04	-12.41	-17.73
11	-x, y+1/2, -z	13.9	0.00	-0.68	-0.74	-0.78	-0.71
12	-x, y+1/2, -z	7.8	-0.96	-2.52	-1.80	-2.12	-2.10
13	x-1, y, z	9.7	-8.42	-9.39	-5.52	-6.82	-9.00
14	x-1, y, z	17.3	0.00	0.09	0.16	0.11	0.12
15	-x, y+1/2, 1-z	18.0	0.00	-0.54	-0.53	-0.55	-0.60
16	-x, y+1/2, 1-z	22.0	0.00	-0.34	0.14	0.16	0.11
17	-x, y-1/2, -z	9.1	-2.92	-6.69	-4.66	-5.69	-7.29
18	-x, y+1/2, -z	9.8	-0.17	-1.76	-0.78	-1.21	-1.38
19	1-x, y-1/2, -z	5.2	-52.70	-56.93	-52.85	-57.24	-57.74
20	1-x, y-1/2, -z	12.5	-12.16	-18.29	-15.82	-18.54	-20.78

21	1-x, y-1/2, -z	9.8	0.00	-0.13	0.26	0.05	0.12
22	x, y-1, z	8.4	-0.01	-2.85	-2.06	-2.29	-1.13
23	x, y-1, z	15.4	0.00	-0.42	-0.40	-0.33	-0.14
24	1-x, y-1/2, 1-z	15.5	0.00	-0.75	-0.62	-0.61	-0.66
25	x, y, z-1	13.3	-13.57	-17.52	-13.09	-13.79	-18.41
26	1-x, y+1/2, -z	5.2	-54.78	-56.93	-52.84	-57.24	-57.75
27	1-x, y+1/2, -z	13.1	-1.47	-6.96	-6.28	-7.05	-7.41
28	1-x, y+1/2, -z	10.4	0.00	-1.40	-1.09	-1.31	-1.27
29	1-x, y+1/2, 1-z	15.9	0.00	-0.27	-0.14	-0.13	-0.18
30	1-x, y-1/2, -z	10.2	0.00	-1.07	-0.49	-0.58	-0.58
31	x, y+1, z	8.4	-0.01	-2.78	-1.92	-2.29	-1.13
32	x, y+1, z	16.2	0.00	-0.21	-0.14	-0.09	-0.05
33	x+1, y, z	9.7	-8.42	-9.39	-5.52	-6.82	-9.00
34	x+1, y, z	15.8	0.00	-0.40	-0.35	-0.39	-0.50
35	x+1, y, z	8.9	0.00	-2.43	-1.81	-2.27	-2.13
36	x+1, y, z	8.5	-4.43	-3.13	-1.98	-2.26	-3.44
ΣE_{dim}, kJ/mol			-276.34	-327.69	-257.35	-288.38	-325.73

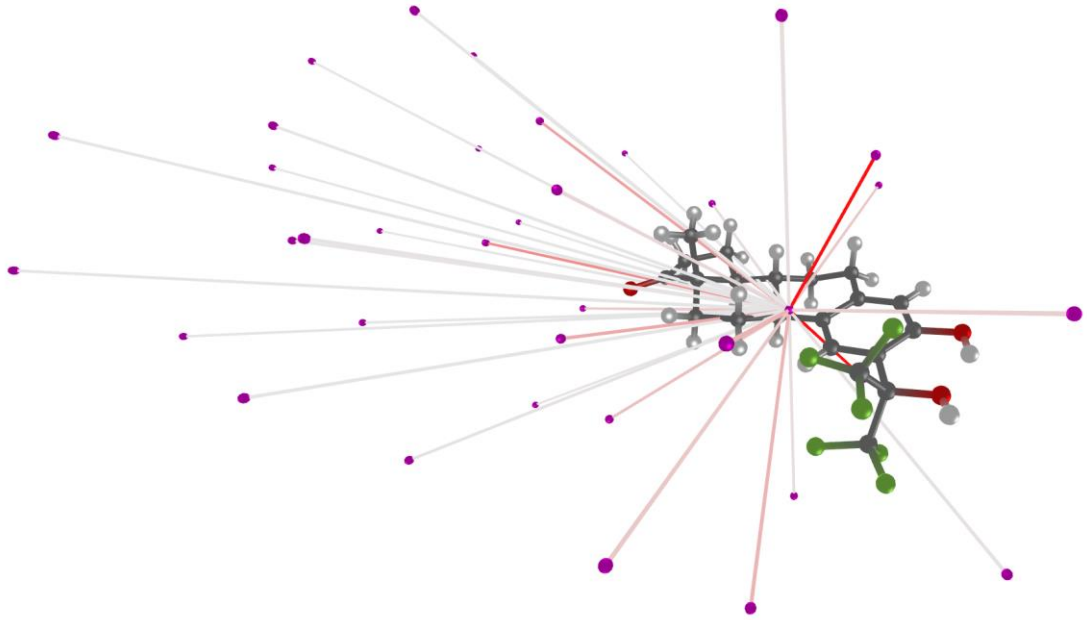

Figure 4S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of compound **3**.

Table 2S. Pair interaction energy and distance in the molecular cluster of compound **3**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
0	x, y, z	13.4	-21.27	-26.34	-20.63	-22.53	-28.41
2	x, y, z	6.9	-36.33	-20.46	-13.61	-15.67	-19.32
3	x, y, z	19.1	0.00	-0.46	-0.12	-0.11	-0.14
4	-x, y-1/2, -z	13.9	0.00	-0.79	-0.74	-0.81	-0.79
5	-x, y-1/2, -z	25.6	0.00	0.18	0.09	0.21	0.26
6	-x, y-1/2, -z	19.5	0.00	-0.31	0.00	0.04	0.00
7	-x, y-1/2, 1-z	8.5	-28.18	-18.69	-11.12	-13.56	-18.75
8	-x, y-1/2, 1-z	9.5	-0.89	-2.09	-0.74	-1.23	-1.78
9	x-1, y, z-1	27.5	0.00	-0.03	-0.06	0.01	0.01
10	-x, y+1/2, -z	13.4	0.00	-0.57	-0.54	-0.53	-0.47
11	-x, y+1/2, -z	25.6	0.00	0.18	0.09	0.20	0.26
12	-x, y+1/2, -z	19.4	0.00	-0.20	0.10	0.16	0.12
13	x-1, y, z	15.8	0.00	-0.41	-0.35	-0.40	-0.51
14	x-1, y, z	9.7	-5.21	-10.57	-6.82	-8.18	-10.59
15	-x, y+1/2, 1-z	8.5	-28.17	-18.70	-11.12	-13.56	-18.75
16	-x, y+1/2, 1-z	9.3	-0.13	-6.35	-5.04	-5.99	-6.23
17	-x, y-1/2, -z	7.4	-1.08	-10.53	-8.63	-9.98	-10.94
18	-x, y+1/2, -z	7.5	-1.64	-4.13	-3.06	-3.62	-4.11
19	1-x, y-1/2, -z	13.1	-1.47	-6.96	-6.28	-7.05	-7.41

20	1-x, y-1/2, -z	25.6	0.00	-0.08	-0.14	-0.10	-0.09
21	1-x, y-1/2, -z	21.2	0.00	-0.34	-0.08	0.00	-0.05
22	x, y-1, z	16.2	0.00	-0.21	-0.14	-0.09	-0.05
23	x, y-1, z	8.4	-0.01	-2.77	-1.85	-2.07	-0.99
24	1-x, y-1/2, 1-z	5.2	-62.25	-53.73	-49.70	-52.24	-54.63
25	x, y, z-1	26.6	0.00	-0.09	-0.12	-0.07	-0.09
26	1-x, y+1/2, -z	12.5	-12.14	-18.29	-15.82	-18.56	-20.79
27	1-x, y+1/2, -z	25.6	0.00	-0.08	-0.15	-0.10	-0.09
28	1-x, y+1/2, -z	21.2	0.00	-0.32	-0.02	0.02	-0.01
29	1-x, y+1/2, 1-z	5.2	-62.25	-53.73	-49.70	-52.24	-54.63
30	1-x, y-1/2, -z	10.1	-0.07	-0.93	-0.59	-0.75	-0.74
31	x, y+1, z	15.4	0.00	-0.42	-0.40	-0.33	-0.14
32	x, y+1, z	8.4	-0.01	-2.77	-1.85	-2.07	-0.99
33	x+1, y, z	17.3	0.00	0.09	0.16	0.11	0.12
34	x+1, y, z	9.7	-5.28	-10.57	-6.82	-8.18	-10.59
35	x+1, y, z	8.5	-4.05	-3.02	-2.00	-2.32	-3.44
36	x+1, y, z	20.5	0.00	-0.34	0.00	0.03	-0.01
ΣE_{dim}, kJ/mol			-270.43	-274.85	-217.81	-241.55	-274.72

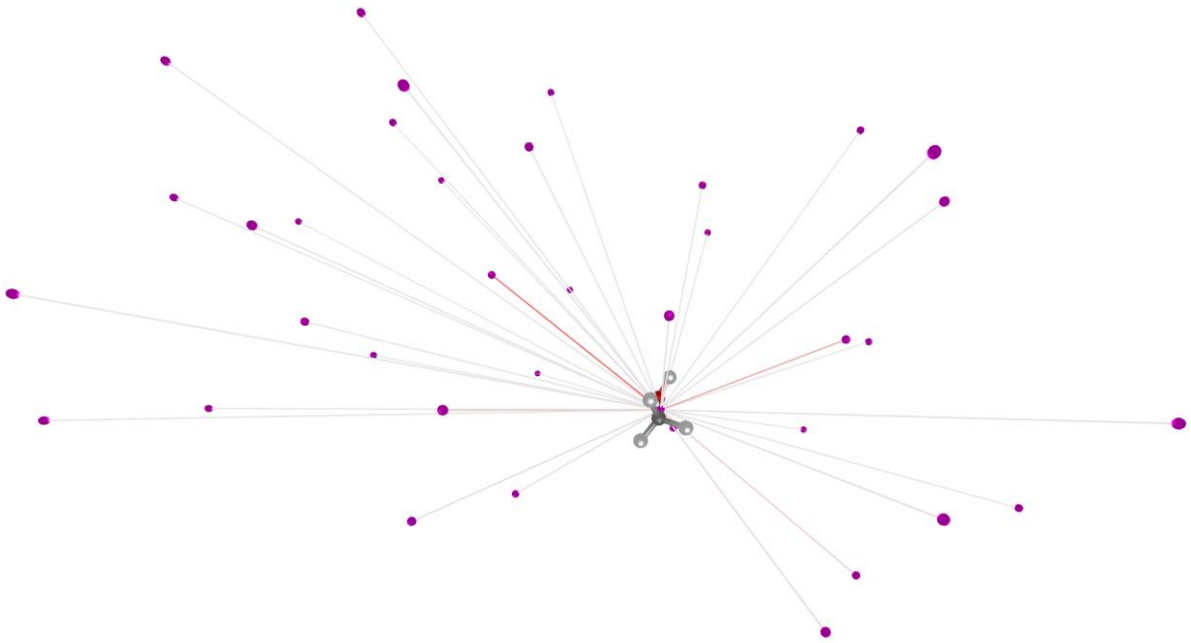

Figure 5S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of compound **3**.

Table 3S. Pair interaction energy and distance in the molecular cluster of compound **3**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
0	x, y, z	8.9	-38.22	-41.14	-31.02	-33.25	-37.88
1	x, y, z	6.9	-36.35	-20.46	-13.60	-15.67	-19.32
3	x, y, z	13.2	0.00	0.00	-0.06	-0.07	-0.07
4	-x, y-1/2, -z	7.8	-0.96	-2.52	-1.77	-2.09	-2.10
5	-x, y-1/2, -z	19.4	0.00	-0.20	0.12	0.16	0.12
6	-x, y-1/2, -z	13.9	0.00	0.15	0.10	0.11	0.10
7	-x, y-1/2, 1-z	9.3	0.00	-6.35	-5.04	-5.99	-6.23
8	-x, y-1/2, 1-z	14.1	0.00	0.12	0.05	0.06	0.06
9	x-1, y, z-1	21.0	0.00	-0.38	0.00	0.00	-0.04
10	-x, y+1/2, -z	7.1	-3.89	-7.40	-5.90	-6.99	-8.20
11	-x, y+1/2, -z	19.5	0.00	-0.31	-0.01	0.03	0.00
12	-x, y+1/2, -z	13.9	0.00	0.15	0.10	0.11	0.10
13	x-1, y, z	8.9	0.00	-2.43	-1.81	-2.27	-2.13
14	x-1, y, z	8.5	-4.04	-3.03	-2.00	-2.32	-3.44
15	-x, y+1/2, 1-z	9.5	-0.89	-2.08	-0.73	-1.22	-1.78
16	-x, y+1/2, 1-z	14.1	0.00	0.12	0.05	0.06	0.06
17	-x, y-1/2, -z	4.1	-35.26	-25.95	-18.29	-20.04	-23.01
18	-x, y+1/2, -z	4.5	-2.38	-1.01	-0.25	-0.53	-0.82
19	1-x, y-1/2, -z	10.4	0.00	-1.40	-1.10	-1.33	-1.27
20	1-x, y-1/2, -z	21.2	0.00	-0.33	-0.01	0.01	-0.03

21	1-x, y-1/2, -z	18.3	0.00	0.09	0.04	0.05	0.03
22	x, y-1, z	12.7	0.00	-0.52	0.04	0.05	0.03
23	x, y-1, z	10.7	0.00	-0.11	0.19	0.25	0.22
24	1-x, y-1/2, 1-z	10.6	0.00	-0.70	-0.25	-0.25	-0.34
25	x, y, z-1	21.5	0.00	-0.42	-0.02	-0.03	-0.06
26	1-x, y+1/2, -z	9.9	-0.01	-0.64	-0.29	-0.42	-0.37
27	1-x, y+1/2, -z	21.2	0.00	-0.33	-0.08	0.00	-0.05
28	1-x, y+1/2, -z	18.3	0.00	0.09	0.04	0.05	0.03
29	1-x, y+1/2, 1-z	10.7	0.00	-0.87	-0.36	-0.37	-0.37
30	1-x, y-1/2, -z	11.5	0.00	-0.08	-0.15	-0.16	-0.14
31	x, y+1, z	11.8	0.00	-0.42	0.12	0.06	0.05
32	x, y+1, z	11.0	0.00	-0.55	-0.12	-0.14	-0.16
33	x+1, y, z	16.3	0.00	-0.41	0.06	0.05	0.03
34	x+1, y, z	14.5	0.00	-0.33	0.09	0.06	0.10
35	x+1, y, z	9.7	0.00	0.25	0.22	0.23	0.18
36	x+1, y, z	17.2	0.00	0.05	-0.02	-0.02	-0.02
ΣE_{dim}, kJ/mol			-122.02	-119.71	-81.69	-91.80	-106.72

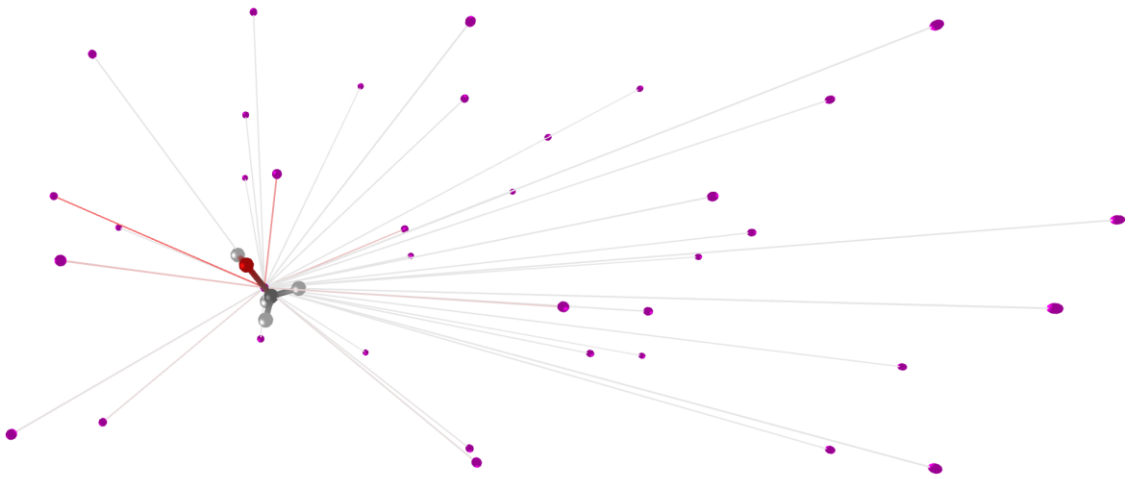

Figure 6S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of compound **3**.

Table 4S. Pair interaction energy and distance in the molecular cluster of compound **3**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
0	x, y, z	6.8	-5.86	-11.99	-8.78	-10.52	-12.34
1	x, y, z	19.1	0.00	-0.46	-0.10	-0.09	-0.11
2	x, y, z	13.2	0.00	0.00	-0.06	-0.07	-0.07
4	-x, y-1/2, -z	9.8	0.00	-1.76	-0.77	-1.21	-1.38
5	-x, y-1/2, -z	7.5	-1.63	-4.13	-3.05	-3.62	-4.12
6	-x, y-1/2, -z	4.5	-2.38	-1.01	-0.25	-0.53	-0.82
7	-x, y-1/2, 1-z	21.8	0.00	-0.36	0.00	0.07	-0.03
8	-x, y-1/2, 1-z	27.0	0.00	0.06	0.01	0.02	0.01
9	x-1, y, z-1	9.1	0.00	-1.69	-1.25	-1.57	-1.62
10	-x, y+1/2, -z	9.1	-2.92	-6.68	-4.65	-5.69	-7.29
11	-x, y+1/2, -z	7.4	-0.50	-10.64	-8.65	-9.99	-10.93
12	-x, y+1/2, -z	4.1	-35.26	-25.95	-18.29	-20.04	-23.00
13	x-1, y, z	8.5	-4.43	-3.13	-1.98	-2.26	-3.44
14	x-1, y, z	20.5	0.00	-0.34	0.00	0.03	-0.01
15	-x, y+1/2, 1-z	21.8	0.00	-0.40	-0.01	0.01	-0.04
16	-x, y+1/2, 1-z	27.0	0.00	0.06	0.01	0.01	0.00
17	-x, y-1/2, -z	13.9	0.00	0.01	0.02	0.02	0.02
18	-x, y+1/2, -z	13.9	0.00	0.04	0.05	0.03	0.04
19	1-x, y-1/2, -z	10.8	0.00	-0.86	-0.33	-0.37	-0.36
20	1-x, y-1/2, -z	10.1	0.00	0.06	0.38	0.48	0.45

21	1-x, y-1/2, -z	11.6	0.00	0.18	0.09	0.09	0.09
22	x, y-1, z	11.4	0.00	-0.33	0.05	0.07	0.05
23	x, y-1, z	20.9	0.00	-0.42	-0.05	-0.03	-0.06
24	1-x, y-1/2, 1-z	21.7	0.00	-0.39	-0.01	0.00	-0.02
25	x, y, z-1	8.9	-62.38	-40.76	-29.89	-32.23	-36.91
26	1-x, y+1/2, -z	10.2	0.00	-1.08	-0.50	-0.58	-0.59
27	1-x, y+1/2, -z	10.1	-0.07	-0.93	-0.59	-0.75	-0.74
28	1-x, y+1/2, -z	11.5	0.00	-0.08	-0.15	-0.16	-0.14
29	1-x, y+1/2, 1-z	21.7	0.00	-0.39	-0.02	0.01	-0.05
30	1-x, y-1/2, -z	16.8	0.00	0.05	0.06	0.05	0.04
31	x, y+1, z	10.1	0.00	-0.10	0.43	0.46	0.43
32	x, y+1, z	20.9	0.00	-0.38	-0.03	0.00	-0.02
33	x+1, y, z	14.4	0.00	-0.54	-0.11	-0.10	-0.12
34	x+1, y, z	22.4	0.00	-0.46	-0.11	-0.10	-0.11
35	x+1, y, z	15.6	0.00	0.02	-0.03	-0.04	-0.04
36	x+1, y, z	9.7	0.00	0.03	0.02	0.02	0.01
ΣE_{dim}, kJ/mol			-115.43	-114.75	-78.54	-88.58	-103.23

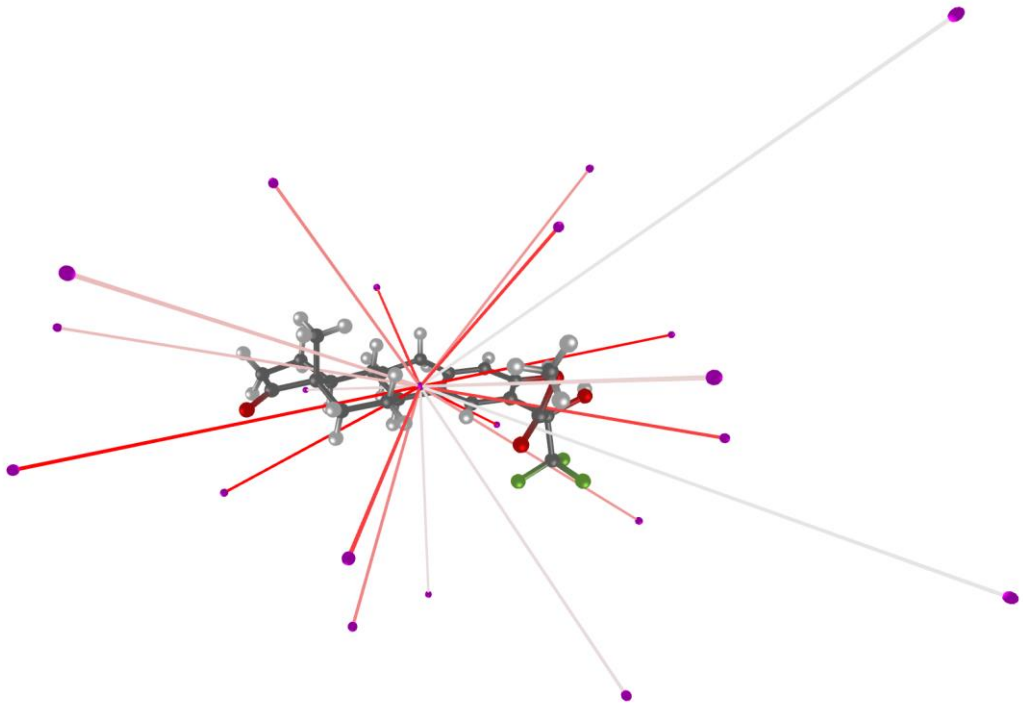

Figure 7S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of compound **5**.

Table 5S. Pair interaction energy and distance in the molecular cluster of compound **5**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
1	1-x, y-1/2, 3/2-z	9.6	-56.06	-36.16	-26.18	-30.45	-37.38
2	x-1/2, 1/2-y, 1-z	12.5	-2.22	-8.13	-6.60	-7.41	-8.14
3	x-1, y, z	11.7	-7.69	-4.72	-3.06	-3.62	-4.67
4	1/2-x, 2-y, z-1/2	16.4	0.00	-0.51	-0.28	-0.33	-0.34
5	1-x, y+1/2, 3/2-z	9.6	-56.06	-36.15	-26.17	-30.45	-37.38
6	x-1/2, 3/2-y, 1-z	7.3	-39.37	-31.83	-27.63	-30.26	-32.93
7	1/2-x, 2-y, z+1/2	16.4	0.00	-0.51	-0.28	-0.32	-0.34
8	x-1/2, 3/2-y, 2-z	11.3	0.00	-1.68	-1.56	-1.76	-1.22
9	x, y-1, z	12.2	-39.25	-45.57	-35.59	-38.68	-41.75
10	3/2-x, 1-y, z-1/2	8.0	-20.60	-20.60	-15.25	-18.81	-20.74
11	2-x, y-1/2, 3/2-z	8.3	-34.01	-42.17	-35.84	-38.22	-41.63
12	x+1/2, 1/2-y, 1-z	12.5	-2.22	-8.11	-6.59	-7.40	-8.12
13	3/2-x, 1-y, z+1/2	8.0	-20.60	-20.58	-15.25	-18.80	-20.75
14	3/2-x, 2-y, z-1/2	10.5	-8.86	-15.81	-12.60	-14.16	-16.27
15	2-x, y+1/2, 3/2-z	8.3	-34.00	-42.18	-35.80	-38.27	-41.62
16	x+1/2, 3/2-y, 1-z	7.3	-37.29	-31.96	-27.86	-30.26	-32.92
17	3/2-x, 2-y, z+1/2	10.5	-8.86	-15.81	-12.60	-14.16	-16.27
18	x+1/2, 3/2-y, 2-z	11.3	0.00	-1.71	-1.57	-1.81	-1.22
19	x, y+1, z	12.2	-39.25	-45.57	-35.60	-38.68	-41.75

20	x+1, y, z	11.7	-7.69	-4.71	-3.08	-3.64	-4.66
ΣE_{dim}, kJ/mol			-414.01	-414.48	-329.38	-367.47	-410.11

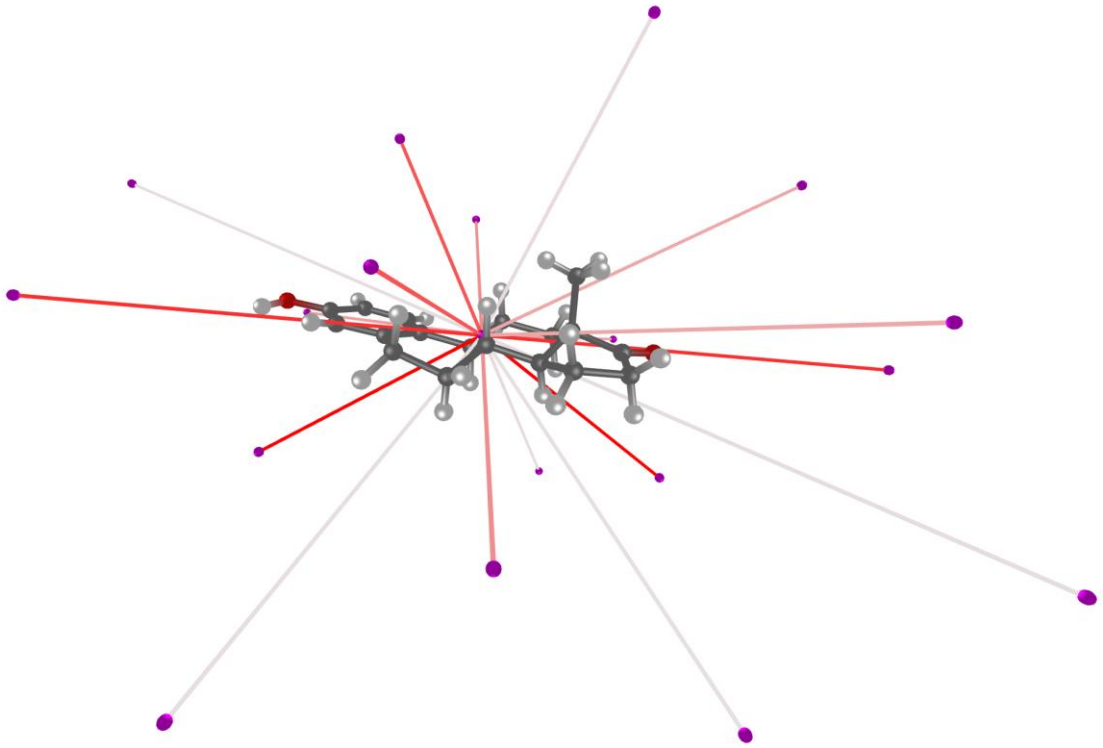

Figure 8S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of polymorph **I**.

Table 6S. Pair interaction energy and distance in the molecular cluster of polymorph **I**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
1	-3/2-x, -y, z-1/2	10.9	-6.82	-11.45	-8.97	-9.94	-12.16
2	-x-1, y-1/2, -1/2-z	9.3	-0.07	-2.00	-1.62	-2.05	-1.28
3	-3/2-x, -y, z+1/2	10.9	-6.80	-11.45	-8.99	-9.98	-12.16
4	x-1/2, 1/2-y, -z-1	9.9	-10.61	-12.39	-10.34	-11.07	-12.47
5	x-1/2, 1/2-y, -z	7.5	-21.64	-38.14	-34.18	-35.70	-39.41
6	-x-1, y+1/2, -1/2-z	9.3	-0.06	-2.00	-1.62	-2.05	-1.28
7	x-1/2, 1/2-y, 1-z	11.2	0.00	-1.00	-0.83	-1.05	-0.78
8	-1/2-x, -y, z-1/2	6.1	-19.49	-24.39	-21.54	-22.09	-24.98
9	-1/2-x, -y, z+1/2	6.1	-19.49	-24.40	-21.58	-22.10	-24.98
10	x+1/2, 1/2-y, -z-1	9.9	-10.62	-12.39	-10.32	-11.05	-12.47
11	x+1/2, 1/2-y, -z	7.5	-19.24	-38.16	-34.26	-35.70	-39.41
12	x-1, y, z	12.2	-37.33	-35.64	-27.07	-29.75	-32.92
13	x+1/2, 1/2-y, 1-z	11.2	0.00	-1.05	-0.90	-1.10	-0.82
14	x-1, y, z+1	14.3	0.00	-1.57	-1.08	-1.38	-1.77
15	x, y, z-1	7.5	-9.66	-16.10	-13.12	-13.51	-15.57
16	x, y, z+1	7.5	-9.66	-16.12	-13.12	-13.52	-15.57

17	x+1, y, z-1	14.3	0.00	-1.57	-1.07	-1.38	-1.76
18	x+1, y, z	12.2	-37.33	-35.62	-27.07	-29.74	-32.92
ΣE_{dim}, kJ/mol			-208.82	-285.42	-237.69	-253.16	-282.70

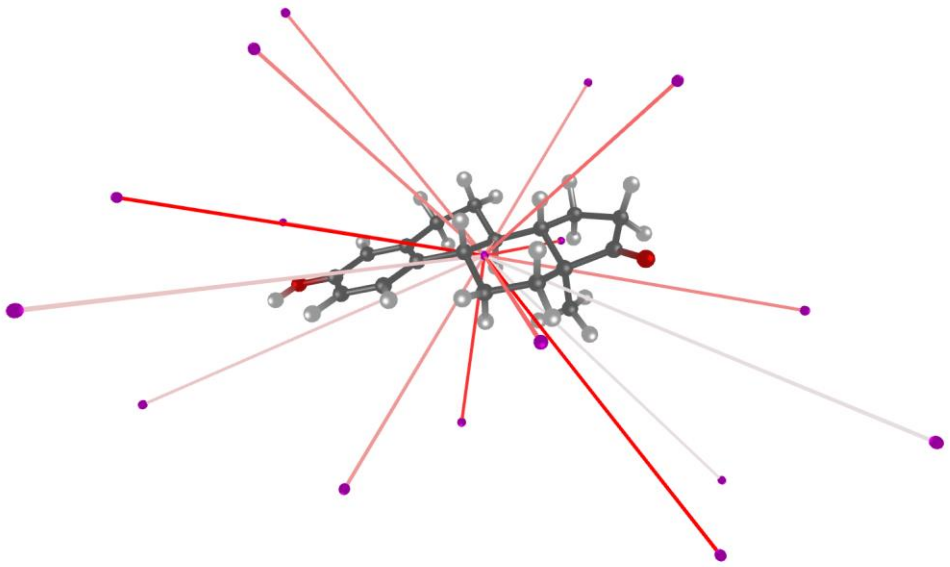

Figure 9S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of polymorph **II**.

Table 7S. Pair interaction energy and distance in the molecular cluster of polymorph **II**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
1	x-1/2, -1/2-y, 1-z	7.5	-19.42	-21.66	-18.34	-19.54	-17.09
2	x-1, y, z	7.7	-8.80	-14.47	-11.42	-11.87	-11.30
3	x-1/2, 1/2-y, 1-z	5.8	-24.63	-28.27	-26.21	-27.11	-24.09
4	3/2-x, -y, z-1/2	9.8	-9.06	-16.47	-13.97	-15.16	-14.50
5	2-x, y-1/2, 1/2-z	8.7	-16.13	-16.75	-14.30	-14.97	-11.61
6	3/2-x, -y, z+1/2	9.8	-9.06	-16.47	-13.99	-15.16	-14.51
7	x+1/2, -1/2-y, 1-z	7.5	-19.42	-21.66	-18.35	-19.54	-17.09
8	2-x, y-1/2, 3/2-z	12.3	0.00	-1.36	-1.12	-1.33	-1.05
9	2-x, y+1/2, 1/2-z	8.7	-16.13	-16.75	-14.32	-14.98	-11.62
10	x+1/2, 1/2-y, 1-z	5.8	-24.63	-28.27	-26.21	-27.09	-24.08
11	2-x, y+1/2, 3/2-z	12.3	0.00	-1.36	-1.11	-1.33	-1.05
12	5/2-x, -y, z-1/2	10.3	-46.21	-44.46	-33.70	-36.49	-37.34
13	3-x, y-1/2, 1/2-z	12.1	-2.08	-6.45	-4.77	-5.27	-4.78
14	5/2-x, -y, z+1/2	10.3	-46.22	-44.46	-33.70	-36.49	-37.33
15	3-x, y+1/2, 1/2-z	12.1	-2.08	-6.45	-4.76	-5.27	-4.78

16	x+1, y, z	7.7	-8.81	-14.47	-11.42	-11.85	-11.28
ΣE_{dim}, kJ/mol			-252.68	-299.79	-247.70	-263.44	-243.50

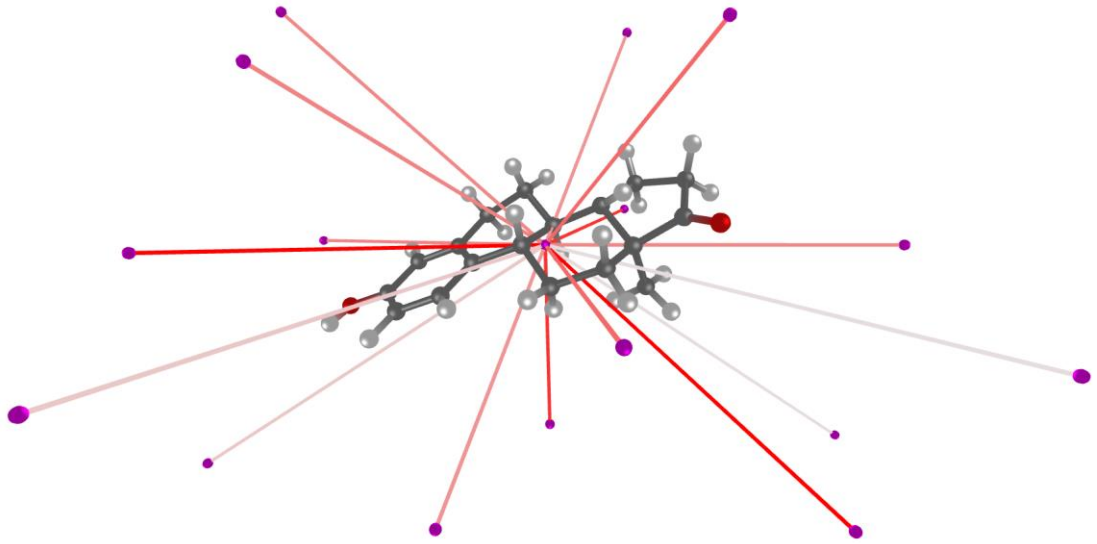

Figure 10S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of polymorph **II**.

Table 8S. Pair interaction energy and distance in the molecular cluster of polymorph **II**(r.t.).

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
1	x-1/2, 1/2-y, 1-z	7.6	-16.22	-21.04	-18.10	-19.09	-21.51
2	x-1/2, 1/2-y, 2-z	7.8	-9.27	-14.53	-11.67	-12.26	-14.41
3	1/2-x, 1-y, z-1/2	5.8	-21.55	-28.29	-26.10	-27.54	-29.43
4	x-1/2, 3/2-y, 1-z	9.8	-7.81	-15.94	-13.71	-14.79	-17.09
5	1/2-x, 1-y, z+1/2	8.7	-14.33	-16.44	-14.26	-14.91	-16.17
6	1-x, y-1/2, 1/2-z	9.8	-7.81	-15.94	-13.70	-14.79	-17.09
7	x+1/2, 1/2-y, 1-z	7.6	-16.23	-21.03	-18.05	-19.07	-21.52
8	1-x, y-1/2, 3/2-z	12.4	-0.04	-1.29	-1.10	-1.29	-1.19
9	x+1/2, 1/2-y, 2-z	8.7	-13.89	-16.44	-14.25	-14.90	-16.17
10	x, y, z-1	5.8	-21.56	-28.30	-26.12	-27.56	-29.42
11	1-x, y+1/2, 1/2-z	12.4	0.00	-1.29	-1.10	-1.29	-1.19
12	3/2-x, 1-y, z-1/2	10.3	-43.08	-43.87	-33.48	-36.18	-41.34
13	x+1/2, 3/2-y, 1-z	12.1	-1.50	-5.87	-4.37	-4.93	-5.89
14	1-x, y+1/2, 3/2-z	10.3	-43.08	-43.87	-33.48	-36.19	-41.35
15	3/2-x, 1-y, z+1/2	12.1	-1.50	-5.87	-4.37	-4.93	-5.89
16	x, y, z+1	7.8	-9.27	-14.53	-11.67	-12.26	-14.41
ΣE_{dim}, kJ/mol			-227.14	-294.51	-245.52	-261.95	-294.07

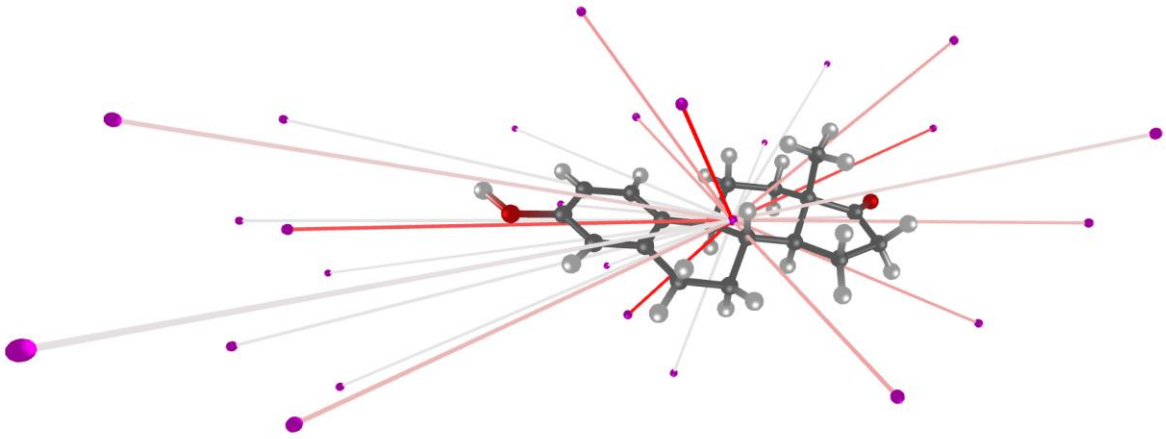

Figure 11S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of polymorph **III**.

Table 9S. Pair interaction energy and distance in the molecular cluster of polymorph **III**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
1	x, y, z	11.1	0.00	-1.10	-0.91	-1.15	-0.90
2	-x, y-1/2, -z	16.4	0.00	-0.39	-0.26	-0.38	-0.41
3	-x, y-1/2, 1-z	12.0	-40.57	-35.42	-26.79	-29.54	-33.25
4	-x, y-1/2, -z	14.1	0.00	-5.73	-4.84	-5.54	-5.97
5	-x, y-1/2, 2-z	11.6	-7.34	-10.85	-8.31	-9.66	-12.43
6	-x, y-1/2, 1-z	15.0	0.00	-1.45	-1.08	-1.34	-1.39
7	-x, y+1/2, -z	16.4	0.00	-0.45	-0.33	-0.42	-0.47
8	-x, y+1/2, 1-z	12.0	-40.58	-35.46	-26.80	-29.54	-33.26
9	-x, y+1/2, -z	9.9	-8.98	-14.34	-11.93	-13.21	-15.38
10	x-1, y, z	8.1	-6.29	-16.11	-13.97	-15.38	-16.77
11	-x, y+1/2, 2-z	11.6	-7.34	-10.85	-8.31	-9.66	-12.42
12	-x, y+1/2, 1-z	11.2	0.00	-3.41	-2.96	-3.51	-3.17
13	x-1, y, z+1	4.9	-33.61	-44.09	-41.82	-42.97	-45.71
14	1-x, y-1/2, -z	21.1	0.00	0.01	0.08	0.02	0.02
15	1-x, y-1/2, -z-1	19.3	0.00	0.06	0.18	0.06	0.03
16	1-x, y-1/2, 1-z	16.3	0.00	-0.05	0.00	-0.03	0.00
17	1-x, y-1/2, -z	15.2	0.00	-0.29	-0.33	-0.39	-0.33
18	1-x, y+1/2, -z-1	16.5	0.00	-0.30	-0.32	-0.33	-0.36
19	x, y, z-1	7.6	-12.11	-15.36	-11.58	-12.20	-14.43

20	x, y, z-1	18.2	0.00	-0.06	0.00	-0.02	-0.05
21	1-x, y+1/2, -z	11.4	0.00	-4.13	-3.84	-4.45	-4.45
22	1-x, y+1/2, 1-z	10.3	-6.89	-14.44	-12.13	-13.12	-15.36
23	x, y, z+1	7.6	-12.14	-15.24	-11.60	-12.20	-14.41
24	x, y, z+1	5.5	-19.68	-38.93	-37.95	-38.93	-41.93
25	x+1, y, z-1	14.0	0.00	-0.10	-0.01	-0.07	-0.02
26	x+1, y, z	9.3	0.00	-0.58	-0.60	-0.63	0.16
ΣE_{dim}, kJ/mol			-195.52	-269.04	-226.40	-244.60	-272.67

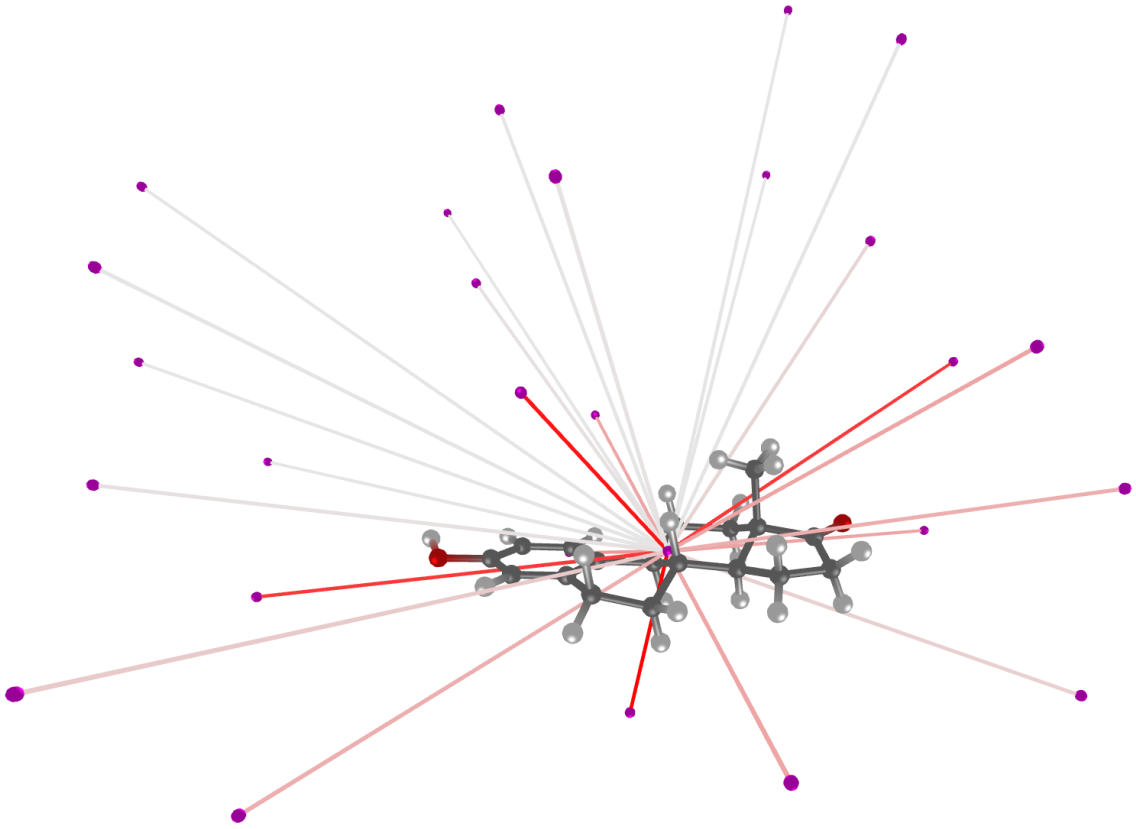

Figure 12S. A schematic diagram illustrating the distances to the center of the neighboring molecules in the molecular cluster used for the lattice energy calculation of polymorph **III**.

Table 10S. Pair interaction energy and distance in the molecular cluster of polymorph **III**.

№	Symmetry operation	R, Å	EML, kJ/mol	B3LYP-D4, kJ/mol	DLPNO-CCDC(T), kJ/mol	PWPB95, kJ/mol	R2SCAN-3c, kJ/mol
0	x, y, z	11.1	0.00	-1.07	-1.06	-1.19	-0.90
2	-x, y-1/2, -z	9.9	-9.00	-14.35	-11.92	-13.22	-15.38
3	-x, y-1/2, 1-z	11.2	-0.60	-3.40	-2.97	-3.52	-3.18
4	-x, y-1/2, -z	16.0	0.00	0.06	-0.07	-0.05	-0.01
5	-x, y-1/2, 2-z	16.3	0.00	-0.06	-0.17	-0.06	-0.11
6	-x, y-1/2, 1-z	20.8	0.00	0.08	0.03	0.04	0.01

7	-x, y+1/2, -z	14.1	0.00	-5.77	-4.96	-5.52	-5.96
8	-x, y+1/2, 1-z	15.0	0.00	-1.40	-1.04	-1.27	-1.39
9	-x, y+1/2, -z	16.0	0.00	0.03	-0.04	-0.05	0.01
10	x-1, y, z	9.3	0.00	-0.44	-0.58	-0.60	0.19
11	-x, y+1/2, 2-z	19.2	0.00	0.04	0.09	-0.01	0.01
12	-x, y+1/2, 1-z	20.8	0.00	0.09	0.06	0.04	0.04
13	x-1, y, z+1	14.0	0.00	0.06	-0.01	0.05	0.03
14	1-x, y-1/2, -z	11.4	-0.19	-4.13	-3.83	-4.44	-4.46
15	1-x, y-1/2, -z-1	11.6	-6.56	-12.02	-10.18	-11.61	-13.98
16	1-x, y-1/2, 1-z	10.3	-6.89	-14.44	-12.13	-13.12	-15.36
17	1-x, y-1/2, -z	12.0	-37.00	-41.12	-31.40	-34.34	-38.60
18	1-x, y+1/2, -z-1	11.6	-6.57	-11.98	-10.17	-11.62	-13.98
19	x, y, z-1	5.5	-19.68	-38.92	-37.95	-38.94	-41.92
20	x, y, z-1	7.6	-8.91	-15.06	-11.82	-12.04	-14.43
21	1-x, y+1/2, -z	12.0	-36.99	-41.16	-31.39	-34.35	-38.59
22	1-x, y+1/2, 1-z	16.4	0.00	-0.23	-0.29	-0.29	-0.35
23	x, y, z+1	18.2	0.00	-0.04	0.05	-0.04	-0.06
24	x, y, z+1	7.6	-8.91	-15.08	-11.79	-12.07	-14.42
25	x+1, y, z-1	4.9	-33.61	-44.09	-41.85	-42.98	-45.72
26	x+1, y, z	8.1	-5.61	-16.11	-13.97	-15.38	-16.77
ΣE_{dim}, kJ/mol			-180.53	-280.53	-239.35	-256.58	-285.28