Data-driven evaluation for multi-criteria selection of covalent organic frameworks for membrane-based hydrogen separation

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Supporting Information

Table S1: Database of 1242 COFs including Scores

Name	Number	Type	Dimension	Topology	Stacking	Interpenetration	Surface Area (m^2/g)	Density (g/cm^3)	Pore Size (nm)	Norm. Surface	Norm. Density	Norm. Pore Size	Density Score	Topo Score	Dense Pore Score	Score Combi
1-22n-COF	1	(1-22)n COF with AA stacking	2D	sql	AA	-	838	0.97	6.0	0.08	0.49	0.06	0.43	0.79	4.72	4.27
12C4-COF	2	12C4-COF with AA stacking	2D	hcb	AA	-	2414	0.46	19.7	0.24	0.23	0.20	1.86	1.94	5.85	5.16
15C5-COF	3	15C5-COF with AA stacking	2D	hcb	AA	-	2503	0.49	16.9	0.25	0.24	0.17	1.89	2.08	5.67	5.26
18C6-COF	4	18C6-COF with AA stacking	2D	hcb	AA	-	2262	0.57	13.6	0.23	0.28	0.14	1.62	1.95	5.54	5.15
2D-BPTA-COF	5	2D-BPTA-COF	2D	sql	-	-	1463	0.83	8.2	0.15	0.41	0.08	0.86	1.34	5.01	4.66
2D-NiPc-BTDA-COF	6	2D-NiPc-BTDA-COF	2D	sql	-	-	1192	0.97	12.3	0.12	0.49	0.12	0.61	1.05	4.53	4.25
3D-BMTA-COF	7	3D-BMTA-COF	3D	dia	-	-	1374	0.83	10.0	0.14	0.42	0.10	0.80	1.24	5.03	4.55
3D-COOH-COF	8	3D-COOH-COF	3D	dia	-	-	0	0.93	4.8	0.00	0.46	0.05	0.00	0.00	5.36	3.93
3D-CuPor-COF	9	3D-CuPor-COF	3D	pts	-	-	5817	0.33	16.5	0.58	0.17	0.16	4.85	4.86	3.49	7.08
3D-HNU5-2	10	3D-HNU5 two-interpenetrated	3D	dia	-	2	7796	0.31	11.5	0.78	0.15	0.12	6.60	6.90	1.86	8.24
3D-HNU5-3	11	3D-HNU5 three-interpenetrated	3D	dia	-	3	7445	0.46	6.3	0.74	0.23	0.06	5.73	6.97	1.97	8.07
3D-HNU5-4	12	3D-HNU5 four-interpenetrated	3D	dia	-	4	2327	0.62	7.7	0.23	0.31	0.08	1.61	2.15	5.31	5.32

3D-HNU5-5	13	3D-HNU5 five-interpenetrated	3D	dia	-	5	1367	0.77	5.9	0.14	0.38	0.06	0.84	1.29	5.31	4.74
3D-HNU5-non	14	3D-HNU5 non-interpenetrated	3D	dia	-	1	5206	0.32	14.3	0.52	0.16	0.14	4.38	4.46	4.03	6.86
3D-IL-COF-1	15	3D-IL-COF-1	3D	dia	-	-	3176	0.50	7.5	0.32	0.25	0.08	2.38	2.94	5.11	5.86
3D-IL-COF-2	16	3D-IL-COF-2	3D	dia	-	-	1465	0.72	7.9	0.15	0.36	0.08	0.94	1.35	5.45	4.77
3D-IL-COF-3	17	3D-IL-COF-3	3D	dia	-	-	1771	0.67	10.0	0.18	0.33	0.10	1.18	1.59	5.49	4.92
3D-OH-COF	18	3D-OH-COF	3D	dia	-	-	1938	0.77	7.1	0.19	0.38	0.07	1.20	1.80	4.97	4.99
3D-Por-COF	19	3D-Por-COF	3D	pts	-	-	6105	0.31	16.3	0.61	0.16	0.16	5.15	5.11	3.29	7.25
3D-Py-COF	20	3D-Py-COF	3D	pts	-	-	7310	0.28	13.5	0.73	0.14	0.13	6.29	6.33	2.31	7.97
3D-TPE-COF	21	3D-TPE-COF	3D	dia	-	-	439	0.95	6.0	0.04	0.48	0.06	0.23	0.41	5.00	4.09
sonoCOF-G11	985	sonoCOF-G11	2D	bex	-	-	2524	0.56	13.3	0.25	0.28	0.13	1.82	2.19	5.38	5.30
sonoCOF-G3	987	sonoCOF-G3	2D	bex	-	-	1830	0.67	17.2	0.18	0.33	0.17	1.22	1.52	5.45	4.73
sonoCOF-H3	992	sonoCOF-H3	2D	bex	-	-	1972	0.62	16.3	0.20	0.31	0.16	1.36	1.65	5.55	4.88
TCOF-AA	1028	TCOF with AA slipped stacking.	2D	bex	AA	-	2208	0.58	13.9	0.22	0.29	0.14	1.57	1.90	5.54	5.11
TCOF-AB	1029	TCOF with AB slipped stacking.	2D	bex	AB	-	2449	0.72	7.9	0.24	0.36	0.08	1.56	2.26	4.82	5.26
ICOF-1	260	ICOF-1	2D	fes	-	-	2146	0.58	15.2	0.21	0.29	0.15	1.52	1.82	5.56	5.03
A2B2-Por-COF	28	A2B2-Por-COF	2D	sql	-	-	1963	0.57	18.5	0.20	0.28	0.19	1.40	1.60	5.75	4.86
AB-COF	29	AB-COF	2D	hcb	-	-	1847	0.75	10.4	0.18	0.37	0.10	1.15	1.65	5.10	4.86
ACOF-1	30	ACOF-1	2D	hcb	-	-	1564	0.83	9.8	0.16	0.42	0.10	0.91	1.41	4.92	4.65
AEM-COF-1	31	AEM-COF-1	2D	hcb	-	-	1902	0.48	29.3	0.19	0.24	0.29	1.45	1.34	6.15	4.59
AEM-COF-2	32	AEM-COF-2	2D	hcb	-	-	1316	0.59	32.3	0.13	0.29	0.32	0.93	0.89	6.13	4.10
APT-DHTA-COF-AA	33	TAPT-DHTA-COF-AA	2D	hcb	-	-	2073	0.43	29.9	0.21	0.22	0.30	1.63	1.45	6.21	4.71
APT-DHTA-COF-AB	34	TAPT-DHTA-COF-AB	2D	hcb	-	-	3341	0.50	12.3	0.33	0.25	0.12	2.50	2.93	4.99	5.80
ATFG-COF	35	ATFG-COF	2D	hcb	-	-	1314	0.94	10.6	0.13	0.47	0.11	0.69	1.17	4.59	4.40
AzO-COF	36	AzO-COF	2D	hcb	-	-	2454	0.37	31.9	0.25	0.19	0.32	2.00	1.67	6.15	4.90

BBO-COF	37	AA-stacking mode of BBO-COF	2D	hcb	-	-	1137	0.94	11.5	0.11	0.47	0.12	0.60	1.01	4.69	4.28
BBO-COF-1	38	BBO-COF-1	2D	hcb	-	-	1460	0.90	13.0	0.15	0.45	0.13	0.81	1.27	4.71	4.44
BBO-COF-2	39	BBO-COF-2	2D	hcb	-	-	1963	0.48	28.9	0.20	0.24	0.29	1.50	1.40	6.13	4.64
BCCTP-COF	40	BCCTP-COF	2D	hcb	-	-	1722	0.64	16.9	0.17	0.32	0.17	1.17	1.43	5.64	4.72
B-COF-1	41	B-COF-1 with AA stacking	2D	hcb	-	-	2042	0.59	21.3	0.20	0.30	0.21	1.43	1.61	5.59	4.79
B-COF-2	42	B-COF-2 with AA stacking	2D	hcb	-	-	2051	0.57	21.8	0.21	0.29	0.22	1.46	1.60	5.67	4.80
BCTB-BCTA-COF	43	BCTB-BCTA COF	2D	sql	-	-	1936	0.62	15.8	0.19	0.31	0.16	1.34	1.63	5.57	4.88
BCTB-PD-COF	44	BCTB-PD COF	2D	sql	-	-	2291	0.48	22.8	0.23	0.24	0.23	1.74	1.77	5.87	4.98
BCzP-COF	45	BCzP-COF	2D	sql	-	-	1842	0.66	14.1	0.18	0.33	0.14	1.24	1.58	5.47	4.84
BDT-COF	46	BDT-COF	2D	hcb	-	-	1755	0.50	30.1	0.18	0.25	0.30	1.31	1.23	6.17	4.47
ICOF-2	261	ICOF-2	2D	fes	-	-	2383	0.54	17.2	0.24	0.27	0.17	1.74	1.97	5.55	5.13
BDT-OEt_COF	48	BDT-OEt-COF	2D	hcb	-	-	1788	0.60	23.7	0.18	0.30	0.24	1.25	1.36	5.74	4.58
BF-COF-1	49	BF-COF-1	3D	ctn	-	-	5219	0.44	8.4	0.52	0.22	0.08	4.08	4.78	3.73	6.92
BF-COF-2	50	BF-COF-2	3D	ctn	-	-	4330	0.52	8.5	0.43	0.26	0.08	3.20	3.96	4.19	6.39
BITA-PDA-COF-AA	51	BITA-PDA COF with AA packing	2D	htb	AA	-	2067	0.51	31.5	0.21	0.26	0.32	1.54	1.42	5.90	4.58
BITA-PDA-COF-AB	52	BITA-PDA COF with AB packing	2D	htb	AB	-	3541	0.54	10.2	0.35	0.27	0.10	2.58	3.18	4.71	5.92
BLP-2H	53	BLP-2(H)	2D	hcb	-	-	1115	0.90	9.5	0.11	0.45	0.10	0.61	1.01	4.87	4.37
BND-TFB	54	BND-TFP COF	2D	hcb	-	-	1778	0.58	22.8	0.18	0.29	0.23	1.27	1.37	5.85	4.63
Brick-wall-COF	55	brick-wall-COF	2D	sql	-	-	2786	0.54	16.1	0.28	0.27	0.16	2.04	2.34	5.28	5.37
BTA-COF1	56	BTA-COF1	2D	hcb	-	-	1431	0.78	16.2	0.14	0.39	0.16	0.87	1.20	5.22	4.45
BTA-COF2	57	BTA-COF2	2D	hcb	-	-	1904	0.42	35.4	0.19	0.21	0.35	1.50	1.23	6.39	4.47
BTA-COF3	58	BTA-COF3	2D	hcb	-	-	1915	0.44	32.9	0.19	0.22	0.33	1.49	1.28	6.29	4.53
BTA-COF4_AAI	59	BTA-COF4 AA_I	2D	hcb	-	-	937	1.04	9.0	0.09	0.52	0.09	0.45	0.85	4.34	4.16
BTA-COF4_AAII	60	BTA-COF4 AA_II	2D	hcb	-	-	917	1.05	9.0	0.09	0.52	0.09	0.44	0.83	4.33	4.14
BTMA-TAPA-COF	61	BTMA-TAPA-COF	2D	hcb	-	-	1461	0.79	11.3	0.15	0.40	0.11	0.88	1.30	5.16	4.60

BTP-COF	62	BTP-COF	2D	hcb	-	-	1928	0.42	34.6	0.19	0.21	0.35	1.52	1.26	6.38	4.51
BTT-DAB-COF	63	BTT-DAB-COF	2D	hcb	-	-	1823	0.59	22.5	0.18	0.29	0.23	1.29	1.41	5.77	4.65
BTT-DADP-COF	64	BTT-DADP-COF	2D	hcb	-	-	1936	0.48	29.5	0.19	0.24	0.30	1.47	1.36	6.13	4.60
BTT-TAB-CO	65	BTT-TAB-COF	2D	hcb	-	-	1511	0.75	14.9	0.15	0.38	0.15	0.94	1.29	5.29	4.56
BTT-TAPT-COF	66	BTT-TAPT-COF	2D	hcb	-	-	1650	0.70	15.7	0.16	0.35	0.16	1.07	1.39	5.41	4.65
BZL-COF	67	BZL-COF	2D	hcb	-	-	1872	0.43	35.0	0.19	0.21	0.35	1.47	1.22	6.39	4.46
C2N-h2D	68	C2N-h2D	2D	hcb	-	-	0	1.78	3.6	0.00	0.89	0.04	0.00	0.00	1.08	3.11
C4-SHz-COF	69	C4-SHz-COF	2D	hcb	-	-	2174	0.58	16.1	0.22	0.29	0.16	1.55	1.82	5.56	5.03
Car-ETTA-COF	70	Car-ETTA COF	2D	sql	-	-	1408	0.84	8.5	0.14	0.42	0.08	0.82	1.29	4.98	4.61
CCOF-1	71	CCOF-1	2D	sql	-	-	3984	0.53	9.6	0.40	0.26	0.10	2.93	3.60	4.43	6.18
CCOF-2	72	CCOF-2	2D	sql	-	-	8557	0.12	22.9	0.86	0.06	0.23	8.06	6.60	1.36	8.48
CCOF-3	73	CCOF 3	2D	hcb	-	-	1664	0.76	14.6	0.17	0.38	0.15	1.03	1.42	5.18	4.64
CCOF-4	74	CCOF 4	2D	hcb	-	-	851	1.01	12.1	0.09	0.50	0.12	0.42	0.75	4.54	4.05
CCOF-5	75	CCOF 5	3D	dia	-	-	1139	0.83	5.6	0.11	0.42	0.06	0.67	1.07	5.18	4.57
CCOF-6	76	CCOF 6	3D	dia	-	-	621	0.89	5.7	0.06	0.44	0.06	0.34	0.59	5.21	4.25
CCOF-CuTPP1	77	CCOF-CuTPP (1) with P1 mode	2D	sql	-	-	6631	0.25	17.8	0.66	0.12	0.18	5.81	5.45	2.95	7.54
CCOF-CuTPP2	78	CCOF-CuTPP (1) with P41 mode	2D	sql	-	-	1137	1.01	9.7	0.11	0.51	0.10	0.56	1.03	4.37	4.27
CCOF-MPC	79	CCOF-MPC	2D	hcb	-	-	0	0.87	5.4	0.00	0.43	0.05	0.00	0.00	5.67	3.97
CCOF-TpBD	80	CCOF-TpBD	2D	hcb	-	-	1937	0.53	23.7	0.19	0.27	0.24	1.42	1.48	5.91	4.72
CCOF-TpBD-Me2	81	CCOF-TpBD-Me2	2D	hcb	-	-	1671	0.60	21.9	0.17	0.30	0.22	1.17	1.31	5.83	4.58
CCOF-TpPa-1	82	CCOF-TpPa-1	2D	hcb	-	-	1610	0.72	14.8	0.16	0.36	0.15	1.03	1.37	5.37	4.64
CCOF-TpTab	83	CCOF-TpTab	2D	hcb	-	-	1402	0.83	11.4	0.14	0.42	0.11	0.82	1.24	5.02	4.53
CC-TAPH-COF	84	CC-TAPH-COF	2D	sql	-	-	4355	0.49	9.3	0.44	0.24	0.09	3.29	3.95	4.27	6.41
CF3-TFP-TAPB	85	CF3-TFP-TAPB	2D	hcb	-	-	2235	0.52	19.4	0.22	0.26	0.19	1.65	1.80	5.74	5.01
CF3-TFP-TTA	86	CF3-TFP-TTA	2D	hcb	-	-	1897	0.59	19.0	0.19	0.29	0.19	1.34	1.54	5.72	4.79
COF-1	87	COF-1	2D	hcb	-	-	0	0.91	4.2	0.00	0.45	0.04	0.00	0.00	5.45	3.97
COF-10	88	COF-10	2D	hcb	-	-	1949	0.45	31.5	0.19	0.22	0.32	1.51	1.33	6.25	4.58
COF-102	89	COF-102	3D	ctn	-	-	5129	0.42	9.0	0.51	0.21	0.09	4.05	4.66	3.85	6.87

COF-103	90	COF-103	3D	ctn	-	-	5315	0.39	9.7	0.53	0.19	0.10	4.28	4.80	3.77	6.98
COF-105	91	COF-105	3D	ctn	-	-	6645	0.18	18.8	0.66	0.09	0.19	6.06	5.40	3.06	7.58
COF-108	92	COF-108	3D	bor	-	-	6387	0.17	27.5	0.64	0.09	0.27	5.84	4.63	3.31	7.20
COF-112	93	COF-112	3D	dia	-	-	0	1.42	3.6	0.00	0.71	0.04	0.00	0.00	2.92	3.48
CoTAPP-BDTA-COF-AA	730	AA-COF for CoTAPP-BDTA-COF	2D	fes	-	-	1488	0.77	15.9	0.15	0.39	0.16	0.91	1.25	5.22	4.50
COF-11A	95	COF-11Å	2D	hcb	-	-	515	0.88	8.4	0.05	0.44	0.08	0.29	0.47	5.31	4.13
COF-1-2	96	COF-1	2D	hcb	-	-	2653	0.30	37.7	0.27	0.15	0.38	2.25	1.65	6.23	4.89
COF-120	97	COF-120, Pawley refined	2D	hcb	-	-	2252	0.43	27.7	0.23	0.21	0.28	1.77	1.63	6.08	4.87
COF-121	98	COF-121, Pawley refined	2D	hcb	-	-	2459	0.35	34.6	0.25	0.17	0.35	2.03	1.61	6.22	4.84
COF-122	99	COF-122, modeled against WAXS	2D	hcb	-	-	2374	0.26	55.5	0.24	0.13	0.55	2.06	1.06	6.62	4.26
COF-14A	100	COF-14Å	2D	hcb	-	-	1355	0.79	10.5	0.14	0.40	0.11	0.82	1.21	5.22	4.57
COF-16A	101	COF-16Å	2D	hcb	-	-	1936	0.74	12.7	0.19	0.37	0.13	1.22	1.69	5.09	4.85
COF-18A	102	COF-18Å	2D	hcb	-	-	1705	0.74	14.7	0.17	0.37	0.15	1.08	1.45	5.24	4.67
COF-2	103	COF-2	3D	pts	-	-	7633	0.18	34.6	0.76	0.09	0.35	6.96	4.99	2.16	7.60
COF-202	104	COF-202	3D	ctn	-	-	4240	0.52	9.9	0.42	0.26	0.10	3.13	3.82	4.26	6.30
COF-300_dia-c5	105	dia-c5 COF-300	3D	dia	-	-	3301	0.55	9.4	0.33	0.27	0.09	2.40	2.99	4.87	5.82
COF-300_dia-c7	106	dia-c7 COF-300	3D	dia	-	-	426	1.04	4.5	0.04	0.52	0.05	0.20	0.41	4.59	4.04
COF-300-SC_dia-c7	107	single crstal COF-300	3D	dia	-	-	1888	0.74	9.0	0.19	0.37	0.09	1.19	1.72	5.13	4.94
COF-300-SC-hydrated_dia-c7	108	single crstal COF-300-hydrated	3D	dia	-	-	280	1.12	4.3	0.03	0.56	0.04	0.12	0.27	4.30	3.90
COF-316	109	COF-316	2D	hcb	-	-	1137	1.14	13.0	0.11	0.57	0.13	0.49	0.99	3.81	4.04
COF-318	110	COF-318	2D	hcb	-	-	1020	1.14	13.0	0.10	0.57	0.13	0.44	0.89	3.85	3.98
COF-320-298K	111	COF-320	3D	dia	-	-	1816	0.70	8.5	0.18	0.35	0.08	1.18	1.66	5.31	4.95
COF-366	112	COF-366	2D	sql	-	-	4020	0.36	20.5	0.40	0.18	0.20	3.29	3.20	4.90	6.03
COF-366-Co	113	COF-366-Co	2D	sql	-	-	2260	0.50	20.8	0.23	0.25	0.21	1.70	1.79	5.82	5.01

COF-366-F4-Co	114	COF-366-(F)4-Co	2D	sql	-	-	1885	0.61	18.7	0.19	0.30	0.19	1.31	1.53	5.65	4.77
COF-366-F-Co	115	COF-366-F-Co	2D	sql	-	-	2142	0.55	19.0	0.21	0.27	0.19	1.55	1.73	5.71	4.95
COF-366-OMe2-Co	116	COF-366-(OMe)2-Co	2D	sql	-	-	2354	0.55	18.2	0.24	0.27	0.18	1.71	1.93	5.55	5.08
COF-367-Co	117	COF-367-Co	2D	sql	-	-	3449	0.43	19.7	0.34	0.21	0.20	2.71	2.77	5.15	5.70
COF-3BD	118	COF 3BD	2D	hcb	-	-	2243	0.41	31.0	0.22	0.21	0.31	1.78	1.55	6.16	4.78
COF-3PD	119	COF 3PD	2D	hcb	-	-	2038	0.51	23.4	0.20	0.25	0.23	1.52	1.56	5.94	4.81
COF-42	120	COF-42	2D	hcb	-	-	2647	0.56	17.2	0.26	0.28	0.17	1.91	2.19	5.29	5.25
COF-43	121	COF-43	2D	hcb	-	-	2603	0.35	32.5	0.26	0.17	0.32	2.15	1.76	6.11	4.98
COF-432	122	COF-432	2D	hcb	-	-	1209	0.90	6.0	0.12	0.45	0.06	0.67	1.14	4.84	4.53
COF-5	123	COF-5	2D	hcb	-	-	1707	0.58	23.7	0.17	0.29	0.24	1.21	1.30	5.87	4.56
COF-505	124	COF-505	3D	dia	-	-	0	1.44	3.7	0.00	0.72	0.04	0.00	0.00	2.82	3.45
COF-506-Cu	125	COF-506-Cu	3D	dia	-	-	6156	0.36	12.6	0.62	0.18	0.13	5.06	5.38	3.16	7.34
COF-6	126	COF-6	2D	hcb	-	-	1128	1.00	9.2	0.11	0.50	0.09	0.57	1.03	4.45	4.29
COF-66	127	COF-66	2D	sql	-	-	4453	0.28	27.0	0.45	0.14	0.27	3.83	3.25	4.77	6.13
COF-8	128	COF-8	2D	sql	-	-	1601	0.70	16.5	0.16	0.35	0.17	1.04	1.34	5.47	4.61
COF-921	129	COF-921	2D	sql	-	-	1617	0.73	17.6	0.16	0.36	0.18	1.03	1.33	5.34	4.55
CoTAPP-BDTA-COF-AB	731	AB-COF for CoTAPP-BDTA-COF	2D	fes	-	-	928	0.87	5.5	0.09	0.44	0.05	0.52	0.88	5.12	4.43
COF-AO	131	COF-AO	2D	hcb	-	-	2153	0.60	18.3	0.22	0.30	0.18	1.50	1.76	5.48	4.92
COF-ASB	132	COF-ASB	2D	hcb	-	-	2609	0.41	25.5	0.26	0.20	0.25	2.08	1.94	5.88	5.13
COF-BABD-BZ	133	COF-BABD-BZ	2D	hcb	-	-	5124	0.46	12.5	0.51	0.23	0.13	3.94	4.48	3.75	6.73
COF-BABD-DB	134	COF-BABD-DB	2D	hcb	-	-	3856	0.54	11.6	0.39	0.27	0.12	2.81	3.41	4.48	6.04
CoTAPP-PATA-COF-AB	732	AB-COF for CoTAPP-PATA-COF	2D	fes	-	-	933	0.92	5.3	0.09	0.46	0.05	0.50	0.88	4.89	4.39
mcm-CdPc-3N	820	mcm-CdPc-3N	2D	fes	-	-	2848	0.29	22.4	0.28	0.15	0.22	2.43	2.21	6.10	5.46
COF-BTA-PDA	137	COFBTA-PDA	2D	hcb	-	-	2403	0.52	17.1	0.24	0.26	0.17	1.78	1.99	5.62	5.17
COF-C	138	COF-C	2D	hcb	-	-	3463	0.33	25.3	0.35	0.17	0.25	2.88	2.59	5.44	5.64
COF-DL229	139	COF-DL229	3D	dia	-	-	2303	0.62	11.1	0.23	0.31	0.11	1.59	2.05	5.30	5.20

COF-DL229_2	140	COF-DL229 2-fold interpenetrated	3D	dia	-	2	8393	0.16	17.6	0.84	0.08	0.18	7.74	6.92	1.48	8.51
COF-DL229_3	141	COF-DL229 3-fold interpenetrated	3D	dia	-	3	8475	0.24	10.7	0.85	0.12	0.11	7.47	7.57	1.34	8.68
COF-DL229_5	142	COF-DL229 5-fold interpenetrated	3D	dia	-	5	6762	0.37	11.3	0.68	0.19	0.11	5.49	6.00	2.63	7.67
COF-DL229_6	143	COF-DL229 6-fold interpenetrated	3D	dia	-	6	3560	0.47	10.2	0.36	0.23	0.10	2.73	3.20	4.94	6.01
COF-DL229_7	144	COF-DL229 7-fold interpenetrated	3D	dia	-	7	2581	0.58	10.2	0.26	0.29	0.10	1.84	2.32	5.28	5.41
COF-DL229_non	145	COF-DL229 non-interpenetrated	3D	dia	-	1	8535	0.08	31.9	0.85	0.04	0.32	8.20	5.82	1.41	8.23
COF-ETTA-ETTCA-AA	146	COF-ETTA-ETTCA	2D	sql	-	-	2615	0.51	14.9	0.26	0.26	0.15	1.94	2.23	5.49	5.35
COF-F	147	COF-F	2D	hcb	-	-	1680	0.56	27.1	0.17	0.28	0.27	1.21	1.22	6.00	4.47
COF-F6	148	COF-F6	2D	hcb	-	-	797	1.09	10.6	0.08	0.54	0.11	0.36	0.71	4.21	4.00
TP-COF-BZ	536	TP-COF-BZ	2D	fxt	-	-	1945	0.44	36.6	0.19	0.22	0.37	1.52	1.23	6.29	4.44
COF-HQ	150	COF-HQ	2D	hcb	-	-	1693	0.78	17.2	0.17	0.39	0.17	1.04	1.40	5.08	4.55
COF-JLU2	151	COF-JLU2	2D	hcb	-	-	1307	0.94	10.2	0.13	0.47	0.10	0.69	1.17	4.60	4.41
COF-JLU3	152	COF-JLU3	2D	hcb	-	-	2771	0.54	14.6	0.28	0.27	0.15	2.02	2.37	5.28	5.41
COF-JLU4	153	COF-JLU4	2D	hcb	-	-	1679	0.62	21.6	0.17	0.31	0.22	1.15	1.32	5.72	4.57
COF-K	154	COF-K	2D	sql	-	-	605	1.00	9.5	0.06	0.50	0.10	0.30	0.55	4.71	4.02
COF-LZU1	155	COF-LZU1	2D	hcb	-	-	2212	0.57	16.0	0.22	0.29	0.16	1.58	1.86	5.56	5.05
COF-LZU8	156	COF-LZU8	2D	hcb	-	-	498	0.92	9.0	0.05	0.46	0.09	0.27	0.45	5.13	4.06
COF-m-3Ph	157	COF-m-3Ph	2D	hcb	-	-	1501	0.78	11.2	0.15	0.39	0.11	0.92	1.33	5.18	4.64
COF-Me-AA	158	COF-Me AA stacking mode	2D	hcb	-	-	2543	0.32	35.7	0.25	0.16	0.36	2.14	1.63	6.27	4.88

COF-Naph	159	COF-Naph	2D	hcb	-	-	1879	0.73	11.7	0.19	0.37	0.12	1.19	1.66	5.14	4.85
COF-NHC	160	COF-NHC	2D	hcb	-	-	931	0.89	17.4	0.09	0.45	0.17	0.51	0.77	5.01	4.05
COF-NUST-1	161	COF-NUST-1	2D	hcb	-	-	6043	0.29	23.9	0.60	0.14	0.24	5.17	4.60	3.38	7.02
COF-O	162	COF-O	2D	hcb	-	-	3939	0.30	25.8	0.39	0.15	0.26	3.35	2.92	5.15	5.90
COF-p-2Ph	163	COF-p-2Ph	2D	hcb	-	-	1836	0.53	24.1	0.18	0.26	0.24	1.35	1.39	6.01	4.67
COF-p-3Ph	164	COF-p-3Ph	2D	hcb	-	-	1982	0.42	32.2	0.20	0.21	0.32	1.57	1.34	6.33	4.60
COF-QA-AA	165	COF-QA AA stacking mode	2D	hcb	-	-	4053	0.34	17.7	0.41	0.17	0.18	3.37	3.34	4.95	6.16
COFs	166	COFs	2D	hcb	-	-	2431	0.33	38.2	0.24	0.17	0.38	2.03	1.50	6.31	4.74
COF-SDU1	167	COF-SDU1	2D	hcb	-	-	2577	0.31	38.9	0.26	0.16	0.39	2.17	1.57	6.26	4.81
COF-Tirf-Benz	168	COF-Tirf-Benz	2D	hcb	-	-	3115	0.28	37.7	0.31	0.14	0.38	2.68	1.94	5.91	5.15
COF-TpAab	169	COF-TpAab	2D	hcb	-	-	2088	0.47	26.5	0.21	0.24	0.27	1.59	1.53	6.04	4.77
COF-TpAzo	170	COF-TpAzo	2D	hcb	-	-	2081	0.50	26.1	0.21	0.25	0.26	1.56	1.54	5.95	4.76
TP-COF-DAB	537	TP-COF-DAB	2D	fxt	-	-	1584	0.58	28.0	0.16	0.29	0.28	1.12	1.14	5.97	4.37
COF-TpDb	172	COF-TpDb	2D	hcb	-	-	1704	0.73	13.0	0.17	0.37	0.13	1.08	1.48	5.26	4.73
COF-TpTU	173	COF-TpTU	2D	hcb	-	-	2136	0.54	19.2	0.21	0.27	0.19	1.56	1.73	5.74	4.95
COF-TpU	174	COF-TpU	2D	hcb	-	-	2185	0.44	27.2	0.22	0.22	0.27	1.70	1.59	6.09	4.83
COF-TVBT-PA-AA	175	COF-TVBT-PA calculated based on staggered AA model	2D	hcb	-	-	2624	0.31	39.1	0.26	0.16	0.39	2.21	1.60	6.23	4.83
COF-V	176	COF-V	2D	hcb	-	-	2390	0.43	26.2	0.24	0.21	0.26	1.88	1.76	5.98	4.98
CoPc-PorDBA-COF	177	CoPc-PorDBA	2D	sql	-	-	4128	0.31	25.5	0.41	0.15	0.26	3.49	3.07	4.96	5.99
CorMeO-COF	178	CorMeO-COF	2D	sql	-	-	2268	0.45	21.5	0.23	0.23	0.21	1.75	1.78	5.97	5.03
CPF-1	179	CPF-1	2D	sql	-	-	5087	0.29	24.0	0.51	0.14	0.24	4.35	3.87	4.20	6.54
CPF-2	180	CPF-2	2D	sql	-	-	5177	0.30	22.5	0.52	0.15	0.23	4.39	4.01	4.09	6.61
CS-COF	181	CS-COF	2D	hcb	-	-	1070	0.84	11.6	0.11	0.42	0.12	0.62	0.95	5.17	4.35
CTC-COF	182	CTC-COF	2D	hcb	-	-	1513	0.72	18.8	0.15	0.36	0.19	0.97	1.23	5.43	4.47
CTF-0	183	CTF-0	2D	hcb	-	-	0	1.67	2.6	0.00	0.83	0.03	0.00	0.00	1.65	3.25
CTF-1	184	CTF-1	2D	hcb	-	-	1004	1.02	8.9	0.10	0.51	0.09	0.49	0.91	4.41	4.21
CTF-2-AA	185	CTF-2-AA	2D	hcb	AA	-	1251	0.91	11.0	0.13	0.45	0.11	0.69	1.11	4.79	4.39

CTF-2-AB	186	CTF-2-AB	2D	hcb	AB	-	0	0.91	4.8	0.00	0.45	0.05	0.00	0.00	5.48	3.95
CTF-fuma	187	CTF-FUM	2D	hcb	-	-	1045	1.03	6.7	0.10	0.52	0.07	0.51	0.97	4.33	4.29
CTF-NDC	188	CTF-DCN	2D	hcb	-	-	0	1.33	4.3	0.00	0.67	0.04	0.00	0.00	3.33	3.54
CuP-2-3-DHPh-COF	189	CuP-2,3-DHPh COF	2D	sql	-	-	2088	0.54	18.8	0.21	0.27	0.19	1.52	1.69	5.78	4.94
CuP-BPyPh-COF	190	CuP-BPyPh COF	2D	sql	-	-	2506	0.41	25.1	0.25	0.21	0.25	1.99	1.88	5.96	5.09
CuP-COF	191	CuP-COF	2D	sql	-	-	1619	0.67	18.7	0.16	0.33	0.19	1.08	1.32	5.58	4.58
CuP-DHNAPh-COF	192	CuP-DHNAPh COF	2D	sql	-	-	2154	0.50	21.6	0.22	0.25	0.22	1.61	1.69	5.87	4.93
CuP-Ph-COF	193	CuP-Ph COF	2D	sql	-	-	1826	0.60	19.5	0.18	0.30	0.19	1.27	1.47	5.70	4.72
CuP-PyTTPh-COF	194	CuP-PyTTPh COF	2D	sql	-	-	1646	0.71	14.1	0.16	0.35	0.14	1.06	1.41	5.40	4.69
CuP-SQ_COF	195	CuP-SQ COF	2D	sql	-	-	3240	0.52	12.9	0.32	0.26	0.13	2.40	2.82	5.01	5.71
CuP-TFPh50-COF	196	CuP-TFPh50	2D	sql	-	-	1640	0.68	17.7	0.16	0.34	0.18	1.08	1.35	5.51	4.61
CuP-TFPh-COF	197	CuP-TFPh COF	2D	sql	-	-	1690	0.70	17.0	0.17	0.35	0.17	1.10	1.40	5.42	4.64
DAAQ-TFP-COF	198	DAAQ-TFP COF	2D	hcb	-	-	1739	0.61	22.3	0.17	0.31	0.22	1.21	1.35	5.74	4.59
DABQ-TFP-COF	199	DABQ-TFP-COF	2D	hcb	-	-	1492	0.79	15.2	0.15	0.39	0.15	0.90	1.27	5.15	4.50
DAB-TFP_COF	200	DAQ-TFP COF	2D	hcb	-	-	1643	0.71	16.1	0.16	0.35	0.16	1.06	1.38	5.41	4.63
D-A-COF	201	DA-COF	2D	hcb	-	-	1646	0.66	19.4	0.16	0.33	0.19	1.11	1.33	5.62	4.59
DaTp-COF	202	DaTP	2D	hcb	-	-	875	1.11	21.9	0.09	0.56	0.22	0.39	0.68	4.04	3.67
DBA-3D-COF	203	DBA-3D-COF 1	3D	bor	-	-	6945	0.13	30.8	0.69	0.07	0.31	6.48	4.80	2.85	7.41
DBA-COF_1	204	DBA-COF 1	2D	hcb	-	-	1965	0.48	29.4	0.20	0.24	0.29	1.50	1.39	6.11	4.62
DBA-COF_2	205	DBA-COF 2	2D	hcb	-	-	2127	0.40	34.4	0.21	0.20	0.34	1.70	1.40	6.30	4.63
DCuPc-ANDI-COF	206	DCuPc-ANDI-COF	2D	sql	-	-	1595	0.56	27.4	0.16	0.28	0.27	1.15	1.16	6.04	4.41
DCuPc-APDI-COF	207	DCuPc-APDI-COF	2D	sql	-	-	1591	0.52	32.0	0.16	0.26	0.32	1.18	1.08	6.22	4.32
DCuPc-APyrDI-COF	208	DCuPc-APyrDI-COF	2D	sql	-	-	1629	0.55	28.6	0.16	0.27	0.29	1.18	1.16	6.08	4.41
DhaTab	209	DhaTab	2D	hcb	-	-	1944	0.47	30.5	0.19	0.24	0.30	1.49	1.35	6.16	4.59
DhaTab-23	210	2,3-DhaTab	2D	hcb	-	-	997	0.85	28.5	0.10	0.42	0.29	0.58	0.71	5.19	3.80
DhaTab-25	211	2,5-DhaTab	2D	hcb	-	-	2212	0.42	29.6	0.22	0.21	0.30	1.75	1.56	6.16	4.80
DhaTph	212	DhaTph	2D	sql	-	-	1812	0.59	19.1	0.18	0.30	0.19	1.28	1.47	5.76	4.74

DhaTph-23	213	2,3-DhaTph	2D	sql	-	-	1771	0.64	17.7	0.18	0.32	0.18	1.20	1.46	5.59	4.71
DhaTph-25	214	2,5-DhaTph	2D	sql	-	-	4382	0.35	18.5	0.44	0.18	0.18	3.61	3.57	4.63	6.29
DhaTta-23	215	2,3-DhaTta	2D	hcb	-	-	937	0.87	28.9	0.09	0.43	0.29	0.53	0.67	5.13	3.73
DL-COF-1	216	DL-COF-1	3D	ctn	-	-	7239	0.19	16.1	0.72	0.10	0.16	6.55	6.07	2.50	7.95
DL-COF-2	217	DL-COF-2	3D	ctn	-	-	6602	0.21	16.1	0.66	0.11	0.16	5.90	5.54	3.04	7.61
DmaTph	218	DmaTph	2D	sql	-	-	2337	0.55	15.2	0.23	0.27	0.15	1.70	1.98	5.57	5.17
DmaTph-23	219	2,3-DmaTph	2D	sql	-	-	1842	0.65	16.5	0.18	0.32	0.17	1.25	1.54	5.52	4.78
DMTA-TPB1_2prime	220	DMTA-TPB1/2'	2D	hcb	-	-	1972	0.49	25.6	0.20	0.25	0.26	1.49	1.47	6.05	4.72
DMTA-TPB1_3prime	221	DMTA-TPB1/3'	2D	hcb	-	-	1920	0.51	24.5	0.19	0.26	0.25	1.43	1.45	6.02	4.71
DMTA-TPB1_4prime	222	DMTA-TPB1/4'	2D	hcb	-	-	1886	0.52	23.3	0.19	0.26	0.23	1.40	1.45	6.02	4.73
DMTA-TPB1_5prime	223	DMTA-TPB1/5'	2D	hcb	-	-	1841	0.52	24.1	0.18	0.26	0.24	1.36	1.40	6.04	4.68
DMTA-TPB2	224	DMTA-TPB2	2D	hcb	-	-	1449	0.62	20.9	0.14	0.31	0.21	1.00	1.15	5.92	4.48
DMTA-TPB3	225	DMTA-TPB3	2D	hcb	-	-	1470	0.63	19.4	0.15	0.32	0.19	1.01	1.19	5.83	4.52
DMTA-TPB4	226	DMTA-TPB4	2D	hcb	-	-	632	1.05	5.6	0.06	0.52	0.06	0.30	0.60	4.45	4.10
DNiPc-ANDI-COF	227	DNiPc-ANDI-COF	2D	sql	-	-	1599	0.56	27.4	0.16	0.28	0.27	1.15	1.16	6.05	4.42
DNiPc-APDI-COF	228	DNiPc-APDI-COF	2D	sql	-	-	1568	0.52	32.0	0.16	0.26	0.32	1.16	1.07	6.24	4.31
DNiPc-APyrDI-COF	229	DNiPc-APyrDI-COF	2D	sql	-	-	1634	0.55	28.6	0.16	0.27	0.29	1.19	1.17	6.09	4.41
HAT-COF	250	HAT-COF	2D	hxl	-	-	1734	0.75	9.9	0.17	0.37	0.10	1.09	1.56	5.18	4.82
DPP-TAPP-COF	231	DPP-TAPP-COF	2D	sql	-	-	1362	0.70	18.6	0.14	0.35	0.19	0.89	1.11	5.61	4.42
DPP-TFP	232	DPP-TFP-Eclipsed	2D	hcb	-	-	1510	0.72	17.5	0.15	0.36	0.18	0.97	1.25	5.44	4.51
DTP-ANDI-COF	233	DTP-ANDI-COF	2D	hcb	-	-	1842	0.38	43.9	0.18	0.19	0.44	1.50	1.03	6.62	4.23
DTP-APyrDI-COF	234	DTP-APyrDI-COF	2D	hcb	-	-	1888	0.36	44.6	0.19	0.18	0.45	1.54	1.05	6.64	4.24
EB-COF-Br	235	EB-COF:Br	2D	hcb	-	-	1336	0.93	10.6	0.13	0.47	0.11	0.71	1.20	4.62	4.42
EB-COF-Cl	236	EB-COF:Cl	2D	hcb	-	-	1490	0.85	10.6	0.15	0.42	0.11	0.86	1.33	4.89	4.58

EB-COF-F	237	EB-COF:F	2D	hcb	-	-	1594	0.82	10.6	0.16	0.41	0.11	0.94	1.43	4.96	4.66
EB-COF-I	238	EB-COF:I	2D	hcb	-	-	1195	1.02	10.6	0.12	0.51	0.11	0.58	1.07	4.31	4.26
EDTFP-1	239	EDTFP-1	2D	hcb	-	-	2556	0.39	27.4	0.26	0.20	0.27	2.06	1.86	5.99	5.07
HAT-NTBCA-COF	252	HAT-NTBCA-COF	2D	hxl	-	-	1692	0.75	11.4	0.17	0.37	0.11	1.06	1.50	5.20	4.76
HBC-COF	253	HBC-COF	2D	hxl	-	-	1515	0.81	11.0	0.15	0.41	0.11	0.90	1.35	5.04	4.61
F-COF	242	F-COF	2D	hcb	-	-	1128	0.89	17.2	0.11	0.45	0.17	0.62	0.93	4.91	4.15
FL-COF-1	243	FL-COF-1	2D	hcb	-	-	2091	0.55	19.5	0.21	0.27	0.19	1.52	1.68	5.74	4.91
FLT-COF-1	244	FLT-COF 1 – Eclipsed	2D	hcb	-	-	2025	0.45	24.8	0.20	0.23	0.25	1.57	1.52	6.17	4.82
GS-COF-1-AA	245	GS-COF-1	2D	hcb	AA	-	1160	0.91	12.1	0.12	0.45	0.12	0.63	1.02	4.84	4.31
GS-COF-1-AB	246	GS-COF-1	2D	hcb	AB	-	0	1.00	4.1	0.00	0.50	0.04	0.00	0.00	5.01	3.88
GS-COF-2-AA	247	GS-COF-2	2D	hcb	AA	-	1229	0.89	12.3	0.12	0.45	0.12	0.68	1.08	4.85	4.35
GS-COF-2-AB	248	GS-COF-2	2D	hcb	AB	-	0	0.98	4.5	0.00	0.49	0.04	0.00	0.00	5.11	3.89
H2P-COF	249	H2P-COF	2D	sql	-	-	4417	0.33	20.3	0.44	0.16	0.20	3.69	3.52	4.67	6.27
HPB-COF	257	HPB-COF	2D	hxl	-	-	2071	0.73	7.1	0.21	0.37	0.07	1.31	1.92	5.02	5.09
HAT-NTBA-COF	251	HAT-NTBA-COF	2D	kgd	-	-	1195	0.93	7.9	0.12	0.47	0.08	0.64	1.10	4.70	4.43
V-2D-COF-4_AA	757	V-2D-COF-4_slipAA	2D	hxl	-	-	1556	0.71	16.3	0.16	0.36	0.16	1.00	1.30	5.43	4.58
4PE-1P	22	4PE-1P	2D	kgm	-	-	2344	0.52	24.3	0.23	0.26	0.24	1.73	1.77	5.66	4.92
HCC-H2P-COF	254	HCC-H2P-COF	2D	sql	-	-	4134	0.39	15.7	0.41	0.19	0.16	3.33	3.49	4.73	6.21
HHTP-DPB-COF	255	HHTP-DPB COF	2D	hcb	-	-	2277	0.34	41.2	0.23	0.17	0.41	1.89	1.34	6.42	4.57
HO2C-H2P-COFs	256	HO2C-H2P-COF	2D	sql	-	-	4927	0.42	10.9	0.49	0.21	0.11	3.90	4.39	4.02	6.72
4PE-1P-COF	23	4PE-1P-COF	2D	kgm	-	-	3221	0.39	25.3	0.32	0.20	0.25	2.59	2.41	5.46	5.46
HP-COF-1	258	HP-COF-1	2D	hcb	-	-	2003	0.63	14.8	0.20	0.32	0.15	1.37	1.71	5.46	4.92
HP-COF-2	259	HP-COF-2	2D	hcb	-	-	2429	0.53	17.2	0.24	0.27	0.17	1.78	2.01	5.55	5.17
4PE-1P-COF-oxidation	24	4PE-1P-oxi	2D	kgm	-	-	2721	0.45	25.0	0.27	0.23	0.25	2.10	2.04	5.62	5.16
4PE-2P	25	4PE-2P	2D	kgm	-	-	2458	0.44	32.3	0.25	0.22	0.32	1.92	1.66	5.89	4.82
IISERP-COF3	262	IISERP-COF3	2D	hcb	-	-	7075	0.22	22.2	0.71	0.11	0.22	6.31	5.51	2.61	7.66
IISERP-CON1	263	IISERP-CON1	2D	hcb	-	-	1760	0.79	9.8	0.18	0.39	0.10	1.07	1.59	4.99	4.80
ILCOF-1	264	ILCOF-1	2D	sql	-	-	3865	0.32	21.2	0.39	0.16	0.21	3.24	3.05	5.14	5.97

ILCOF-1b	265	ILCOF-1	2D	sql	-	-	1693	0.69	16.5	0.17	0.34	0.17	1.11	1.41	5.45	4.66
IMDEA-2	266	IMDEA-COF-2	2D	hcb	-	-	1739	0.66	18.5	0.17	0.33	0.18	1.17	1.42	5.55	4.66
Intercalated-COF-5	267	Intercalated-COF 5 with AA stacking	2D	sql	-	-	1407	0.77	8.0	0.14	0.39	0.08	0.86	1.29	5.28	4.69
iPrTAPB-TFP	268	iPrTAPB-TFP	2D	hcb	-	-	712	0.98	7.5	0.07	0.49	0.07	0.36	0.66	4.74	4.15
iPrTAPB-TFPB	269	iPrTAPB-TFPB	2D	hcb	-	-	1738	0.61	15.9	0.17	0.31	0.16	1.21	1.46	5.73	4.78
JNU-1	270	JNU-1	2D	hcb	-	-	2370	0.34	35.9	0.24	0.17	0.36	1.97	1.52	6.34	4.77
JUC-511-1	271	JUC-511 based on P4 space group	2D	sql	-	-	1929	0.51	26.4	0.19	0.26	0.26	1.44	1.42	6.01	4.66
JUC-512-1	272	JUC-512 based on P4 space group	2D	sql	-	-	1956	0.51	26.2	0.20	0.26	0.26	1.45	1.44	5.98	4.68
JUC-527	273	JUC-527	2D	hcb	-	-	2274	0.42	25.6	0.23	0.21	0.26	1.79	1.69	6.09	4.94
JUC-528	274	JUC-528	2D	hcb	-	-	2574	0.33	33.0	0.26	0.17	0.33	2.15	1.72	6.19	4.96
JUC-530	275	JUC-530	3D	dia	-	-	829	0.95	9.6	0.08	0.47	0.10	0.44	0.75	4.82	4.18
JUC-531	276	JUC-531	3D	dia	-	-	1038	0.87	13.2	0.10	0.43	0.13	0.59	0.90	5.07	4.25
JUC-550-2-fold	277	JUC-550 2-fold interpenetrated	3D	dia	-	2	8331	0.22	12.5	0.83	0.11	0.12	7.41	7.29	1.48	8.57
JUC-550-3-fold	278	JUC-550 3-fold interpenetrated	3D	dia	-	3	8105	0.33	10.4	0.81	0.16	0.10	6.78	7.26	1.59	8.41
JUC-550-non	279	JUC-550 non-interpenetrated	3D	dia	-	1	8662	0.10	29.0	0.87	0.05	0.29	8.25	6.15	1.27	8.36
JUC-551-2-fold	280	JUC-551 2-fold interpenetrated	3D	dia	-	2	8232	0.23	12.0	0.82	0.12	0.12	7.28	7.24	1.56	8.52
JUC-551-3-fold	281	JUC-551 3-fold interpenetrated	3D	dia	-	3	8190	0.34	10.7	0.82	0.17	0.11	6.81	7.32	1.51	8.44
JUC-551-non	282	JUC-551 non-interpenetrated	3D	dia	-	1	8766	0.10	28.3	0.88	0.05	0.28	8.32	6.29	1.17	8.43
JUC-552-3-fold	283	JUC-552 3-fold interpenetrated	3D	dia	-	3	7571	0.36	9.8	0.76	0.18	0.10	6.19	6.83	1.99	8.13
JUC-552-non	284	JUC-552 non-interpenetrated	3D	dia	-	1	8235	0.11	28.5	0.82	0.05	0.29	7.79	5.89	1.67	8.15

JUC-560-1	285	JUC-560 calculated based on the eclipsed sql net	2D	sql	-	-	2042	0.46	27.0	0.20	0.23	0.27	1.57	1.49	6.12	4.75
JUC-560-2	286	JUC-560 calculated based on the staggered sql net	2D	sql	-	-	3225	0.52	13.4	0.32	0.26	0.13	2.39	2.79	5.03	5.69
JUC-561-1	287	JUC-561 calculated based on ffc net	3D	ffc	-	-	3348	0.38	23.3	0.33	0.19	0.23	2.71	2.57	5.39	5.60
JUC-561-3	288	JUC-561 calculated based on fjh net	3D	fjh	-	-	7688	0.13	27.2	0.77	0.06	0.27	7.19	5.59	2.16	7.90
JUC-564	289	JUC-564	3D	stp	-	-	7433	0.11	47.7	0.74	0.05	0.48	7.03	3.89	2.43	7.18
LZU-111	290	LZU111	3D	dia	-	-	2895	0.62	8.7	0.29	0.31	0.09	2.00	2.64	4.90	5.57
LZU-190	291	LZU-190	2D	hcb	-	-	1586	0.80	14.0	0.16	0.40	0.14	0.95	1.36	5.05	4.57
LZU-191	292	LZU-191	2D	hcb	-	-	1860	0.50	28.1	0.19	0.25	0.28	1.39	1.34	6.09	4.58
LZU-192	293	LZU-192	2D	sql	-	-	1579	0.74	16.9	0.16	0.37	0.17	1.00	1.31	5.31	4.54
LZU-301-activated	294	LZU-301	3D	dia	-	-	0	0.99	4.7	0.00	0.50	0.05	0.00	0.00	5.03	3.87
LZU-301-solvated	295	LZU-301-sol	3D	dia	-	-	1686	0.73	8.3	0.17	0.37	0.08	1.07	1.55	5.28	4.86
LZU-70	296	LZU-70	2D	hcb	-	-	2183	0.43	26.1	0.22	0.21	0.26	1.72	1.61	6.14	4.88
LZU-72	297	LZU-72	2D	hcb	-	-	2429	0.46	20.9	0.24	0.23	0.21	1.87	1.92	5.83	5.13
LZU-76	298	LZU-76	2D	hcb	-	-	2787	0.39	22.3	0.28	0.19	0.22	2.25	2.17	5.81	5.34
LZU-79	299	LZU79	3D	dia	-	-	2485	0.59	13.6	0.25	0.30	0.14	1.75	2.15	5.28	5.24
MC-COF-NiPc-E1E7	300	MC-COF-NiPc-E1E7	2D	sql	-	-	1462	0.76	15.1	0.15	0.38	0.15	0.91	1.24	5.29	4.52
MC-COF-TP-E11E22	301	MC-COF-TP-E11E22	2D	hcb	-	-	1730	0.61	20.2	0.17	0.30	0.20	1.21	1.38	5.76	4.65

MC-COF-TP-E11E71	302	MC-COF-TP-E11E71	2D	hcb	-	-	1824	0.54	25.2	0.18	0.27	0.25	1.34	1.36	5.98	4.62
MC-COF-TP-E11E72	303	MC-COF-TP-E11E72	2D	hcb	-	-	1884	0.52	24.9	0.19	0.26	0.25	1.40	1.41	6.02	4.68
MC-COF-TP-E12E21	304	MC-COF-TP-E12E21	2D	hcb	-	-	1674	0.63	20.0	0.17	0.31	0.20	1.15	1.34	5.72	4.61
MC-COF-TP-E12E71	305	MC-COF-TP-E12E71	2D	hcb	-	-	1769	0.55	22.0	0.18	0.27	0.22	1.29	1.38	5.99	4.68
MC-COF-TP-E1E3E7	306	MC-COF-TP-E1E3E7	2D	hcb	-	-	1808	0.54	22.7	0.18	0.27	0.23	1.32	1.40	5.99	4.68
MC-COF-TP-E22E31	307	MC-COF-TP-E22E31	2D	hcb	-	-	1660	0.58	25.1	0.17	0.29	0.25	1.18	1.24	5.92	4.50
MC-COF-TP-E22E41	308	MC-COF-TP-E22E41	2D	hcb	-	-	1691	0.61	22.9	0.17	0.30	0.23	1.18	1.30	5.79	4.55
MF-1a	309	MF-1a	2D	hcb	-	-	1516	0.64	23.8	0.15	0.32	0.24	1.03	1.16	5.76	4.40
MF-2a	310	MF-2a	2D	hcb	-	-	1457	0.80	14.1	0.15	0.40	0.14	0.87	1.25	5.11	4.50
MPCOF	311	MPCOF	2D	hcb	-	-	1445	0.94	6.9	0.14	0.47	0.07	0.77	1.35	4.55	4.58
N0_phenyl-COF	312	N0–COF	2D	hcb	-	-	2043	0.52	22.4	0.20	0.26	0.22	1.51	1.59	5.89	4.83
N1_pyridyl-COF	313	N1–COF	2D	hcb	-	-	1979	0.54	21.5	0.20	0.27	0.21	1.45	1.55	5.87	4.81
N2_pyrimidyl-COF	314	N2–COF	2D	hcb	-	-	2120	0.50	22.4	0.21	0.25	0.22	1.59	1.65	5.90	4.89
N2-COF	315	N2-COF	2D	hcb	-	-	2215	0.49	23.4	0.22	0.24	0.23	1.68	1.70	5.89	4.92
N3_triazine-COF	316	N3–COF	2D	hcb	-	-	2008	0.53	21.5	0.20	0.27	0.22	1.48	1.58	5.87	4.83
N3-COF	317	N3-COF	2D	hcb	-	-	1658	0.77	11.2	0.17	0.38	0.11	1.02	1.47	5.13	4.72
N-COF	318	N-COF	2D	hcb	-	-	0	0.73	5.6	0.00	0.36	0.06	0.00	0.00	6.35	4.10
NiPc-COF	319	NiPc-COF	2D	sql	-	-	1328	0.82	17.1	0.13	0.41	0.17	0.78	1.10	5.12	4.33
NN-TAPH-COF	320	NN-TAPH-COF	2D	sql	-	-	3931	0.49	9.3	0.39	0.24	0.09	2.97	3.56	4.58	6.20
NPN-1	321	NPN-1	3D	dia	-	-	958	1.05	5.3	0.10	0.52	0.05	0.46	0.91	4.30	4.27
NPN-2	322	NPN-2	3D	dia	-	-	1125	0.98	5.3	0.11	0.49	0.05	0.57	1.07	4.53	4.43
NPN-3	323	NPN-3	3D	dia	-	-	941	1.05	6.1	0.09	0.53	0.06	0.45	0.88	4.30	4.23
NS-COF	324	NS-COF	2D	hcb	-	-	4241	0.59	6.7	0.42	0.29	0.07	2.99	3.96	4.06	6.33
NTU-BDA-THTA	325	NTU-BDA-THTA	2D	hcb	-	-	1674	0.69	16.2	0.17	0.34	0.16	1.10	1.40	5.47	4.67
NTU-COF-1	326	NTU-COF-1	2D	hcb	-	-	1916	0.58	18.7	0.19	0.29	0.19	1.36	1.56	5.74	4.82
NTU-COF-2	327	NTU-COF-2	2D	hcb	-	-	2117	0.45	24.8	0.21	0.23	0.25	1.64	1.59	6.09	4.86

NUS-10	328	NUS-10	2D	hcb	-	-	2049	0.71	13.4	0.20	0.36	0.13	1.32	1.77	5.11	4.91
NUS-14	329	NUS-14	2D	hcb	-	-	2327	0.40	30.7	0.23	0.20	0.31	1.86	1.61	6.14	4.84
NUS-15	330	NUS-15	2D	hcb	-	-	2337	0.39	31.5	0.23	0.19	0.31	1.88	1.60	6.18	4.84
NUS-2	331	NUS-2	2D	hcb	-	-	1136	1.03	7.8	0.11	0.52	0.08	0.55	1.05	4.30	4.30
NUS-3	332	NUS-3	2D	hcb	-	-	1774	0.69	18.3	0.18	0.34	0.18	1.16	1.45	5.40	4.65
NUS-50	333	NUS-50	2D	hcb	-	-	1916	0.55	22.8	0.19	0.28	0.23	1.39	1.48	5.86	4.72
NUS-51	334	NUS-51	2D	hcb	-	-	1881	0.55	22.7	0.19	0.28	0.23	1.36	1.45	5.89	4.71
NUS-9	335	NUS-9	2D	hcb	-	-	2449	0.58	12.7	0.24	0.29	0.13	1.73	2.14	5.34	5.26
OH-H2P-COF	336	HO-H2P-COF	2D	sql	-	-	4400	0.35	18.5	0.44	0.18	0.19	3.63	3.58	4.62	6.29
OH-TAPH-COF	337	OH-TAPH-COF	2D	sql	-	-	4369	0.34	18.5	0.44	0.17	0.19	3.63	3.56	4.68	6.29
OH-TFP-TTA	338	OH-TFP-TTA	2D	hcb	-	-	1722	0.64	18.5	0.17	0.32	0.18	1.17	1.40	5.63	4.67
OH-TPBP-COF	339	AA-stacking mode of OH-TPBP-COF	2D	sql	-	-	1941	0.69	10.4	0.19	0.34	0.10	1.27	1.74	5.28	4.97
OMe-OH-TPBP-COF	340	AA-stacking mode of OMe-OH-TPBP-COF	2D	sql	-	-	1737	0.77	9.0	0.17	0.39	0.09	1.07	1.58	5.08	4.83
OMe-TPBP-COF	341	AA-stacking mode of OMe-TPBP-COF	2D	sql	-	-	1817	0.71	9.9	0.18	0.35	0.10	1.17	1.64	5.29	4.91
PC-COF	342	PC-COF	2D	hcb	-	-	3056	0.28	41.1	0.31	0.14	0.41	2.62	1.80	5.96	5.01
P-COF	343	P-COF	2D	hcb	-	-	1801	0.70	12.3	0.18	0.35	0.12	1.17	1.58	5.34	4.83
P-COF-1-AA	344	P-COF-1 model arranged in A-A stacking mode	2D	hcb	AA	-	5069	0.24	29.0	0.51	0.12	0.29	4.47	3.60	4.35	6.43
P-COF-1-AB	345	P-COF-1 model arranged in A-B stacking mode	2D	hcb	AB	-	7486	0.24	14.3	0.75	0.12	0.14	6.60	6.41	2.22	8.08
P-COF-2-AA	346	P-COF-2 model arranged in A-A stacking mode	2D	hcb	-	-	7853	0.17	34.4	0.79	0.08	0.34	7.19	5.15	1.97	7.72
Pc-PBBA-COF	347	Pc-PBBA-COF	2D	sql	-	-	1391	0.79	16.8	0.14	0.40	0.17	0.84	1.16	5.21	4.40
PCTF-1	348	PCTF-1	2D	hcb	-	-	1872	0.63	13.7	0.19	0.32	0.14	1.28	1.61	5.57	4.89

PCTF-2	349	PCTF-2	2D	hcb	-	-	2280	0.48	21.5	0.23	0.24	0.22	1.74	1.79	5.88	5.02
PCTF-3	350	PCTF-3	2D	hcb	-	-	2364	0.40	27.8	0.24	0.20	0.28	1.89	1.71	6.10	4.94
PCTF-4	351	PCTF-4	2D	hcb	-	-	1942	0.58	17.9	0.19	0.29	0.18	1.37	1.59	5.70	4.85
P-DpTaDm-COF-12	352	P-DpTaDm-COF (12)	2D	hcb	-	-	2023	0.52	25.6	0.20	0.26	0.26	1.50	1.51	5.92	4.73
Ph-AnCD-COF	353	Ph-AnCD-COF	2D	hcb	-	-	5283	0.31	23.7	0.53	0.15	0.24	4.46	4.03	3.99	6.62
Ph-An-COF	354	Ph-An-COF	2D	hcb	-	-	1701	0.62	22.3	0.17	0.31	0.22	1.18	1.32	5.74	4.56
PI-2-COF	355	PI-2-COF	2D	hcb	-	-	2196	0.49	23.4	0.22	0.24	0.23	1.66	1.68	5.91	4.91
PI-3-COF	356	PI-3-COF	2D	hcb	-	-	1652	0.77	11.2	0.17	0.38	0.11	1.02	1.47	5.14	4.72
PI-COF	357	PI-COF	2D	sql	-	-	2653	0.46	21.7	0.27	0.23	0.22	2.04	2.08	5.66	5.22
PI-COF-1	358	PI-COF-1	2D	hcb	-	-	1446	0.64	17.7	0.14	0.32	0.18	0.98	1.19	5.82	4.55
PI-COF-1-unflat	359	PI-COF-1	2D	hcb	-	-	2942	0.54	19.4	0.29	0.27	0.19	2.15	2.37	5.16	5.35
PI-COF-2	360	PI-COF-2	2D	hcb	-	-	2091	0.55	20.9	0.21	0.28	0.21	1.51	1.65	5.72	4.87
PI-COF-2-unflat	361	PI-COF-2	2D	hcb	-	-	2544	0.49	23.5	0.25	0.24	0.24	1.92	1.95	5.63	5.08
PI-COF-3	362	PI-COF-3	2D	hcb	-	-	3197	0.39	32.1	0.32	0.19	0.32	2.58	2.17	5.49	5.25
PI-COF-4	363	PI-COF-4	3D	dia	-	-	5107	0.28	17.5	0.51	0.14	0.18	4.40	4.21	4.22	6.75
PI-COF-5	364	PI-COF-5	3D	dia	-	-	4120	0.51	11.2	0.41	0.26	0.11	3.07	3.66	4.38	6.21
PI-COF-SR	365	PI-COF-SR	2D	hcb	-	-	1693	0.52	29.3	0.17	0.26	0.29	1.25	1.20	6.13	4.44
POR-COF	366	POR-COF	2D	sql	-	-	1218	0.91	13.3	0.12	0.46	0.13	0.66	1.06	4.78	4.30
Por-COF-jmca	367	Por-COF	2D	sql	-	-	3725	0.58	9.0	0.37	0.29	0.09	2.64	3.39	4.45	6.01
PPPP-1	368	PPPP-1	2D	sql	-	-	1641	0.55	27.1	0.16	0.27	0.27	1.19	1.20	6.06	4.46
PPPP-2	369	PPPP-2	2D	sql	-	-	1565	0.57	26.0	0.16	0.29	0.26	1.12	1.16	6.01	4.43
PP-TzDa	370	PP-TzDa in perfect AA	2D	hcb	AA	-	2256	0.65	16.9	0.23	0.33	0.17	1.52	1.87	5.21	4.97
PP-TzDa-AA	371	PP-TzDa in slipped AA	2D	hcb	-	-	1792	0.73	13.1	0.18	0.37	0.13	1.13	1.56	5.20	4.77
PP-TzDa-AB	372	PP-TzDa in staggered AB	2D	hcb	AB	-	2401	0.70	7.3	0.24	0.35	0.07	1.56	2.22	4.93	5.28
PPy-COF	373	PPy-COF	2D	hcb	-	-	1332	0.87	13.7	0.13	0.43	0.14	0.75	1.15	4.90	4.39
PR100-COF	374	PPy-COF	2D	hcb	-	-	2783	0.38	26.1	0.28	0.19	0.26	2.25	2.06	5.84	5.23
P-StPtDm-COF-6	375	P-StPtDm-COF (6)	2D	hcb	-	-	1502	0.64	23.6	0.15	0.32	0.24	1.02	1.15	5.77	4.40

P-StPtTp-COF-8	376	P-StPtTp-COF (8)	2D	hcb	-	-	1735	0.58	23.5	0.17	0.29	0.23	1.23	1.33	5.88	4.59
P-StTaDm-COF-2	377	P-StTaDm-COF (2)	2D	hcb	-	-	1513	0.64	23.6	0.15	0.32	0.24	1.03	1.16	5.76	4.40
P-StTaTp-COF-4	378	P-StTaTp-COF (4)	2D	hcb	-	-	1682	0.58	23.6	0.17	0.29	0.24	1.19	1.28	5.89	4.55
P-StTtDm-COF-10	379	P-StTtDm-COF (10)	2D	hcb	-	-	1471	0.66	23.5	0.15	0.33	0.23	0.99	1.13	5.73	4.38
PV-COF	380	PV-COF	2D	sql	-	-	1796	0.69	14.2	0.18	0.34	0.14	1.18	1.54	5.38	4.79
Py-1P_F-COF	381	Py-1PF COF	2D	sql	-	-	1833	0.65	16.4	0.18	0.32	0.16	1.24	1.53	5.52	4.78
Py-1P-COF	382	Py-1P COF	2D	sql	AA	-	1967	0.59	17.3	0.20	0.29	0.17	1.39	1.63	5.67	4.88
Py-1P-COF-AB	383	Py-1P COF in quasi-AB stacking mode	2D	sql	AB	-	4931	0.50	9.6	0.49	0.25	0.10	3.70	4.46	3.80	6.68
Py-22-BPYPH_COF	384	Py-2,2'-BPyPh-COF	2D	sql	-	-	2507	0.45	20.6	0.25	0.23	0.21	1.94	1.99	5.79	5.18
Py-23-BPYPH_COF	385	Py-2,3-BPyPh-COF	2D	sql	-	-	2243	0.47	22.9	0.22	0.24	0.23	1.71	1.73	5.93	4.96
Py-23-DHPh_COF	386	Py-2,3-DHPh-COF	2D	sql	-	-	1699	0.67	17.3	0.17	0.34	0.17	1.13	1.41	5.50	4.66
Py-2PE-COF	387	Py-2PE COF	2D	sql	-	-	2371	0.44	24.1	0.24	0.22	0.24	1.85	1.80	5.94	5.02
Py-33-BPYPH_COF	388	Py-3,3-BPyPh COF	2D	sql	-	-	1957	0.54	21.5	0.20	0.27	0.22	1.43	1.54	5.89	4.80
Py-3PE_BTD-COF	389	Py-3PEBTD COF	2D	sql	-	-	2364	0.41	29.2	0.24	0.20	0.29	1.88	1.67	6.09	4.90
Py-3PE-COF	390	Py-3PE COF	2D	sql	-	-	2455	0.41	27.2	0.25	0.20	0.27	1.95	1.79	6.01	5.00
Py-4T_TPD-COF	391	Py-4TTPD COF	2D	sql	-	-	2176	0.50	24.3	0.22	0.25	0.24	1.63	1.65	5.85	4.85
Py-4T_TT-COF	392	Py-4TTT COF	2D	sql	-	-	1914	0.57	23.5	0.19	0.29	0.23	1.37	1.46	5.78	4.68
Py-a4T_Me-COF	393	Py-a4TMe COF	2D	sql	-	-	2030	0.51	25.7	0.20	0.26	0.26	1.51	1.51	5.94	4.73
Py-a4T-COF	394	Py-a4T COF	2D	sql	-	-	2084	0.54	23.0	0.21	0.27	0.23	1.52	1.60	5.76	4.81
Py-An-COF	395	Py-An COF	2D	sql	-	-	2147	0.51	20.6	0.21	0.26	0.21	1.60	1.70	5.85	4.94
Py-Azine-COF	396	Py-Azine COF	2D	sql	-	-	1827	0.68	14.9	0.18	0.34	0.15	1.21	1.56	5.41	4.79
Py-BSZ-COF	397	Py-BSZ-COF	2D	sql	-	-	2020	0.51	23.6	0.20	0.26	0.24	1.50	1.54	5.93	4.79
Py-DBA-COF-1	398	Py-DBA-COF-1	2D	hcb	-	-	1904	0.45	33.6	0.19	0.22	0.34	1.48	1.26	6.30	4.50

Py-DBA-COF-2	399	Py-DBA-COF-2	2D	hcb	-	-	1973	0.39	38.3	0.20	0.20	0.38	1.59	1.22	6.45	4.44
Py-DHPh-COF	400	Py-DHPh COF	2D	sql	-	-	2376	0.51	18.8	0.24	0.26	0.19	1.77	1.93	5.67	5.11
Py-MV-DBA-COF	401	Py-MV-DBA-COF	2D	hcb	-	-	1723	0.47	34.3	0.17	0.23	0.34	1.32	1.13	6.33	4.36
Py-pII	402	Py-pII COF	2D	sql	-	-	2260	0.48	21.2	0.23	0.24	0.21	1.72	1.78	5.88	5.01
Py-pTII	403	Py-pTII COF	2D	sql	-	-	2233	0.53	19.1	0.22	0.27	0.19	1.64	1.81	5.70	5.01
PyTA-BC	404	PyTA-BC	2D	sql	-	-	1147	0.95	10.6	0.11	0.47	0.11	0.60	1.03	4.65	4.31
PyTA-BC-Ph-COF	405	PyTA-BC-Ph COF	2D	sql	-	-	1753	0.72	12.7	0.18	0.36	0.13	1.12	1.53	5.28	4.78
Py-TPE-COF	406	Py-TPE-COF	2D	sql	-	-	1716	0.75	11.8	0.17	0.37	0.12	1.08	1.51	5.19	4.76
PyTTA-BFBIm-iCOF	407	PyTTA-BFBIm-iCOF	2D	sql	-	-	1496	0.87	14.9	0.15	0.44	0.15	0.84	1.27	4.80	4.43
Py-tTII	408	Py-tTII COF	2D	sql	-	-	2130	0.54	19.7	0.21	0.27	0.20	1.55	1.71	5.74	4.93
QH-COF-1	409	QH-COF-1	2D	hcb	-	-	2576	0.38	29.7	0.26	0.19	0.30	2.09	1.81	6.03	5.02
RT-COF-1	410	RT-COF-1	2D	hcb	-	-	1587	0.78	11.8	0.16	0.39	0.12	0.97	1.40	5.15	4.66
SA-COF	411	SA-COF	2D	hcb	-	-	1713	0.72	12.0	0.17	0.36	0.12	1.10	1.51	5.32	4.78
Salen-COF	412	Salen-COF	2D	hcb	-	-	3348	0.36	25.7	0.33	0.18	0.26	2.75	2.49	5.46	5.54
SB-PORPy-COF	413	SB-PORPy	2D	sql	-	-	1589	0.74	13.0	0.16	0.37	0.13	1.00	1.38	5.31	4.67
S-CuTAPBN-COF	414	(S)-CuTAPBN-COF	2D	sql	-	-	4948	0.43	12.2	0.49	0.21	0.12	3.89	4.35	3.97	6.68
S-DpTaDm-COF-11	415	S-DpTaDm-COF (11)	2D	sql	-	-	2193	0.46	25.9	0.22	0.23	0.26	1.69	1.63	6.01	4.86
SiCOF-Li	416	SiCOF-Li	2D	hcb	-	-	1539	0.82	13.5	0.15	0.41	0.14	0.91	1.33	4.98	4.54
4PE-3P	26	4PE-3P	2D	kgm	-	-	2802	0.36	39.2	0.28	0.18	0.39	2.30	1.70	5.92	4.87
4PE-TT	27	4PE-TT	2D	kgm	-	-	2234	0.53	27.6	0.22	0.26	0.28	1.65	1.62	5.72	4.76
SIOC-COF-3	419	SIOC-COF-3	2D	hcb	-	-	2316	0.66	7.3	0.23	0.33	0.07	1.55	2.15	5.14	5.28
SIOC-COF-4	420	SIOC-COF-4	2D	hcb	-	-	3786	0.56	7.3	0.38	0.28	0.07	2.72	3.51	4.46	6.11
SIOC-COF-5	421	SIOC-COF-5	2D	sql	-	-	1142	0.91	6.9	0.11	0.45	0.07	0.62	1.06	4.84	4.46
SIOC-COF-6	422	SIOC-COF-6	2D	sql	-	-	1915	0.68	12.5	0.19	0.34	0.13	1.26	1.67	5.32	4.90
SIOC-COF-7	423	SIOC-COF-7	2D	sql	-	-	1372	0.82	9.8	0.14	0.41	0.10	0.81	1.24	5.09	4.57
sp2c-COF	424	sp2c-COF	2D	sql	-	-	1851	0.65	16.5	0.19	0.32	0.17	1.25	1.54	5.51	4.78

sp2c-COF-1	425	AA-stacking mode of sp2c-COF	2D	sql	-	-	1963	0.61	17.2	0.20	0.30	0.17	1.37	1.62	5.60	4.86
sp2c-COF-2	426	refined unit cell parameters for sp2c-COF	2D	sql	-	-	1849	0.65	16.3	0.18	0.33	0.16	1.25	1.55	5.49	4.78
sp2c-COF-4	427	AA-stacking mode of sp2c-COF-4	2D	hcb	-	-	2650	0.35	30.7	0.27	0.18	0.31	2.18	1.84	6.05	5.05
sp2c-COF-4-2	428	refined unit cell parameters for sp2c-COF-4	2D	hcb	-	-	2643	0.36	30.6	0.26	0.18	0.31	2.17	1.83	6.05	5.05
BDT-ETTA-COF	47	BDT-COF	2D	kgm	-	-	2289	0.49	31.7	0.23	0.24	0.32	1.73	1.56	5.84	4.71
COF-119	94	COF-119, Pawley refined	2D	kgm	-	-	2130	0.54	24.6	0.21	0.27	0.25	1.55	1.61	5.73	4.78
SP-3D-COF-1	431	SP-3D-COF 1	3D	dia	-	-	4273	0.40	13.2	0.43	0.20	0.13	3.43	3.71	4.59	6.34
SP-3D-COF-2	432	SP-3D-COF 2	3D	dia	-	-	2980	0.47	16.7	0.30	0.24	0.17	2.28	2.48	5.36	5.52
SP-COF-ED	433	SP-COF-ED with AA	2D	sql	-	-	2783	0.44	18.5	0.28	0.22	0.18	2.18	2.27	5.64	5.40
Star-COF-1	434	Star-COF-1	2D	hcb	-	-	1371	0.59	30.6	0.14	0.29	0.31	0.97	0.95	6.10	4.18
Star-COF-2	435	Star-COF-2	2D	hcb	-	-	1496	0.50	37.4	0.15	0.25	0.37	1.12	0.94	6.39	4.13
Star-COF-3	436	Star-COF-3	2D	hcb	-	-	1602	0.45	40.2	0.16	0.23	0.40	1.24	0.96	6.50	4.15
S-TmPtDm-COF-5	437	S-TmPtDm-COF (5)	2D	hcb	-	-	2239	0.46	25.8	0.22	0.23	0.26	1.72	1.66	5.97	4.88
S-TmPtTp-COF-7	438	S-TmPtTp-COF (7)	2D	hcb	-	-	2457	0.40	27.3	0.25	0.20	0.27	1.97	1.79	6.04	5.01
S-TmTaDm-COF-1	439	S-TmTaDm-COF (1)	2D	hcb	-	-	2193	0.46	25.9	0.22	0.23	0.26	1.69	1.63	6.01	4.86
S-TmTaTp-COF-3	440	S-TmTaTp-COF (3)	2D	hcb	-	-	2476	0.39	28.1	0.25	0.20	0.28	1.99	1.78	6.05	5.00
S-TmTtDm-COF-9	441	S-TmTtDm-COF (9)	2D	hcb	-	-	2176	0.47	26.0	0.22	0.23	0.26	1.67	1.61	6.00	4.84
TANG-COF-AA-1	442	TANG-COF AA-1 stacking	2D	hcb	-	-	4905	0.31	24.9	0.49	0.16	0.25	4.14	3.69	4.30	6.40

TAPBB-COF	443	TAPBB-COF	2D	sql	AA	-	4897	0.49	9.9	0.49	0.25	0.10	3.69	4.41	3.85	6.66
TAPBB-COF-AB	444	TAPBB-COF AB model	2D	sql	AB	-	4897	0.49	9.9	0.49	0.25	0.10	3.69	4.41	3.85	6.66
TAPB-BMTTPA-COF	445	TAPB-BMTTPA-COF	2D	hcb	-	-	2244	0.47	25.1	0.22	0.23	0.25	1.72	1.68	5.94	4.90
TAPB-BPDA-COF	446	TAPB-BPDA COF	2D	hcb	-	-	2400	0.33	38.2	0.24	0.17	0.38	2.00	1.48	6.34	4.72
TAPB-OMeTA-COF-AB	447	TAPB-OMeTA COF in quasi-AB stacking mode	2D	hcb	-	-	3916	0.46	13.6	0.39	0.23	0.14	3.01	3.38	4.68	6.09
TAPB-PDA-COF	448	TAPB-PDA COF	2D	hcb	-	-	2415	0.37	31.0	0.24	0.19	0.31	1.97	1.67	6.17	4.91
TAPB-TA-COF-AB	449	TAPB-TA COF in quasi-AB stacking mode	2D	hcb	-	-	6084	0.38	16.9	0.61	0.19	0.17	4.93	5.06	3.18	7.16
TAPB-TFP	450	TAPB-TFP	2D	hcb	-	-	1496	0.77	12.0	0.15	0.39	0.12	0.92	1.32	5.23	4.62
TAPB-TFPA-COF	451	TAPB-TFPA COF	2D	hcb	-	-	2045	0.57	17.8	0.20	0.29	0.18	1.46	1.68	5.68	4.91
TAPB-TFPB	452	TAPB-TFPB	2D	hcb	-	-	1973	0.54	19.3	0.20	0.27	0.19	1.44	1.59	5.87	4.87
TAPB-TIDA-COF	453	TAPB-TIDA COF	2D	hcb	-	-	2205	0.48	27.7	0.22	0.24	0.28	1.68	1.59	5.93	4.79
TAPP-TFPP-COF-AA	454	TAPP–TFPP–COF	2D	sql	-	-	1497	0.77	13.2	0.15	0.38	0.13	0.92	1.30	5.25	4.59
TAPT-BMTA-COF-AA	455	TAPT-BMTA-COF of the AA-stacking mode	2D	hcb	AA	-	1893	0.55	23.8	0.19	0.28	0.24	1.37	1.44	5.86	4.68
TAPT-BTCA-COF-AB	456	TAPT-BTCA COF in quasi-AB stacking mode	2D	hcb	AB	-	1898	0.74	5.6	0.19	0.37	0.06	1.20	1.79	5.12	5.05
TAPT-DHTA-COF	457	TAPT-DHTA-COF	2D	hcb	-	-	2066	0.44	29.8	0.21	0.22	0.30	1.61	1.45	6.20	4.70
TAT-COF-1	458	TAT-COF-1	2D	hcb	-	-	1989	0.46	28.4	0.20	0.23	0.28	1.54	1.42	6.18	4.69
TAT-COF-2	459	TAT-COF-2	2D	hcb	-	-	1651	0.69	15.4	0.17	0.34	0.15	1.08	1.40	5.47	4.67
TB-COF	460	TB-COF	2D	hcb	-	-	1081	0.94	9.3	0.11	0.47	0.09	0.57	0.98	4.71	4.32
Tb-DANT-COF	461	Tb-DANT-COF	2D	hcb	-	-	1579	0.68	21.2	0.16	0.34	0.21	1.04	1.24	5.55	4.47
TBI-COF	462	TBI-COF	2D	hcb	-	-	2021	0.54	19.0	0.20	0.27	0.19	1.48	1.64	5.83	4.90

TBPB_COF	463	TBPB COF	2D	hcb	-	-	1677	0.66	16.7	0.17	0.33	0.17	1.12	1.40	5.58	4.68
T-COF	464	T-COF 1	2D	hcb	-	-	1695	0.74	12.1	0.17	0.37	0.12	1.07	1.49	5.25	4.75
T-COF_1	465	T-COF 1	2D	hcb	AB	-	1045	1.05	8.2	0.10	0.53	0.08	0.49	0.96	4.24	4.22
T-COF_2	466	T-COF 2	2D	hcb	AB	-	1507	0.77	14.9	0.15	0.38	0.15	0.93	1.28	5.24	4.54
T-COF-1	467	T-COF-1 with AA stacking	2D	hcb	AA	-	1949	0.61	21.1	0.19	0.31	0.21	1.35	1.54	5.59	4.73
T-COF-2	468	T-COF-2 with AA stacking	2D	hcb	AA	-	1989	0.59	21.4	0.20	0.29	0.21	1.40	1.56	5.65	4.76
T-COF-3	469	T-COF 3	2D	hcb	-	-	1272	0.92	12.7	0.13	0.46	0.13	0.69	1.11	4.73	4.34
T-COF-4	470	T-COF 4	2D	hcb	-	-	1538	0.63	24.8	0.15	0.31	0.25	1.05	1.16	5.80	4.39
T-COF-OH	471	T-COF-OH	2D	hcb	-	-	2082	0.38	36.6	0.21	0.19	0.37	1.69	1.32	6.42	4.56
TD-COF	472	[OH]0%-TD-COF	2D	hcb	-	-	2301	0.43	27.3	0.23	0.21	0.27	1.81	1.67	6.06	4.91
TD-COF-5	473	TD-COF-5	2D	hcb	-	-	4465	0.26	28.4	0.45	0.13	0.28	3.90	3.20	4.83	6.13
TD-COF-AA	474	TD-COF	2D	hcb	-	-	1797	0.59	22.8	0.18	0.29	0.23	1.27	1.39	5.79	4.63
TDFP-1	475	TDFP-1	2D	hcb	-	-	2429	0.53	13.1	0.24	0.26	0.13	1.79	2.11	5.58	5.30
TEMPO-COF	476	TEMPO-COF	2D	hcb	-	-	1177	0.84	15.8	0.12	0.42	0.16	0.68	0.99	5.11	4.27
TFB-COF	477	TFB-COF	2D	hcb	-	-	2432	0.50	20.7	0.24	0.25	0.21	1.82	1.93	5.67	5.09
TfBD	478	TfBD	2D	hcb	-	-	2335	0.46	24.0	0.23	0.23	0.24	1.80	1.77	5.91	4.99
Tf-DHzDAll-COF	479	Tf-DHzDAll COF	2D	hcb	-	-	1978	0.74	16.3	0.20	0.37	0.16	1.25	1.65	5.07	4.76
Tf-DHzDAll-COF-1	480	DFT-optimized unit cell of eclipsed stacked Tf-DHzDAll-COF	2D	hcb	-	-	2095	0.64	17.3	0.21	0.32	0.17	1.43	1.73	5.38	4.89
Tf-DHzDAll-COF-2	481	DFT-optimized unit cell of antiparallel stacked Tf-DHzDAll-COF	2D	hcb	-	-	1251	0.68	19.0	0.13	0.34	0.19	0.82	1.01	5.77	4.37
Tf-DHzDM-COF	482	Tf-DHzDM COF	2D	hcb	-	-	1863	0.62	19.8	0.19	0.31	0.20	1.29	1.49	5.62	4.72
Tf-DHzDM-COF-1	483	DFT-optimized unit cell of	2D	hcb	-	-	2146	0.54	20.8	0.21	0.27	0.21	1.56	1.70	5.72	4.90

		eclipsed stacked Tf-DHzDM-COF														
Tf-DHzDPr-COF	484	Tf-DHzDPr COF	2D	hcb	-	-	1903	0.74	15.8	0.19	0.37	0.16	1.20	1.60	5.10	4.74
Tf-DHzOAll-COF-A	485	Tf-DHzOAll with antiparallel	2D	hcb	-	-	2095	0.64	17.3	0.21	0.32	0.17	1.43	1.73	5.38	4.89
Tf-DHzOAll-COF-E	486	Tf-DHzOAll with eclipsed	2D	hcb	-	-	1250	0.68	19.0	0.13	0.34	0.19	0.82	1.01	5.76	4.37
TFPA-TAPA-COF	487	TFPA-TAPA-COF	2D	hcb	-	-	2083	0.60	15.4	0.21	0.30	0.15	1.45	1.76	5.52	4.97
TFPA-TAPB-COF	488	TFPA-TAPB-COF	2D	hcb	-	-	2114	0.56	17.2	0.21	0.28	0.17	1.52	1.75	5.68	4.98
TFPA-TGCl-iCOF-3	489	TFPA-TGCl-iCOF c	2D	hcb	-	-	1281	0.94	8.4	0.13	0.47	0.08	0.68	1.17	4.61	4.45
TfpBDH	490	TfpBDH	2D	hcb	-	-	2753	0.63	9.1	0.28	0.32	0.09	1.88	2.50	4.96	5.47
TFPB-DHzDAll-COF	491	TFPB-DHzDAll COF	2D	hcb	-	-	2035	0.50	28.5	0.20	0.25	0.28	1.53	1.46	5.98	4.67
TFPB-DHzDM-COF	492	TFPB-DHzDM COF	2D	hcb	-	-	2040	0.41	34.7	0.20	0.21	0.35	1.62	1.33	6.32	4.57
TFPB-DHzDPr-COF	493	TFPB-DHzDPr COF	2D	hcb	-	-	2079	0.48	28.4	0.21	0.24	0.28	1.58	1.49	6.01	4.70
TFPB-DHzDS-COF	494	TFPB-DHzDS COF	2D	hcb	-	-	2096	0.57	22.8	0.21	0.28	0.23	1.50	1.62	5.67	4.80
TFPB-TAPB-COF	495	TFPB-TAPB-COF	2D	hcb	-	-	2113	0.54	19.6	0.21	0.27	0.20	1.55	1.70	5.77	4.93
TFPB-TAPT_COF	496	TFPB-TAPT COF	2D	hcb	-	-	1992	0.57	18.8	0.20	0.28	0.19	1.43	1.62	5.74	4.87
TFPB-TGCl-iCOF-2	497	TFPB-TGCl-iCOF b	2D	hcb	-	-	1413	0.85	10.8	0.14	0.42	0.11	0.81	1.26	4.95	4.53
TFPB-THz-COF	498	TFPB-THz COF	2D	hcb	-	-	1866	0.64	15.1	0.19	0.32	0.15	1.27	1.58	5.53	4.84
TFP-NDA-COF	499	TFP-NDA-COF	2D	hcb	-	-	1387	0.87	13.6	0.14	0.44	0.14	0.78	1.20	4.86	4.41
TFPPy-DETHz-COF	500	TFPPy-DETHz-COF	2D	sql	-	-	2329	0.54	17.2	0.23	0.27	0.17	1.70	1.93	5.60	5.11
TFPT-BTAN	501	TFPT-BTAN	2D	hcb	-	-	1384	0.81	10.7	0.14	0.40	0.11	0.83	1.24	5.14	4.56
TFPT-COF	502	TFPT-COF	2D	hcb	-	-	2015	0.49	28.6	0.20	0.25	0.29	1.52	1.44	6.01	4.66
TFPT-TGCl-iCOF-1	503	TFPT-TGCl-iCOF a	2D	hcb	-	-	1361	0.86	10.7	0.14	0.43	0.11	0.78	1.21	4.92	4.50
TH-COF-1	504	TH-COF-1	2D	hcb	-	-	1561	0.92	12.1	0.16	0.46	0.12	0.84	1.37	4.55	4.50

Thio-COF	505	Thio-COF	2D	hcb	-	-	2624	0.48	22.2	0.26	0.24	0.22	1.99	2.04	5.59	5.16
TJNU-201	506	TJNU-201	2D	hcb	-	-	2356	0.53	16.7	0.24	0.26	0.17	1.74	1.96	5.64	5.15
TJNU-202	507	TJNU-202	2D	hcb	-	-	2065	0.54	20.1	0.21	0.27	0.20	1.51	1.65	5.80	4.89
TPA-COF	508	TPA-COF	2D	hcb	-	-	1939	0.63	15.4	0.19	0.32	0.15	1.33	1.64	5.51	4.87
TPA-COF-2	509	TPA-COF-2	2D	hcb	-	-	2132	0.56	16.7	0.21	0.28	0.17	1.53	1.78	5.66	5.01
TPA-COF-3	510	TPA-COF-3	2D	hcb	-	-	1810	0.66	15.8	0.18	0.33	0.16	1.21	1.52	5.47	4.77
TPAPC-COF	511	TPAPC-COF	2D	sql	-	-	4395	0.36	20.3	0.44	0.18	0.20	3.61	3.50	4.60	6.23
TPA-TPA-COF	512	TPA-TPA-COF (TPA-COF-1)	2D	hcb	-	-	2289	0.57	15.2	0.23	0.28	0.15	1.64	1.94	5.53	5.12
TPA-TPP-COF	513	TPA-TPP-COF (TPA-COF-2)	2D	hcb	-	-	1813	0.65	16.1	0.18	0.33	0.16	1.22	1.52	5.52	4.77
Tp-Azo	514	Tp-Azo	2D	hcb	-	-	1829	0.56	25.7	0.18	0.28	0.26	1.32	1.36	5.90	4.59
TPB-BMTP-COF	515	TPB-BMTP-COF	2D	hcb	-	-	2815	0.57	15.5	0.28	0.29	0.15	2.01	2.38	5.13	5.37
TpBD	516	TpBD	2D	hcb	-	-	1716	0.59	22.9	0.17	0.30	0.23	1.21	1.32	5.82	4.58
TPB-DBBA-COF-AA	517	AA-stacking mode of TPB-DBBA-COF	2D	hcb	AA	-	2261	0.39	31.5	0.23	0.20	0.32	1.82	1.55	6.22	4.79
TPB-DBBA-COF-AB	518	AB-stacking mode of TPB-DBBA-COF	2D	hcb	AB	-	4659	0.56	12.4	0.47	0.28	0.12	3.36	4.08	3.86	6.40
TP-BDDA-COF	519	TP-BDDA-COF	2D	hcb	-	-	2546	0.35	33.2	0.25	0.18	0.33	2.10	1.70	6.14	4.92
TpBDH	520	TpBDH	2D	hcb	-	-	1407	0.71	21.1	0.14	0.35	0.21	0.91	1.11	5.55	4.36
TPBD-Me2	521	TPBD-ME2	2D	hcb	-	-	1749	0.53	25.5	0.17	0.27	0.26	1.28	1.30	6.06	4.58
TPB-DMeTP-COF-1	522	AA-stacking mode of TPB-DMeTP-COF	2D	hcb	-	-	2246	0.42	28.4	0.22	0.21	0.28	1.77	1.61	6.11	4.85
TPB-DMTP-COF	523	TPB-DMTP-COF	2D	hcb	-	-	2243	0.46	26.6	0.22	0.23	0.27	1.73	1.65	5.97	4.86
TpBD-NH2_2	524	TpBD-NH2	2D	hcb	-	-	1705	0.60	22.2	0.17	0.30	0.22	1.20	1.33	5.82	4.59
TpBD-NHCOCH3_2	525	TpBD-NHCOCH3	2D	hcb	-	-	1335	0.75	18.1	0.13	0.38	0.18	0.83	1.09	5.40	4.37
TpBD-NO2_2	526	TpBD-NO2	2D	hcb	-	-	1517	0.71	21.4	0.15	0.35	0.21	0.98	1.19	5.48	4.41
TpBD-OH2	527	TpPa-(OH)2	2D	hcb	-	-	1843	0.59	21.0	0.18	0.30	0.21	1.30	1.46	5.74	4.70
TpBD-OMe2	528	TpBD-(OMe)2	2D	hcb	-	-	1883	0.64	18.4	0.19	0.32	0.18	1.28	1.54	5.50	4.75

TpBpy-cis-COF	529	cis TpBpy	2D	hcb	-	-	1643	0.65	20.9	0.16	0.32	0.21	1.11	1.30	5.64	4.55
TpBpy-COF	530	TpBpy	2D	hcb	-	-	1888	0.56	22.6	0.19	0.28	0.23	1.36	1.46	5.86	4.71
TPB-TP-COF	531	TPB-TP-COF	2D	hcb	-	-	2957	0.33	29.8	0.30	0.17	0.30	2.46	2.08	5.86	5.25
TPB-TP-COF-oxidation	532	TPB-TP-COF-oxi	2D	hcb	-	-	2373	0.39	30.1	0.24	0.19	0.30	1.91	1.66	6.15	4.90
TP-COF	533	TP-COF	2D	hcb	-	-	1712	0.69	16.2	0.17	0.34	0.16	1.13	1.44	5.45	4.69
TP-COF-AA	534	TP-COF-AA	2D	hcb	AA	-	2012	0.45	29.7	0.20	0.22	0.30	1.56	1.41	6.20	4.67
TP-COF-AB	535	TP-COF-AB	2D	hcb	AB	-	4582	0.45	11.5	0.46	0.22	0.12	3.56	4.05	4.21	6.50
COF-AA-H	130	COF-AA-H	2D	kgm	-	-	2294	0.51	25.7	0.23	0.25	0.26	1.71	1.70	5.74	4.87
COF-BPDA	135	COF-BPDA	2D	kgm	-	-	2489	0.43	32.1	0.25	0.22	0.32	1.95	1.69	5.89	4.85
Tp-DANT-COF	538	Tp-DANT-COF	2D	hcb	-	-	1382	0.73	21.6	0.14	0.37	0.22	0.87	1.08	5.45	4.31
TPE-COF-I	539	TPE-COF-I	2D	sql	-	-	1780	0.76	7.8	0.18	0.38	0.08	1.10	1.64	5.08	4.89
COF-BTA-DHBZ	136	COF-BTA-DHBZ	2D	kgm	-	-	1387	0.75	21.4	0.14	0.38	0.21	0.86	1.09	5.37	4.30
COF-FADA-DAB	149	COF-FADA-DAB with AA stacking	2D	kgm	-	-	2113	0.55	24.1	0.21	0.28	0.24	1.53	1.60	5.70	4.78
COF-TPDA	171	COF-TPDA	2D	kgm	-	-	2616	0.37	38.9	0.26	0.19	0.39	2.13	1.60	6.01	4.77
TP-EDDA-COF	543	TP-EDDA COF	2D	hcb	-	-	2360	0.42	28.5	0.24	0.21	0.28	1.87	1.69	6.04	4.91
DP-COF-ED	230	DP-COF-ED with AA	2D	kgm	-	-	2638	0.38	39.9	0.26	0.19	0.40	2.14	1.58	5.97	4.74
ETTF-DABP-COF-1	240	AA-stacking mode of ETTF-DABP-COF	2D	kgm	-	-	2336	0.46	31.9	0.23	0.23	0.32	1.80	1.59	5.91	4.75
TPE-TAP-COF	546	TPE-TAP-COF	2D	sql	-	-	1493	0.80	11.1	0.15	0.40	0.11	0.89	1.33	5.10	4.61
TpFn	547	TpFn	2D	hcb	-	-	1559	0.65	21.3	0.16	0.33	0.21	1.05	1.23	5.68	4.49
TPHH-COF-AB	548	TPHH-COF AB	2D	hcb	-	-	2379	0.69	8.5	0.24	0.34	0.09	1.56	2.18	5.01	5.25
TpMA	549	TpMA	2D	hcb	-	-	549	1.25	4.7	0.05	0.63	0.05	0.20	0.52	3.53	3.88
TpOMe-Azo	550	TpOMe-Azo	2D	hcb	-	-	887	0.97	25.8	0.09	0.49	0.26	0.46	0.66	4.68	3.70
TpOMe-BD_NO2-2	551	TpOMe-BD(NO2)2	2D	hcb	-	-	698	1.33	20.9	0.07	0.67	0.21	0.23	0.55	3.10	3.39
TpOMe-BPy	552	TpOMe-BPy	2D	hcb	-	-	814	1.15	21.4	0.08	0.57	0.21	0.35	0.64	3.91	3.62
TpOMe-DAQ	553	TpOMe-DAQ	2D	hcb	-	-	701	1.29	20.9	0.07	0.65	0.21	0.25	0.55	3.29	3.43
TpOMe-Pa1	554	TpOMe-Pa1	2D	hcb	-	-	616	1.46	13.2	0.06	0.73	0.13	0.17	0.53	2.52	3.45
TpOMe-PaNO2	555	TpOMe-PaNO2	2D	hcb	-	-	979	1.01	13.3	0.10	0.50	0.13	0.49	0.85	4.47	4.08

TpOMe-Tab	556	TpOMe-Tab	2D	hcb	-	-	1337	0.83	10.5	0.13	0.42	0.10	0.78	1.20	5.07	4.52
TpPa-1	557	TpPa-1	2D	hcb	-	-	1628	0.71	16.1	0.16	0.35	0.16	1.05	1.37	5.42	4.62
TpPa-1-2F	558	TpPa-1-F2	2D	hcb	-	-	1359	0.83	15.6	0.14	0.41	0.16	0.80	1.15	5.08	4.39
TpPa-2	559	TpPa-2	2D	hcb	-	-	1538	0.78	13.8	0.15	0.39	0.14	0.94	1.33	5.16	4.58
TpPa-F4	560	TpPa-F4	2D	hcb	-	-	1077	1.02	14.9	0.11	0.51	0.15	0.53	0.92	4.38	4.07
TpPa-NO2	561	TpPa-NO2	2D	hcb	-	-	1281	0.96	11.4	0.13	0.48	0.11	0.67	1.13	4.53	4.34
TpPa-OH2	562	TpPa-(OH)2	2D	hcb	-	-	1488	0.83	12.7	0.15	0.41	0.13	0.87	1.30	4.99	4.53
TpPa-OMe2	563	TpPa-(OMe)2	2D	hcb	-	-	1155	0.90	10.5	0.12	0.45	0.10	0.63	1.03	4.84	4.36
TpPa-Py	564	TpPa-Py	2D	hcb	-	-	1681	0.72	15.0	0.17	0.36	0.15	1.08	1.43	5.33	4.67
TpPa-SO3H	565	TpPa-SO3H	2D	hcb	-	-	1259	0.94	11.6	0.13	0.47	0.12	0.67	1.11	4.64	4.34
TpPa-SO3H-Py	566	TpPa-SO3H-Py	2D	hcb	-	-	1384	0.86	12.1	0.14	0.43	0.12	0.79	1.22	4.89	4.46
Tp-PaSO3Li-COF	567	Tp-PaSO3Li-COF	2D	hcb	-	-	2248	0.60	14.5	0.22	0.30	0.15	1.58	1.92	5.44	5.09
TP-Por-COF	568	TP-Por-COF	2D	hcb	-	-	1921	0.39	41.4	0.19	0.19	0.41	1.55	1.13	6.52	4.33
Tp-Por-COF-AA	569	Tp-Por COF-AA	2D	hcb	AA	-	1907	0.39	41.2	0.19	0.19	0.41	1.54	1.12	6.53	4.33
Tp-Por-COF-AA-38	570	Tp-Por COF-AA	2D	hcb	-	-	1907	0.39	41.2	0.19	0.19	0.41	1.54	1.12	6.53	4.33
Tp-Por-COF-AB	571	Tp-Por COF-AB	2D	hcb	AB	-	2880	0.45	20.1	0.29	0.23	0.20	2.23	2.30	5.51	5.38
Tp-Stb	572	Tp-Stb	2D	hcb	-	-	1912	0.56	24.8	0.19	0.28	0.25	1.38	1.44	5.84	4.65
TPT-Azine-COF	573	TPT-Azine-COF	2D	hcb	-	-	2459	0.48	22.4	0.25	0.24	0.22	1.87	1.91	5.73	5.08
TPT-BD-COF	574	TPT-BD COF	2D	hcb	-	-	2392	0.39	34.8	0.24	0.19	0.35	1.93	1.56	6.14	4.77
TPT-COF-1	575	TPT-COF-1	2D	hcb	-	-	1505	0.65	19.7	0.15	0.33	0.20	1.01	1.21	5.71	4.51
TPT-COF-2	576	TPT-COF-2	2D	hcb	-	-	1870	0.46	28.9	0.19	0.23	0.29	1.44	1.33	6.27	4.61
TPT-COF-4	577	TPT-COF-4	2D	hcb	-	-	2118	0.58	17.2	0.21	0.29	0.17	1.50	1.75	5.60	4.96
TPT-COF-5	578	TPT-COF-5	2D	hcb	-	-	1986	0.58	18.4	0.20	0.29	0.18	1.41	1.62	5.69	4.86
TPT-COF-6	579	TPT-COF-6	2D	hcb	-	-	1895	0.59	18.5	0.19	0.29	0.19	1.34	1.54	5.72	4.80
TpTD	580	TpTD	2D	hcb	-	-	2156	0.41	31.8	0.22	0.21	0.32	1.71	1.47	6.22	4.71
TPT-DAHQ-COF	581	TPT-DAHQ COF	2D	hcb	-	-	1958	0.47	28.6	0.20	0.24	0.29	1.50	1.40	6.15	4.65
TPT-DHBD-COF	582	TPT-DHBD COF	2D	hcb	-	-	2272	0.42	32.5	0.23	0.21	0.32	1.79	1.53	6.09	4.74
TPT-DMBD-COF	583	TPT-DMBD-COF	2D	hcb	-	-	2763	0.31	36.8	0.28	0.15	0.37	2.34	1.75	6.13	4.97
TpTe-1-COF	584	TpTe-1 AA	2D	hcb	AA	-	2116	0.45	26.0	0.21	0.23	0.26	1.64	1.57	6.11	4.83
TpTe-1-COF-AB	585	TpTe-1 AB	2D	hcb	AB	-	5095	0.45	10.3	0.51	0.23	0.10	3.94	4.57	3.79	6.78
TpTG-Br	586	TpTG-Br	2D	hcb	-	-	0	1.75	3.2	0.00	0.87	0.03	0.00	0.00	1.26	3.15

TpTG-Cl	587	TpTG-Cl	2D	hcb	-	-	0	1.52	3.4	0.00	0.76	0.03	0.00	0.00	2.40	3.38
TpTG-I	588	TpTG-I	2D	hcb	-	-	0	1.99	3.0	0.00	0.99	0.03	0.00	0.00	0.07	2.92
TPT-TAPB-COF	589	TPT-TAPB-COF	2D	hcb	-	-	3055	0.38	22.0	0.31	0.19	0.22	2.47	2.38	5.61	5.48
Tp-Ttba	590	Tp-Ttba	2D	hcb	-	-	1659	0.66	17.4	0.17	0.33	0.17	1.11	1.37	5.60	4.65
TRIPTA	591	TRIPTA	2D	hcb	-	-	1502	0.79	12.4	0.15	0.40	0.12	0.91	1.32	5.13	4.59
TS-COF-1	592	TS-COF-1	2D	hcb	-	-	1720	0.51	29.8	0.17	0.26	0.30	1.28	1.21	6.17	4.46
TS-COF-2	593	TS-COF-2	2D	hcb	-	-	1553	0.80	11.3	0.16	0.40	0.11	0.93	1.38	5.06	4.64
TT-COF	594	TT-COF	2D	hcb	-	-	1610	0.58	26.3	0.16	0.29	0.26	1.15	1.19	5.98	4.44
TTF-COF	595	TTF-COF	2D	sql	-	-	3391	0.41	18.6	0.34	0.21	0.19	2.69	2.76	5.24	5.73
TTF-DMTA-1-COF	596	TTF-DMTA-1 COF with the slipped eclipsed sql net	2D	sql	-	-	2048	0.60	17.3	0.20	0.30	0.17	1.43	1.69	5.55	4.90
TTF-DMTA-COF	597	TTF-DMTA COF with the staircase SP sql net	2D	sql	-	-	1450	0.76	11.3	0.15	0.38	0.11	0.90	1.29	5.30	4.62
TTF-Ph-COF	598	TTF-Ph-COF	2D	sql	-	-	1965	0.64	16.1	0.20	0.32	0.16	1.34	1.65	5.47	4.86
TTF-Py-COF	599	TTF-Py-COF	2D	sql	-	-	1568	0.77	13.3	0.16	0.38	0.13	0.97	1.36	5.20	4.62
TTF-TA-COF-AA	600	TTF-TA COF with AA packing	2D	sql	AA	-	2354	0.53	17.1	0.24	0.27	0.17	1.73	1.95	5.61	5.13
TTF-TA-COF-AB	601	TTF-TA COF with AB packing	2D	sql	AB	-	0	1.09	4.2	0.00	0.54	0.04	0.00	0.00	4.57	3.79
TThPP	602	TThPP	2D	sql	-	-	3780	0.39	17.8	0.38	0.20	0.18	3.04	3.11	5.01	5.96
TTI-COF	603	TTI-COF	2D	hcb	-	-	1959	0.57	18.5	0.20	0.28	0.19	1.40	1.60	5.76	4.86
TzBA	604	TzBA	2D	hcb	-	-	2542	0.34	36.2	0.25	0.17	0.36	2.11	1.62	6.19	4.84
TzDa	605	TzDa	2D	hcb	-	-	1975	0.47	29.2	0.20	0.23	0.29	1.51	1.40	6.15	4.64
VO-TAPT-23-DHTA-COF	606	VO-TAPT-2,3-DHTA COF	2D	hcb	-	-	1040	0.92	24.9	0.10	0.46	0.25	0.56	0.78	4.84	3.85
ZnPc-DPB-COF	607	ZnPc-DPB	2D	sql	-	-	1798	0.55	26.8	0.18	0.27	0.27	1.31	1.32	5.97	4.55
ZnPc-NDI-COF	608	ZnPc-NDI	2D	sql	-	-	1428	0.61	27.2	0.14	0.31	0.27	0.99	1.04	5.96	4.29
ZnP-COF	609	ZnP-COF	2D	sql	-	-	4000	0.36	19.1	0.40	0.18	0.19	3.27	3.24	4.91	6.07
ZnPc-PPE-COF	610	ZnPc-PPE	2D	sql	-	-	2060	0.43	32.2	0.21	0.21	0.32	1.62	1.40	6.23	4.63

ZnPc-Py-COF	611	ZnPc-Py	2D	sql	-	-	1312	0.78	18.5	0.13	0.39	0.19	0.80	1.07	5.30	4.32
EDA-TMT	612	EDA-TMT	2D	hcb	-	-	2568	0.39	28.3	0.26	0.20	0.28	2.07	1.84	5.98	5.04
TDA-TMT	613	TDA-TMT	2D	hcb	-	-	2411	0.39	31.6	0.24	0.19	0.32	1.95	1.65	6.12	4.87
COF-PEG-B1	614	COF-PEG-B1	2D	hcb	-	-	2733	0.55	21.4	0.27	0.27	0.21	1.99	2.15	5.28	5.18
COF-Im	615	COF-Im	2D	hcb	-	-	1396	0.84	8.0	0.14	0.42	0.08	0.81	1.28	4.98	4.62
TAPP-TFPP-COF-AB	616	TAPP–TFPP–COF	2D	sql	-	-	2574	0.77	6.0	0.26	0.38	0.06	1.59	2.42	4.59	5.34
VCOF-PyrBpy	617	VCOF-PyrBpy	2D	sql	-	-	1950	0.59	17.9	0.19	0.30	0.18	1.37	1.60	5.67	4.85
TpBD-3COOH	618	TpBD-3COOH	2D	hcb	-	-	355	1.09	5.6	0.04	0.54	0.06	0.16	0.34	4.39	3.92
COF-C6	619	COF-C6	2D	hcb	-	-	941	1.32	9.0	0.09	0.66	0.09	0.32	0.86	3.09	3.88
COF-F4	620	COF-F4	2D	hcb	-	-	1301	0.84	13.0	0.13	0.42	0.13	0.75	1.13	5.04	4.42
TAPP-BDP-AA	621	the eclipsed AA-stacking unit cell of TAPP-BDP	2D	sql	AA	-	6279	0.21	24.4	0.63	0.11	0.24	5.62	4.75	3.33	7.20
TAPP-BDP-AB	622	the AB-staggered stacking unit cell of TAPP-BDP	2D	sql	AB	-	6377	0.22	20.6	0.64	0.11	0.21	5.67	5.07	3.22	7.35
Amide-COF-AA	623	Amide-COF with AA	2D	hcb	-	-	1720	0.72	12.7	0.17	0.36	0.13	1.10	1.50	5.31	4.76
Imine-COF-AA	624	Imine-COF with AA	2D	hcb	-	-	1744	0.70	12.3	0.17	0.35	0.12	1.14	1.53	5.38	4.81
TAPT-COF-AA	625	the AA-stacking mode of [HO]100%-TAPT-COF	2D	hcb	-	-	2374	0.41	28.9	0.24	0.20	0.29	1.89	1.69	6.08	4.91
TFPPy-DP-COF-amide-AA	626	amide COFs TFPPy-DP with AA stacking	2D	sql	-	-	1787	0.73	14.8	0.18	0.37	0.15	1.13	1.52	5.20	4.72
TFPPy-DP-COF-imine-AA	627	imine COFs TFPPy-DP with AA stacking	2D	sql	-	-	1907	0.70	14.8	0.19	0.35	0.15	1.24	1.62	5.28	4.81

TAPP-ETTB-COF-AA	628	TAPP-ETTB COF calculated based on the AA structure	2D	sql	-	-	2157	0.62	11.8	0.22	0.31	0.12	1.48	1.90	5.39	5.10
Me3TFB-(NH2)2BD	629	Me3TFB-(NH2)2BD	2D	hcb	-	-	2334	0.63	7.5	0.23	0.32	0.07	1.59	2.16	5.24	5.31
Me3TFB-(NH2)2BD-AB	630	Me3TFB-(NH2)2BD-AB	2D	hcb	-	-	2334	0.63	7.5	0.23	0.32	0.07	1.59	2.16	5.24	5.31
Me3TFB-BD	631	Me3TFB-BD	2D	hcb	-	-	1571	0.68	19.4	0.16	0.34	0.19	1.03	1.27	5.55	4.52
Me3TFB-BD-AB	632	Me3TFB-BD-AB	2D	hcb	-	-	1889	0.71	7.2	0.19	0.35	0.07	1.22	1.75	5.23	5.02
Tp-BTD	633	Tp-BTD	2D	hcb	-	-	1897	0.48	26.8	0.19	0.24	0.27	1.44	1.39	6.15	4.66
TzDA-BATN-COF-AA	634	TzDA-BTAN-COF with AA packing	2D	hcb	-	-	2114	0.41	31.9	0.21	0.21	0.32	1.68	1.44	6.26	4.69
Bth-Tp_AA_enol	635	Bth-Tp_AA_enol	2D	hcb	-	-	1285	0.94	9.3	0.13	0.47	0.09	0.68	1.17	4.63	4.43
Bth-Tp_AA_keto	636	Bth-Tp_AA_keto	2D	hcb	-	-	1306	0.93	9.3	0.13	0.46	0.09	0.70	1.18	4.65	4.44
Bth-Tp_AB_enol	637	Bth-Tp_AB_enol	2D	hcb	-	-	0	1.00	4.2	0.00	0.50	0.04	0.00	0.00	5.02	3.88
Bth-Tp_AB_keto	638	Bth-Tp_AB_keto	2D	hcb	-	-	0	1.02	4.2	0.00	0.51	0.04	0.00	0.00	4.91	3.86
Bth-Tp_revAA_enol	639	Bth-Tp_revAA_enol	2D	hcb	-	-	1194	0.97	9.2	0.12	0.49	0.09	0.61	1.08	4.53	4.35
Bth-Tp_revAA_keto	640	Bth-Tp_revAA_keto	2D	hcb	-	-	1234	0.98	9.1	0.12	0.49	0.09	0.63	1.12	4.49	4.37
Bth-Tp_slipAA_enol	641	Bth-Tp_slipAA_enol	2D	hcb	-	-	1191	1.00	7.6	0.12	0.50	0.08	0.60	1.10	4.40	4.37
Bth-Tp_slipAA_keto	642	Bth-Tp_slipAA_keto	2D	hcb	-	-	802	1.11	6.1	0.08	0.56	0.06	0.36	0.75	4.07	4.10
Bth-Tp-COF-AA	643	eclipsed (AA) stacking mode of Bth-Tp-COF	2D	hcb	AA	-	1283	0.94	9.3	0.13	0.47	0.09	0.68	1.16	4.63	4.42
Bth-Tp-COF-AB	644	staggered (AB) stacking mode of Bth-Tp-COF	2D	hcb	AB	-	0	1.00	4.2	0.00	0.50	0.04	0.00	0.00	5.01	3.88

COF-100N3-AA	645	COF-100%N3 with AA-stacking.	2D	hcb	-	-	6203	0.34	16.2	0.62	0.17	0.16	5.16	5.20	3.16	7.28
Phen-COF	646	Phen-COF	2D	hcb	-	-	2357	0.27	49.1	0.24	0.14	0.49	2.04	1.20	6.60	4.43
HEP-TAPB-COF-AA	647	AA-stacking mode of the simulated HEP-TAPB-COF	2D	hcb	-	-	2036	0.54	20.7	0.20	0.27	0.21	1.48	1.62	5.81	4.86
HEP-TAPT-AA	648	AA-stacking mode of the simulated HEP-TAPT-COF	2D	hcb	-	-	2012	0.55	20.4	0.20	0.28	0.20	1.46	1.60	5.78	4.84
NKCOF-118(H)	649	NKCOF-118(H)	2D	sql	-	-	2543	0.37	30.0	0.25	0.18	0.30	2.07	1.78	6.08	5.00
TTAN-COF	650	TTAN-COF	2D	hcb	-	-	1922	0.60	16.7	0.19	0.30	0.17	1.34	1.60	5.64	4.86
TTI-COF	651	TTI-COF	2D	hcb	-	-	1953	0.59	17.7	0.20	0.29	0.18	1.38	1.61	5.68	4.86
TTV-COF	652	TTV-COF	2D	hcb	-	-	1962	0.56	18.4	0.20	0.28	0.18	1.41	1.60	5.78	4.87
v-2D-COF-NS1-AA	653	v-2D-COF-NS1 with Eclipsed (AA) Stacking Mode	2D	hcb	-	-	1799	0.64	20.0	0.18	0.32	0.20	1.22	1.44	5.58	4.66
COF-670-hydrazine	654	COF-670-hydrazine	3D	dia	-	-	0	1.09	4.2	0.00	0.54	0.04	0.00	0.00	4.56	3.79
TAPPCo-B18C6-COF-AA	655	the AA-stacking mode of TAPPCo-B18C6-COF	2D	sql	AA	-	1283	0.96	10.9	0.13	0.48	0.11	0.67	1.14	4.52	4.35
TAPPCo-B18C6-COF-AB	656	the AB-stacking mode of TAPPCo-B18C6-COF	2D	sql	AB	-	2750	0.68	7.2	0.28	0.34	0.07	1.81	2.55	4.78	5.48
TFP-DB-COF-1-AA	657	AA-stacking mode of TFP-DB-COF	2D	hcb	-	-	1029	0.98	13.0	0.10	0.49	0.13	0.53	0.90	4.59	4.15

TFP-DB-COF-AA	658	AA-stacking mode of TFP-DB-COF	2D	hcb	AA	-	1577	0.72	13.0	0.16	0.36	0.13	1.01	1.37	5.39	4.68
TFP-DB-COF-AB	659	AB-stacking mode of TFP-DB-COF	2D	hcb	AB	-	7190	0.35	14.4	0.72	0.17	0.14	5.93	6.15	2.32	7.81
PB-PA-AB	660	PB-PA were calculated based on the AB stacking	2D	hcb	-	-	3028	0.62	7.1	0.30	0.31	0.07	2.08	2.81	4.80	5.68
PT-PA-AB	661	PT-PA were calculated based on the AB stacking	2D	hcb	-	-	2852	0.64	6.9	0.29	0.32	0.07	1.94	2.65	4.86	5.58
Hex-Aza-COF-1	662	Hex-Aza-COF-1	2D	hcb	-	-	1047	1.18	9.4	0.10	0.59	0.09	0.43	0.95	3.68	4.06
Hex-Aza-COF-2	663	Hex-Aza-COF-2	2D	hcb	-	-	248	1.45	4.5	0.02	0.73	0.04	0.07	0.24	2.67	3.54
Hex-Aza-COF-3	664	Hex-Aza-COF-3	2D	hcb	-	-	0	1.18	3.7	0.00	0.59	0.04	0.00	0.00	4.09	3.71
IISERP-COF25	665	IISERP-COF25	2D	hcb	-	-	1621	0.75	11.9	0.16	0.37	0.12	1.01	1.43	5.24	4.70
HAQ-COF	666	HAQ-COF	2D	hcb	-	-	247	1.45	4.5	0.02	0.73	0.04	0.07	0.24	2.67	3.54
H-COF-AA	667	H-COF with AA stacking models	2D	hcb	-	-	2437	0.46	21.5	0.24	0.23	0.22	1.88	1.91	5.83	5.12
DA-COF-1	668	DA-COF-1	2D	hcb	-	-	1676	0.67	16.1	0.17	0.33	0.16	1.12	1.41	5.54	4.69
DA-COF-2	669	DA-COF-2	2D	hcb	-	-	1545	0.73	15.3	0.15	0.37	0.15	0.98	1.31	5.36	4.58
TPDA-COF	670	TPDA-COF	2D	hcb	-	-	8011	0.22	17.3	0.80	0.11	0.17	7.11	6.63	1.77	8.26
COF-QA-2	671	COF-QA-2	2D	hcb	-	-	2119	0.66	12.7	0.21	0.33	0.13	1.42	1.85	5.28	5.02
COF-QA-4	672	COF-QA-4	2D	hcb	-	-	1822	0.68	10.2	0.18	0.34	0.10	1.20	1.64	5.40	4.93
COF-QA-6	673	COF-QA-6	2D	hcb	-	-	2163	0.62	9.8	0.22	0.31	0.10	1.49	1.95	5.42	5.17
COF-QA-EO	674	COF-QA-EO	2D	hcb	-	-	1590	0.70	10.0	0.16	0.35	0.10	1.04	1.43	5.48	4.80
CoP-BDT-COF-AA	675	the AA-stacking mode of CoP-BDT-COF	2D	sql	-	-	2447	0.45	22.4	0.24	0.22	0.22	1.90	1.90	5.87	5.10

CoP-BDTEO-COF-AA	676	the AA-stacking mode of CoP-BDTEO-COF	2D	sql	-	-	2517	0.51	16.9	0.25	0.26	0.17	1.87	2.09	5.56	5.24
HPB-COF	677	simulated AA-stacking model of 1,3,5-HPB-COF	2D	hcb	-	-	1912	0.75	7.7	0.19	0.37	0.08	1.20	1.76	5.08	4.98
NKCOF-112-M	678	NKCOF-112-M	2D	hcb	-	-	2310	0.48	22.7	0.23	0.24	0.23	1.76	1.79	5.86	5.00
NKCOF-113-M	679	NKCOF-113-M	2D	hcb	-	-	2115	0.37	36.2	0.21	0.19	0.36	1.72	1.35	6.42	4.60
NKCOF-114-M	680	NKCOF-114-M	2D	hcb	-	-	2241	0.28	50.1	0.22	0.14	0.50	1.93	1.12	6.68	4.34
Co-PorBpy	681	Co-PorBpy	2D	sql	-	-	4963	0.29	24.5	0.50	0.15	0.25	4.23	3.75	4.30	6.45
TPB-COF	682	TPB-COF	2D	hcb	-	-	2233	0.50	19.9	0.22	0.25	0.20	1.67	1.79	5.81	5.02
TPB-TPT-COF	683	TPB-TPT-COF	2D	hcb	-	-	2146	0.53	19.7	0.21	0.27	0.20	1.57	1.72	5.76	4.95
TPT-COF-AB	684	TPT-COF with the antiparallel stacking model	2D	hcb	-	-	1926	0.57	18.9	0.19	0.29	0.19	1.37	1.56	5.75	4.82
Py-ClTP-BT-COF	685	Py-ClTP-BT-COF	2D	sql	-	-	1953	0.51	23.8	0.20	0.26	0.24	1.45	1.49	5.98	4.75
Py-FTP-BT-COF	686	Py-FTP-BT-COF	2D	sql	-	-	1990	0.49	26.0	0.20	0.25	0.26	1.50	1.47	6.03	4.72
Py-HTP-BT-COF	687	Py-HTP-BT-COF	2D	sql	-	-	2082	0.47	27.4	0.21	0.24	0.27	1.59	1.51	6.05	4.75
g-C52N6-COF	688	g-C52N6-COF	2D	hcb	-	-	1751	0.60	18.4	0.18	0.30	0.18	1.22	1.43	5.76	4.72
g-C54N6-COF	689	g-C54N6-COF	2D	hcb	-	-	1740	0.61	18.8	0.17	0.30	0.19	1.21	1.41	5.75	4.70
BrCOF-1-AA	690	BrCOF-1 with AA stacking mode	2D	hcb	AA	-	1710	0.57	27.6	0.17	0.29	0.28	1.22	1.24	5.91	4.45
BrCOF-1-AB	691	BrCOF-1 with AB stacking mode	2D	hcb	AB	-	1893	0.66	12.3	0.19	0.33	0.12	1.27	1.66	5.43	4.92
BrCOF-2-AA	692	BrCOF-2 with AA stacking mode	2D	hcb	AA	-	1856	0.54	28.0	0.19	0.27	0.28	1.36	1.34	5.96	4.55
BrCOF-2-AB	693	BrCOF-2 with AB stacking mode	2D	hcb	AB	-	2491	0.62	13.8	0.25	0.31	0.14	1.72	2.15	5.20	5.21

ivCOF-1-Br	694	ivCOF-1-Br	2D	hcb	-	-	992	1.00	7.8	0.10	0.50	0.08	0.50	0.92	4.51	4.26
ivCOF-2-Br	695	ivCOF-2-Br	2D	hcb	-	-	1839	0.66	14.9	0.18	0.33	0.15	1.24	1.57	5.48	4.82
Py-B18C6-COF-AA	696	Py-B18C6-COF-AA	2D	sql	AA	-	1505	0.82	11.9	0.15	0.41	0.12	0.89	1.33	5.01	4.58
Py-B18C6-COF-AB	697	Py-B18C6-COF-AB	2D	sql	AB	-	1979	0.60	9.4	0.20	0.30	0.09	1.38	1.79	5.60	5.10
Py-B24C8-COF-AA	698	Py-B24C8-COF-AA	2D	sql	AA	-	1639	0.77	9.4	0.16	0.38	0.09	1.01	1.48	5.15	4.77
Py-B24C8-COF-AB	699	Py-B24C8-COF-AB	2D	sql	AB	-	1925	0.63	10.3	0.19	0.31	0.10	1.32	1.73	5.53	5.02
NiPc-TFPN-COF-AA	700	NiPc-TFPN COF with AA stacking	2D	sql	AA	-	1141	1.09	9.6	0.11	0.55	0.10	0.52	1.03	4.01	4.19
NiPc-TFPN-COF-AB	701	NiPc-TFPN COF with AB stacking	2D	sql	AB	-	722	1.12	5.1	0.07	0.56	0.05	0.32	0.69	4.07	4.09
COF-C4	702	COF-C4	2D	hcb	-	-	1693	0.79	14.8	0.17	0.40	0.15	1.02	1.44	5.01	4.61
ivCOF-O	703	ivCOF-O	2D	hcb	-	-	1931	0.59	16.8	0.19	0.30	0.17	1.36	1.61	5.67	4.87
vCOF-N	704	vCOF-N	2D	hcb	-	-	2090	0.53	19.5	0.21	0.26	0.19	1.54	1.68	5.83	4.93
DBOV-COF-AA	705	the AA-stacking mode of DBOV-COF	2D	hcb	AA	-	2501	0.36	36.5	0.25	0.18	0.36	2.05	1.59	6.16	4.80
DBOV-COF-ABC	706	the ABC-stacking mode of DBOV-COF	2D	hcb	AB	-	1196	0.87	11.0	0.12	0.44	0.11	0.67	1.06	4.95	4.39
DBOV-DCTMP-COF	707	DBOV-DCTMP-COF	2D	hcb	AA	-	1197	0.87	11.0	0.12	0.44	0.11	0.67	1.07	4.96	4.39

DBOV-DCTMP-COF-AB	708	the AB-stacking mode of DBOV-DCTMP-COF	2D	hcb	AB	-	1398	0.70	14.8	0.14	0.35	0.15	0.91	1.19	5.58	4.55
JUC-596-hea	709	JUC-596 calculated based on the hea net	3D	hea	-	-	7385	0.15	26.0	0.74	0.08	0.26	6.82	5.46	2.42	7.76
JUC-597-hea	710	JUC-597 calculated based on the hea net	3D	hea	-	-	7084	0.16	25.9	0.71	0.08	0.26	6.51	5.25	2.68	7.60
BT-PTO-COF-AA	711	the AA-stacking model of BT-PTO COF	2D	hcb	-	-	1733	0.66	20.3	0.17	0.33	0.20	1.16	1.38	5.54	4.60
NKCOF-113	712	NKCOF-113	2D	hcb	-	-	2178	0.37	37.4	0.22	0.18	0.37	1.78	1.36	6.38	4.60
RhCp-NKCOF-113	713	RhCp-NKCOF-113	2D	hcb	-	-	1800	0.51	31.5	0.18	0.25	0.31	1.34	1.23	6.12	4.45
JUC-590-4	714	JUC-590 based on the 4-fold interpenetrated dia net	3D	dia	-	-	7893	0.23	17.1	0.79	0.11	0.17	6.99	6.54	1.87	8.20
JUC-590-5	715	JUC-590 based on the 5-fold interpenetrated dia net	3D	dia	-	-	6017	0.34	16.8	0.60	0.17	0.17	4.99	5.01	3.30	7.16
JUC-591-6	716	JUC-591based on the 6-fold interpenetrated dia net	3D	dia	-	-	4407	0.44	14.2	0.44	0.22	0.14	3.45	3.78	4.37	6.34
JUC-591-7	717	JUC-591based on the 7-fold interpenetrated dia net	3D	dia	-	-	1020	0.98	7.2	0.10	0.49	0.07	0.52	0.95	4.58	4.31

JUC-591-8	718	JUC-591based on the 8-fold interpenetrated dia net	3D	dia	-	-	1498	0.78	6.5	0.15	0.39	0.07	0.91	1.40	5.19	4.77
1-NUS-2	719	Δ-NUS-2	2D	hcb	-	-	1008	1.09	8.5	0.10	0.54	0.08	0.46	0.92	4.10	4.16
1-TpPa-1	720	Δ-TpPa-1	2D	hcb	-	-	1626	0.72	15.0	0.16	0.36	0.15	1.04	1.38	5.34	4.64
1-TpPa-2	721	Δ-TpPa-2	2D	hcb	-	-	1652	0.75	12.8	0.17	0.37	0.13	1.03	1.44	5.23	4.69
2-NUS-2	722	Λ-NUS-2	2D	hcb	-	-	1022	1.08	8.5	0.10	0.54	0.08	0.47	0.93	4.13	4.18
2-TpPa-1	723	Λ-TpPa-1	2D	hcb	-	-	1644	0.72	13.4	0.16	0.36	0.13	1.05	1.42	5.34	4.70
2-TpPa-2	724	Λ-TpPa-2	2D	hcb	-	-	1666	0.75	11.2	0.17	0.37	0.11	1.04	1.48	5.23	4.75
RuCOF-ETTA-soc	725	RuCOF-ETTA with soc topology	3D	soc	-	-	2839	0.46	12.4	0.28	0.23	0.12	2.18	2.49	5.51	5.59
RuCOF-ETTA-stp	726	RuCOF-ETTA with stp topology	3D	stp	-	-	3727	0.50	15.1	0.37	0.25	0.15	2.79	3.17	4.69	5.91
RuCOF-ETTBA-stp	727	RuCOF-ETTBA with stp topology	3D	stp	-	-	5675	0.27	24.0	0.57	0.13	0.24	4.91	4.31	3.74	6.85
RuCOF-TPB-soc	728	RuCOF-TPBwith soc topology	3D	soc	-	-	3457	0.39	14.0	0.35	0.20	0.14	2.77	2.97	5.25	5.92
RuCOF-TPB-stp	729	RuCOF-TPB with stp topology	3D	stp	-	-	5037	0.37	18.7	0.50	0.19	0.19	4.09	4.09	4.03	6.58
ETTF-DABP-COF-2	241	refined unit cell parameters for ETTF-DABP-COF	2D	kgm	-	-	2720	0.40	33.0	0.27	0.20	0.33	2.17	1.82	5.81	4.97
SIOC-COF-1	417	SIOC-COF-1	2D	kgm	-	-	2390	0.46	28.5	0.24	0.23	0.29	1.84	1.71	5.86	4.88
SIOC-COF-2	418	SIOC-COF-2	2D	kgm	-	-	2645	0.39	35.2	0.26	0.20	0.35	2.12	1.71	5.91	4.87
NKCOF-52	733	NKCOF-52	2D	hcb	-	-	2107	0.59	14.8	0.21	0.30	0.15	1.49	1.79	5.56	5.02
NKCOF-53	734	NKCOF-53	2D	hcb	-	-	2078	0.69	11.0	0.21	0.34	0.11	1.36	1.85	5.20	5.02
NKCOF-54	735	NKCOF-54	2D	hcb	-	-	1832	0.77	11.2	0.18	0.38	0.11	1.13	1.63	5.03	4.81
TTF-BT-COF-AA	736	TTF-BT-COF with AA stacking	2D	sql	-	-	2235	0.53	23.5	0.22	0.27	0.24	1.64	1.71	5.70	4.88

TP-COF	737	TP-COF	2D	hcb	-	-	1770	0.52	28.7	0.18	0.26	0.29	1.31	1.26	6.07	4.50
CCOF-15	738	CCOF-15	3D	dia	-	-	650	1.03	5.1	0.06	0.52	0.05	0.31	0.62	4.51	4.14
CCOF-16	739	CCOF-16	3D	dia	-	-	1387	0.84	12.0	0.14	0.42	0.12	0.80	1.22	4.98	4.49
2D-COF-1	740	2D-COF-1	2D	sql	-	-	1815	0.77	9.3	0.18	0.39	0.09	1.11	1.65	5.02	4.85
2D-COF-2	741	2D-COF-2	2D	sql	-	-	2104	0.67	11.3	0.21	0.34	0.11	1.40	1.87	5.24	5.04
2D-COF-3	742	2D-COF-3	2D	sql	-	-	2092	0.69	11.5	0.21	0.35	0.12	1.37	1.85	5.16	5.01
FZU-100-AA	743	FZU-100 (AA 1D Structure)	2D	sql	-	-	1113	0.85	11.5	0.11	0.43	0.11	0.64	0.99	5.09	4.36
FZU-101-AA	744	FZU-101 (AA1D Structure)	2D	sql	-	-	897	1.05	9.1	0.09	0.53	0.09	0.43	0.82	4.32	4.13
FZU-102-AA	745	FZU-102 (AA 1D Structure)	2D	sql	-	-	866	0.95	9.5	0.09	0.47	0.09	0.46	0.78	4.80	4.20
FZU-103-AA	746	FZU-103 (AA 1D Structure)	2D	sql	-	-	1218	0.83	11.6	0.12	0.42	0.12	0.71	1.08	5.12	4.43
Co-BFBim-COF-AA	747	the reversible AA stacking structure of the Co-BFBim-COF	2D	sql	-	-	2148	0.45	25.3	0.21	0.23	0.25	1.66	1.60	6.07	4.86
Co-iBFBim-COF-I-AA	748	the reversible AA stacking structure of the Co-iBFBim-COF-I	2D	sql	-	-	2005	0.53	22.3	0.20	0.26	0.22	1.48	1.56	5.89	4.81
COF-923-AA	749	COF-923 based on the AA-stacking	2D	hcb	-	-	2728	0.31	38.6	0.27	0.15	0.39	2.31	1.68	6.16	4.90
COF-932-AA	750	COF-932 based on the AA-stacking	2D	hcb	-	-	2674	0.31	39.0	0.27	0.15	0.39	2.27	1.63	6.21	4.86
H-COF-AA	751	H-COF with AA stacking models.	2D	hcb	-	-	2038	0.59	19.1	0.20	0.30	0.19	1.43	1.65	5.60	4.85

ODA-COF-AA	752	ODA-COF-AA with AA stacking models.	2D	hcb	-	-	2091	0.58	18.4	0.21	0.29	0.18	1.48	1.71	5.60	4.91
Tp-Acr-COF	753	Tp-Acr COF	2D	hcb	-	-	2004	0.55	21.9	0.20	0.27	0.22	1.45	1.57	5.80	4.80
V-2D-COF-1_AA	754	V-2D-COF-1_slipAA	2D	hcb	-	-	2201	0.43	27.8	0.22	0.21	0.28	1.73	1.59	6.12	4.84
V-2D-COF-2_AA	755	V-2D-COF-2_slipAA	2D	hcb	-	-	2083	0.45	28.4	0.21	0.23	0.28	1.61	1.49	6.13	4.74
V-2D-COF-3_AA	756	V-2D-COF-3_slipAA	2D	hcb	-	-	2238	0.36	36.5	0.22	0.18	0.37	1.83	1.42	6.36	4.66
sp2c-COF-5	429	AA-stacking mode of sp2c-COF-5	2D	kgm	-	-	2010	0.50	33.1	0.20	0.25	0.33	1.51	1.34	5.99	4.51
TFB-IQD-COF	758	TFB-IQD COF	2D	hcb	-	-	1607	0.86	10.1	0.16	0.43	0.10	0.92	1.45	4.79	4.64
TP-ND-COF	759	TP-ND COF	2D	hcb	-	-	1545	0.91	8.8	0.15	0.45	0.09	0.85	1.41	4.63	4.60
CN-COF	760	CN	2D	sql	-	-	1839	0.63	17.6	0.18	0.31	0.18	1.26	1.51	5.61	4.76
TUS-64-2	761	TUS-64 calculated based on the 2-fold interpenetrated stp net	3D	stp	-	-	6753	0.21	23.6	0.68	0.11	0.24	6.03	5.16	2.90	7.46
COF1	762	COF1	2D	hcb	-	-	1621	0.56	30.1	0.16	0.28	0.30	1.16	1.13	6.02	4.34
COF2	763	COF2	2D	hcb	-	-	1355	0.81	8.6	0.14	0.41	0.09	0.81	1.24	5.14	4.61
COF3	764	COF3	2D	hcb	-	-	1862	0.80	7.4	0.19	0.40	0.07	1.12	1.72	4.90	4.91
m-Naph-COF-AA-sql	765	the sql AA-stacking mode of m-Naph-COF refined unit cell parameters for	2D	sql	-	-	1617	0.75	12.0	0.16	0.37	0.12	1.01	1.42	5.25	4.70
sp2c-COF-5-2	430	sp2c-COF-5	2D	kgm	-	-	2127	0.47	33.9	0.21	0.24	0.34	1.63	1.41	6.02	4.58
Ti-COF-1	767	Ti-COF-1	3D	soc	-	-	2765	0.49	13.5	0.28	0.25	0.14	2.08	2.39	5.46	5.48

COF-Q-H-AA	768	the unit cell of COF-Q-H with AA packing	2D	hcb	-	-	133	1.21	5.9	0.01	0.61	0.06	0.05	0.13	3.89	3.68
QA-TAPT-COF	769	QA-TAPT-COF	2D	hcb	-	-	2259	0.40	35.4	0.23	0.20	0.35	1.80	1.46	6.17	4.66
QA-TPB-COF	770	QA-TPB-COF	2D	hcb	-	-	2142	0.42	35.6	0.21	0.21	0.36	1.69	1.38	6.20	4.58
BD-TMT-AA	771	BD-TMT-AA	2D	hcb	-	-	2193	0.58	16.5	0.22	0.29	0.16	1.56	1.83	5.56	5.03
DHBD-TMT-AA	772	DHBD-TMT-AA	2D	hcb	-	-	1976	0.67	14.6	0.20	0.34	0.15	1.31	1.69	5.34	4.88
HBD-TMT-AA	773	HBD-TMT-AA	2D	hcb	-	-	2071	0.63	14.4	0.21	0.31	0.14	1.42	1.77	5.45	4.98
TP-COF-AA-1	774	TP-COF with AA stacking	2D	sql	-	-	2020	0.60	16.0	0.20	0.30	0.16	1.41	1.70	5.57	4.93
Por-COF	775	Por-COF	2D	sql	-	-	1723	0.84	9.5	0.17	0.42	0.09	1.00	1.56	4.80	4.74
LiOOC-COF3	776	LiOOC-COF3	2D	hcb	-	-	1541	0.67	16.5	0.15	0.34	0.17	1.02	1.29	5.62	4.60
TB-COF	777	TB-COF	2D	hcb	-	-	2454	0.34	38.2	0.25	0.17	0.38	2.04	1.52	6.28	4.75
TP-TTA-COF	778	TP-TTA-COF	2D	hcb	-	-	1539	0.77	11.9	0.15	0.39	0.12	0.94	1.36	5.18	4.64
GT-COF-3	779	GT-COF-3	2D	hcb	-	-	1785	0.74	19.2	0.18	0.37	0.19	1.12	1.44	5.16	4.57
TPB-BPTA-COF	780	TPB-BPTA-COF	2D	hcb	-	-	2544	0.48	23.5	0.25	0.24	0.23	1.93	1.95	5.67	5.09
PTZ-TFP-COF-AA	781	PTZ-TFP-COF with AA-stacking	2D	hcb	-	-	1395	0.88	10.2	0.14	0.44	0.10	0.78	1.25	4.81	4.51
PD-COF	782	PD-COF	2D	hcb	-	-	1395	0.83	14.9	0.14	0.42	0.15	0.82	1.19	5.03	4.42
TF-COF	783	TF-COF	2D	hcb	-	-	996	1.12	14.0	0.10	0.56	0.14	0.44	0.86	3.96	3.96
Tp-ABA-Pa-1	784	Tp-ABA-Pa-1	2D	hcb	-	-	1602	0.64	24.0	0.16	0.32	0.24	1.09	1.22	5.72	4.44
Tp-ABA-Pa-2	785	Tp-ABA-Pa-2	2D	hcb	-	-	1847	0.57	23.0	0.18	0.28	0.23	1.32	1.42	5.84	4.67
Tp-ABA-TAPB	786	Tp-ABA-TAPB	2D	hcb	-	-	2121	0.50	23.2	0.21	0.25	0.23	1.59	1.63	5.92	4.87
Tp-ABA-TAPT	787	Tp-ABA-TAPT	2D	hcb	-	-	2033	0.51	23.1	0.20	0.26	0.23	1.51	1.56	5.94	4.81
BT-TAPT-COF	788	BT-TAPT-COF	2D	hcb	-	-	1658	0.56	26.3	0.17	0.28	0.26	1.19	1.22	6.00	4.48
TFB-BD-Me-2-AA	789	TFB-BD(Me)2 with eclipsed (AA) stacking mode	2D	hcb	AA	-	2082	0.52	21.6	0.21	0.26	0.22	1.54	1.63	5.84	4.87
TFB-BD-Me-2-AB	790	TFB-BD(Me)2 with eclipsed	2D	hcb	AB	-	3516	0.54	8.0	0.35	0.27	0.08	2.57	3.23	4.74	5.98

		(AB) stacking mode														
PCP-COF	791	PCP-COF	2D	sql	-	-	1657	0.85	7.9	0.17	0.42	0.08	0.95	1.53	4.80	4.74
TPTF-COF	792	TPTF-COF	2D	sql	-	-	1512	0.82	11.0	0.15	0.41	0.11	0.89	1.35	5.00	4.61
COF15C5	793	COF15C5	2D	hcb	-	-	1371	0.77	15.4	0.14	0.38	0.15	0.85	1.16	5.33	4.46
COF18C6	794	COF18C6	2D	hcb	-	-	1435	0.86	11.1	0.14	0.43	0.11	0.82	1.28	4.90	4.53
COF21C7	795	COF21C7	2D	hcb	-	-	1084	0.90	9.5	0.11	0.45	0.10	0.59	0.98	4.89	4.35
COF2OMe	796	COF2OMe	2D	hcb	-	-	2020	0.55	20.9	0.20	0.28	0.21	1.46	1.60	5.78	4.83
BT-COF1	797	BT-COF1	2D	hcb	-	-	1961	0.42	37.8	0.20	0.21	0.38	1.55	1.22	6.36	4.43
BT-COF2	798	BT-COF2	2D	hcb	-	-	1988	0.43	32.9	0.20	0.22	0.33	1.56	1.33	6.29	4.58
TPPY-PBT-COF	799	TPPY-PBT-COF	2D	sql	-	-	1848	0.55	13.0	0.18	0.28	0.13	1.34	1.61	5.89	4.98
DATD-COF-AA	800	DATD COF with AA stacking mode	2D	hcb	-	-	2254	0.44	24.0	0.23	0.22	0.24	1.75	1.71	6.02	4.96
Py-FTP-COF-AA	801	Py-FTP-COF with AA stacking.	2D	sql	-	-	2073	0.49	24.4	0.21	0.25	0.24	1.57	1.57	5.98	4.82
TSCH-BDA	802	TSCH-BDA COF	2D	hcb	-	-	2148	0.51	22.8	0.21	0.25	0.23	1.61	1.66	5.87	4.89
TSCH-DMTA	803	TSCH-DMTA COF	2D	hcb	-	-	1844	0.61	20.1	0.18	0.31	0.20	1.28	1.47	5.66	4.71
TSCH-NDA	804	TSCH-NDA COF	2D	hcb	-	-	2244	0.46	25.8	0.22	0.23	0.26	1.73	1.67	5.97	4.89
TAPB-DMTP-PA-COF-AA	805	Simulated AA-stacking structure of TAPB-DMTP-PA-COF	2D	hcb	-	-	1660	0.57	26.3	0.17	0.28	0.26	1.19	1.22	5.98	4.47
TAPT-TP-PA-COF-AA	806	the AAstacking mode of TAPT-TP-PA-COF	2D	hcb	-	-	1619	0.56	27.5	0.16	0.28	0.27	1.17	1.17	6.05	4.43
BTTZ-por-COF	807	BTTZ-por COF	2D	sql	-	-	1926	0.63	15.7	0.19	0.32	0.16	1.32	1.62	5.53	4.86
FBQD-por-COF	808	FBQD-por-COF	2D	sql	-	-	2270	0.54	17.4	0.23	0.27	0.17	1.65	1.87	5.63	5.07
PTBC-por-COF	809	PTBC-por COF	2D	sql	-	-	2283	0.54	17.5	0.23	0.27	0.17	1.66	1.88	5.62	5.07

TpTch-120	810	the eclipsed AA-stacking unit cell of enol form of synthesized COFs	2D	hcb	-	-	1397	0.90	10.6	0.14	0.45	0.11	0.77	1.25	4.74	4.48
TpTch-90	811	the eclipsed AA-stacking unit cell of keto form of synthesized COFs	2D	hcb	-	-	1389	0.91	10.2	0.14	0.45	0.10	0.76	1.25	4.70	4.48
Hz-TFPTZ-COF-AB	812	Hz-TFPTZ-COF-AB the AA Eclipsed form	2D	hcb	-	-	3492	0.51	9.8	0.35	0.25	0.10	2.61	3.15	4.86	5.95
TiCOF-spn	813	TiCOF-spn with the spn net via Pawley refinement	3D	spn	-	-	3725	0.24	29.7	0.37	0.12	0.30	3.28	2.62	5.52	5.73
TAPD-TDA-COF	814	TAPD-TDA COF	2D	sql	-	-	679	1.05	9.3	0.07	0.53	0.09	0.32	0.62	4.43	4.01
BD-COF	815	BD-COF	2D	hcb	-	-	2093	0.45	27.0	0.21	0.22	0.27	1.62	1.53	6.14	4.79
DBD-COF	816	DBD-COF	2D	hcb	-	-	2273	0.43	25.7	0.23	0.21	0.26	1.78	1.69	6.07	4.94
MB-COF	817	MB-COF	2D	hcb	-	-	2799	0.33	28.4	0.28	0.17	0.28	2.34	2.00	6.01	5.22
Ox-BD-COF	818	Ox-BD-COF	2D	hcb	-	-	2703	0.32	30.6	0.27	0.16	0.31	2.27	1.87	6.13	5.11
Ox-DBD-COF	819	Ox-DBD-COF	2D	hcb	-	-	3025	0.30	30.5	0.30	0.15	0.30	2.57	2.10	5.94	5.30
TPE-COF-II	540	TPE-COF-II	2D	kgm	-	-	2164	0.65	11.7	0.22	0.33	0.12	1.46	1.91	5.29	5.08
mcm-HgPc-3N	821	mcm-HgPc-3N	2D	sql	-	-	2552	0.33	22.4	0.26	0.16	0.22	2.13	1.98	6.23	5.28
mcm-ZnPc-1	822	mcm-ZnPc-1	2D	sql	-	-	2626	0.31	22.2	0.26	0.16	0.22	2.21	2.04	6.22	5.33
mcm-ZnPc-3	823	mcm-ZnPc-3	2D	sql	-	-	3056	0.27	22.2	0.31	0.13	0.22	2.64	2.38	6.01	5.59
mcm-ZnPc-3N	824	mcm-ZnPc-3N	2D	sql	-	-	2981	0.28	22.4	0.30	0.14	0.22	2.56	2.31	6.04	5.54
NUST-21	825	NUST-21	2D	hcb	-	-	2132	0.49	23.0	0.21	0.24	0.23	1.61	1.64	5.95	4.89
NUST-22	826	NUST-22	2D	hcb	-	-	2097	0.50	21.2	0.21	0.25	0.21	1.57	1.65	5.91	4.91
BTEA-COF-AA	827	the AA-stacking mode of BTEA-COF	2D	hcb	-	-	2381	0.54	15.9	0.24	0.27	0.16	1.74	2.00	5.56	5.17

EBA-COF-AA	828	the AA-stacking mode of EBA-COF	2D	hcb	-	-	2637	0.39	27.9	0.26	0.19	0.28	2.13	1.90	5.94	5.10
JUC-557	829	JUC-557	2D	sql	-	-	2900	0.50	15.3	0.29	0.25	0.15	2.18	2.45	5.34	5.49
ETTA-PyTTA-COF	830	ETTA-PyTTA-COF	2D	sql	-	-	2490	0.60	11.7	0.25	0.30	0.12	1.74	2.20	5.26	5.29
TTF-TD-COF-AA	831	TTF-TD-COF calculated based on the eclipsed AA stacking mode.	2D	sql	-	-	2126	0.48	24.6	0.21	0.24	0.25	1.61	1.60	5.98	4.84
JUC-610	832	JUC-610	3D	pts	-	-	8065	0.21	16.1	0.81	0.10	0.16	7.23	6.77	1.73	8.34
COF-1	833	COF-1	3D	pts	-	-	7758	0.18	34.4	0.78	0.09	0.34	7.07	5.09	2.05	7.67
PTz-BTA-COF	834	PTz-BTA-COF	2D	sql	AA	-	1685	0.64	16.8	0.17	0.32	0.17	1.15	1.40	5.67	4.70
PTz-BTA-COF-AB	835	the AB-stacking mode of PTz-BTA-COF	2D	sql	AB	-	2512	0.69	8.9	0.25	0.34	0.09	1.65	2.29	4.91	5.30
PTz-Py-COF-AB	836	the AB-stacking mode of PTz-Py-COF	2D	sql	-	-	377	1.13	4.9	0.04	0.56	0.05	0.16	0.36	4.20	3.91
PTz-TPB-COF	837	PTz-TPB-COF	2D	hcb	AA	-	2341	0.36	29.9	0.23	0.18	0.30	1.92	1.64	6.27	4.91
PTz-TPB-COF-AB	838	the AB-stacking mode of PTz-TPB-COF	2D	hcb	AB	-	3026	0.43	18.5	0.30	0.21	0.18	2.38	2.47	5.49	5.53
JUC-589	839	JUC-589	2D	sql	-	-	3260	0.36	23.7	0.33	0.18	0.24	2.67	2.49	5.53	5.56
Py-OMe3P-COF	840	Py-OMe3P-COF	2D	sql	-	-	2264	0.47	22.3	0.23	0.24	0.22	1.73	1.76	5.92	4.99
P-COF	841	P-COF with AA stacking.	2D	hcb	-	-	1705	0.71	12.1	0.17	0.36	0.12	1.10	1.50	5.34	4.78
T-COF-AA	842	T-COF with AA stacking.	2D	hcb	-	-	1788	0.73	11.8	0.18	0.37	0.12	1.13	1.58	5.21	4.81
R-CuTAPBP-COF	843	(R)-CuTAPBP-COF	2D	sql	-	-	5621	0.36	15.1	0.56	0.18	0.15	4.61	4.77	3.59	7.00
Sb-COF-AA	844	Sb-COF Eclipsed AA	2D	hcb	-	-	2886	0.43	20.8	0.29	0.21	0.21	2.27	2.29	5.59	5.39

Tp-MTABs-AB	845	Tp-MTABs-AB	2D	hcb	-	-	0	1.23	5.5	0.00	0.61	0.05	0.00	0.00	3.86	3.61
dHP-TAB-COF	846	dHP-TAB COF	2D	hcb	-	-	2109	0.36	43.4	0.21	0.18	0.43	1.73	1.19	6.46	4.39
TpPTO-COF-AA	847	eclipsed AA-stacking unit cell of TpPTO-COF	2D	hcb	-	-	1152	0.68	20.6	0.12	0.34	0.21	0.76	0.91	5.84	4.28
COF-TzDa	848	COF-TzDa	2D	hcb	-	-	2051	0.45	28.6	0.21	0.23	0.29	1.59	1.46	6.15	4.72
TpTsc-AA	849	TpTsc-AA	2D	hcb	-	-	1470	0.82	11.9	0.15	0.41	0.12	0.87	1.30	5.05	4.56
TpTt-AA	850	TpTt-AA	2D	hcb	-	-	601	1.25	5.2	0.06	0.63	0.05	0.22	0.57	3.51	3.89
RFCOF-E-AA	851	the AA stacking unit cell of RFCOF-E	2D	hcb	-	-	2079	0.47	26.7	0.21	0.23	0.27	1.59	1.52	6.08	4.77
RFCOF-S-50-AA	852	the AA stacking unit cell of RFCOF-S-50	2D	hcb	-	-	2088	0.46	27.3	0.21	0.23	0.27	1.61	1.52	6.10	4.77
COF-NUST-16-CUT	853	simulated cut net of COF-NUST-16	3D	cut	-	-	7244	0.19	21.5	0.72	0.09	0.22	6.56	5.69	2.50	7.79
COF-NUST-16-TTY	854	simulated tty net of COF-NUST-16	3D	tty	-	-	6286	0.32	15.0	0.63	0.16	0.15	5.29	5.34	3.12	7.38
COF-NUST-17	855	COF-NUST-17	2D	sql	-	-	2305	0.59	16.8	0.23	0.29	0.17	1.63	1.92	5.44	5.06
TFBD-NH2	856	TFBD-NH2	2D	hcb	-	-	2251	0.36	36.0	0.23	0.18	0.36	1.85	1.44	6.36	4.69
TFPA	857	TFPA	2D	hcb	-	-	2080	0.48	27.6	0.21	0.24	0.28	1.58	1.50	6.02	4.73
BTT-AMPD	858	COFBTT-AMPD	2D	hcb	-	-	1915	0.49	27.6	0.19	0.24	0.28	1.45	1.39	6.11	4.64
Py-Na-COF	859	Py-Na-COF	2D	sql	-	-	1036	1.03	6.7	0.10	0.51	0.07	0.50	0.97	4.35	4.29
TUS-84	860	TUS-84	3D	scu	-	-	1124	0.69	9.5	0.11	0.35	0.09	0.74	1.02	5.81	4.59
TUS-84-C	861	TUS-84-C	3D	scu-c	-	-	3155	0.53	13.9	0.32	0.26	0.14	2.32	2.72	5.04	5.63
TAPA-BTD-COF-AA	862	TAPA-BTD-COF-AA	2D	hcb	-	-	2316	0.34	38.4	0.23	0.17	0.38	1.92	1.43	6.36	4.66
TAPA-TPD-COF	863	TAPA-TPD-COF	2D	hcb	-	-	2913	0.27	40.2	0.29	0.14	0.40	2.52	1.74	6.13	4.98
TAPB-BTD-COF	864	TAPB-BTD-COF	2D	hcb	-	-	2248	0.32	40.6	0.22	0.16	0.41	1.89	1.33	6.51	4.58

JUC-616	865	JUC-616	2D	hcb	-	-	2098	0.39	33.1	0.21	0.20	0.33	1.68	1.40	6.34	4.66
JUC-617	866	JUC-617	2D	hcb	-	-	2041	0.41	32.6	0.20	0.20	0.33	1.62	1.38	6.33	4.63
JUC-618	867	JUC-618	2D	hcb	-	-	1881	0.45	32.4	0.19	0.22	0.32	1.46	1.27	6.31	4.52
OH-COOH-COF	868	OH-COOH-COF	2D	hcb	-	-	1250	0.99	12.0	0.13	0.50	0.12	0.63	1.10	4.40	4.27
COOH-COF-2	869	COOH-COF-2	2D	hcb	-	-	1497	0.69	20.3	0.15	0.34	0.20	0.98	1.19	5.58	4.45
COOH-COF-2-AA	870	the AA-stacking mode of COOH-COF-2	2D	hcb	-	-	1175	0.96	12.2	0.12	0.48	0.12	0.61	1.03	4.60	4.26
DDHP-COF	871	DDHP-COF	3D	lvt	-	-	7018	0.21	19.3	0.70	0.11	0.19	6.26	5.66	2.66	7.72
2N-COF	872	2N-COF	2D	sql	-	-	2276	0.44	25.6	0.23	0.22	0.26	1.77	1.69	6.01	4.93
4N-COF	873	4N-COF	2D	sql	-	-	2248	0.44	26.1	0.22	0.22	0.26	1.75	1.66	6.05	4.90
6N-COF	874	6N-COF	2D	sql	-	-	2267	0.44	25.7	0.23	0.22	0.26	1.77	1.68	6.04	4.92
TPE-COF-III	541	TPE-COF-III	2D	kgm	-	-	2134	0.59	16.3	0.21	0.29	0.16	1.51	1.79	5.55	4.99
BTT-TAPB-COF	876	BTT-TAPB-COF	2D	hcb	-	-	1651	0.72	15.4	0.17	0.36	0.15	1.06	1.40	5.34	4.64
BTT-TAT-COF	877	BTT-TAT-COF	2D	hcb	-	-	1570	0.75	15.4	0.16	0.37	0.15	0.98	1.33	5.29	4.58
TFPB-TAPB-COF	878	TFPB-TAPB-COF	2D	hcb	-	-	2216	0.52	18.7	0.22	0.26	0.19	1.64	1.80	5.75	5.02
Tfpa-Mth-COF-AA	879	Tfpa-Mth COF with eclipsed packing	2D	hcb	AA	-	2796	0.45	24.1	0.28	0.23	0.24	2.16	2.12	5.57	5.22
Tfpa-Mth-COF-AB	880	Tfpa-Mth COF with staggered packing	2D	hcb	AB	-	5030	0.44	10.1	0.50	0.22	0.10	3.92	4.52	3.88	6.77
TTPE-COF	881	TTPE-COF	2D	sql	-	-	2072	0.65	10.7	0.21	0.33	0.11	1.40	1.85	5.34	5.06
TP-DMPTU-COF-AA	882	the AA-stacking mode of TP-DMPTU-COF	2D	hcb	AA	-	947	0.84	16.9	0.09	0.42	0.17	0.55	0.79	5.25	4.12
TP-DMPTU-COF-AB	883	the AB-stacking mode of TP-DMPTU-COF	2D	hcb	AB	-	0	0.84	5.2	0.00	0.42	0.05	0.00	0.00	5.79	4.00
TP-DMTU-COF-AA	884	the AA-stacking mode of TP-DMTU-COF	2D	hcb	AA	-	670	1.21	11.0	0.07	0.60	0.11	0.27	0.60	3.70	3.80

TP-DMTU-COF-AB	885	the AB-stacking mode of TP-DMTU-COF	2D	hcb	AB	-	0	1.21	4.2	0.00	0.60	0.04	0.00	0.00	3.97	3.67
TP-TU-COF-AA	886	the AA-stacking mode of TP-TU-COF	2D	hcb	AA	-	692	1.14	10.5	0.07	0.57	0.10	0.30	0.62	3.98	3.89
TP-TU-COF-AB	887	the AB-stacking mode of TP-TU-COF	2D	hcb	AB	-	0	1.14	4.4	0.00	0.57	0.04	0.00	0.00	4.28	3.72
RE-COF-1	888	RE-COF-1	2D	hcb	-	-	1862	0.60	19.1	0.19	0.30	0.19	1.30	1.51	5.70	4.76
RE-COF-2	889	RE-COF-2	2D	hcb	-	-	1904	0.56	22.1	0.19	0.28	0.22	1.37	1.48	5.81	4.72
F-COF-1	890	F-COF-1	2D	hcb	-	-	2069	0.58	17.7	0.21	0.29	0.18	1.47	1.70	5.62	4.92
F-COF-2	891	F-COF-2	2D	hcb	-	-	2275	0.53	18.4	0.23	0.26	0.18	1.68	1.86	5.69	5.06
PD-COF-23	892	PD-COF-23	2D	sql	-	-	2003	0.59	16.4	0.20	0.30	0.16	1.41	1.67	5.63	4.92
PD-COF-23-Ni	893	PD-COF-23-Ni	2D	sql	-	-	1928	0.61	16.4	0.19	0.31	0.16	1.34	1.61	5.59	4.86
CPCOF-2	894	CPOF-2 calculated based on the 9-fold interpenetrated dia net	3D	dia	-	-	3124	0.44	15.7	0.31	0.22	0.16	2.43	2.63	5.35	5.65
CPCOF-3	895	CPOF-3 calculated based on the 11-fold interpenetrated dia net.	3D	dia	-	-	3003	0.44	17.1	0.30	0.22	0.17	2.34	2.49	5.46	5.55
TPB-DHZ-COF	896	the AA-stacking mode of TPB-DHZ-COF	2D	hcb	-	-	2880	0.44	23.5	0.29	0.22	0.24	2.25	2.20	5.57	5.30
TPE-DHZ-COF	897	the AA-stacking mode of TPE-DHZ-COF	2D	sql	-	-	1377	0.75	9.5	0.14	0.37	0.09	0.86	1.25	5.40	4.66
TFBD-Py-COF	898	TFBD-Py-COF	2D	sql	-	-	1054	1.04	7.0	0.11	0.52	0.07	0.51	0.98	4.29	4.28

Tp-Ta-COF	899	Tp-Ta-COF	2D	hcb	-	-	1510	0.79	11.4	0.15	0.40	0.11	0.91	1.34	5.13	4.62
PTDCOF	900	PTDCOF with serrated	2D	hcb	-	-	1100	1.00	8.6	0.11	0.50	0.09	0.55	1.00	4.46	4.29
PTDCOF-AA	901	PTDCOF with AA	2D	hcb	AA	-	1046	1.02	9.1	0.10	0.51	0.09	0.51	0.95	4.38	4.23
PTDCOF-AB	902	PTDCOF with AB	2D	hcb	AB	-	0	1.02	4.2	0.00	0.51	0.04	0.00	0.00	4.92	3.86
TCPB-DMTA-COF-AA	903	TCPB-DMTA-COF-AA	2D	hcb	AA	-	2082	0.49	27.1	0.21	0.24	0.27	1.57	1.52	5.99	4.74
TCPB-DMTA-COF-AB	904	TCPB-DMTA-COF-AB	2D	hcb	AB	-	2678	0.50	11.1	0.27	0.25	0.11	2.00	2.38	5.47	5.50
TpTab-COF	905	TpTab-COF	2D	hcb	-	-	1132	0.89	11.0	0.11	0.44	0.11	0.63	1.01	4.93	4.35
3D-COF-1	906	3D-COF-1	3D	dia	-	-	3055	0.51	7.5	0.31	0.26	0.07	2.27	2.83	5.16	5.79
3D-COF-10	907	3D-COF-10	3D	dia	-	-	3157	0.51	9.8	0.32	0.25	0.10	2.36	2.85	5.11	5.78
TAPA-PCBA	908	TAPA-PCBA with eclipsed arrangement	2D	hcb	-	-	2839	0.43	16.9	0.28	0.22	0.17	2.22	2.36	5.61	5.48
S-NHC-Au-SA-COF	909	(S)-NHC-Au-SA-COF	2D	hcb	-	-	3583	0.48	15.8	0.36	0.24	0.16	2.73	3.02	4.89	5.84
COF-1-ffc	910	COF-1 with the noninterpenetrated ffc topology	3D	ffc	-	1	8156	0.05	58.8	0.82	0.03	0.59	7.95	3.36	1.80	7.26
COF-1-ffc-1	911	COF-1 with the interpenetrated ffc topology	3D	ffc	-	2	8620	0.09	34.8	0.86	0.05	0.35	8.22	5.62	1.32	8.17
COF-1-tbo	912	COF-1 with the noninterpenetrated tbo topology	3D	tbo	-	1	7906	0.06	60.9	0.79	0.03	0.61	7.66	3.09	2.03	7.06
COF-1-tbo-1	913	COF-1 with the interpenetrated tbo topology	3D	tbo	-	2	8318	0.12	31.9	0.83	0.06	0.32	7.82	5.66	1.58	8.08

COF-2-ffc	914	COF-2 with the noninterpenetrated ffc topology	3D	ffc	-	1	7789	0.05	58.8	0.78	0.03	0.59	7.58	3.21	2.15	7.08
COF-2-ffc-2	915	COF-2 with the interpenetrated ffc topology	3D	ffc	-	2	7972	0.10	34.3	0.80	0.05	0.34	7.57	5.24	1.92	7.86
COF-2-tbo	916	COF-1 with the noninterpenetrated tbo topology	3D	tbo	-	1	7622	0.06	61.4	0.76	0.03	0.61	7.37	2.94	2.30	6.90
COF-2-tbo-1	917	COF-1 with the interpenetrated tbo topology	3D	tbo	-	2	7931	0.13	31.9	0.79	0.06	0.32	7.43	5.40	1.94	7.88
3D-CageCOF-1	918	3D-CageCOF-1	3D	acs	-	-	4090	0.49	11.8	0.41	0.25	0.12	3.08	3.61	4.46	6.20
COF-DB	919	COF-DB	2D	hcb	-	-	2192	0.43	32.5	0.22	0.22	0.32	1.72	1.48	6.11	4.69
COF-DT	920	COF-DT	2D	hcb	-	-	2275	0.41	33.3	0.23	0.20	0.33	1.81	1.52	6.15	4.73
CCOF-17	921	CCOF 17	2D	sql	-	-	3958	0.36	19.3	0.40	0.18	0.19	3.25	3.19	4.96	6.04
CCOF-17-R	922	CCOF 17-R	2D	sql	-	-	3677	0.38	18.7	0.37	0.19	0.19	2.98	2.99	5.13	5.90
CCOF-18	923	CCOF 18	2D	sql	-	-	3892	0.37	19.8	0.39	0.18	0.20	3.18	3.12	4.99	5.99
CCOF-18-R	924	CCOF 18-R	2D	sql	-	-	4052	0.35	20.5	0.41	0.18	0.20	3.34	3.22	4.90	6.06
3D-ceq-COF	925	3D-ceq-COF calculated based on the non-interpenetrated ceq net	3D	ceq	-	1	3095	0.39	23.2	0.31	0.20	0.23	2.49	2.38	5.56	5.46
3D-ceq-COF-2	926	3D-ceq-COF calculated based on the 2-fold interpenetrated ceq net	3D	ceq	-	2	3933	0.51	11.0	0.39	0.26	0.11	2.92	3.50	4.51	6.12

TAPB-COF	927	TAPB-COF	2D	hcb	-	-	2652	0.27	45.5	0.27	0.13	0.45	2.30	1.45	6.36	4.69
TAPB-COF-P	928	TAPB-COF-P	2D	hcb	-	-	2398	0.33	40.8	0.24	0.16	0.41	2.01	1.42	6.36	4.65
OH-TPB-BPTA-COF	929	OH-TPB-BPTA-COF	2D	hcb	-	-	1402	0.75	10.8	0.14	0.37	0.11	0.88	1.25	5.38	4.63
OH-TPB-BPTA-COF-DFTB	930	OH-TPB-BPTA-COF-DFTB	2D	hcb	-	-	1346	0.77	10.6	0.13	0.39	0.11	0.83	1.20	5.31	4.58
COF-609	931	COF-609	2D	hcb	-	-	1963	0.54	21.1	0.20	0.27	0.21	1.43	1.55	5.87	4.81
COF-609-Im	932	COF-609-Im	2D	hcb	-	-	2213	0.36	37.7	0.22	0.18	0.38	1.82	1.38	6.39	4.62
COF-609-THQ	933	COF-609-THQ	2D	hcb	-	-	2498	0.39	32.6	0.25	0.19	0.33	2.02	1.68	6.05	4.89
c-HBC-COF-AA	934	AA-stacking mode of c-HBC-COF	2D	sql	AA	-	1046	0.93	10.7	0.10	0.47	0.11	0.56	0.93	4.78	4.27
c-HBC-COF-AB	935	AB-stacking mode of c-HBC-COF	2D	sql	AB	-	0	0.93	4.9	0.00	0.47	0.05	0.00	0.00	5.33	3.92
TPE-COF-IV	542	TPE-COF-IV	2D	kgm	-	-	2692	0.51	15.9	0.27	0.25	0.16	2.01	2.26	5.45	5.36
DHP-COF-AA-slip	937	slipped AA-stacking mode of DHP-COF	2D	sql	-	-	2682	0.48	20.4	0.27	0.24	0.20	2.04	2.14	5.56	5.25
TDCOF-1-A	938	TDCOF-1-A	2D	hcb	-	-	2558	0.21	65.4	0.26	0.11	0.65	2.29	0.89	6.66	4.11
TDCOF-1-S-AA	939	TDCOF-1-S-AA	2D	hcb	-	-	2543	0.21	63.9	0.25	0.10	0.64	2.28	0.92	6.68	4.14
TDCOF-2	940	TDCOF-2	2D	hcb	-	-	2701	0.19	69.2	0.27	0.10	0.69	2.44	0.83	6.59	4.08
TDCOF-3-A	941	TDCOF-3-A.	2D	hcb	-	-	2761	0.16	88.9	0.28	0.08	0.89	2.55	0.31	6.67	3.56
TDCOF-3-S	942	TDCOF-3-S	2D	hcb	-	-	2751	0.16	86.9	0.28	0.08	0.87	2.54	0.36	6.68	3.61
TDpolymer-1-A	943	TDpolymer-1-A	2D	hcb	-	-	2579	0.21	65.5	0.26	0.10	0.66	2.31	0.89	6.64	4.11
TDpolymer-2-AA	944	eclipsed AA stacking mode for TDpolymer-2	2D	hcb	-	-	2904	0.15	93.0	0.29	0.07	0.93	2.69	0.20	6.58	3.52
TDpolymer-3-A	945	TDpolymer-3-A	2D	hcb	-	-	2562	0.20	70.0	0.26	0.10	0.70	2.30	0.77	6.69	3.98
TDpolymer-4	946	TDpolymer-4	2D	hcb	-	-	2775	0.15	88.9	0.28	0.08	0.89	2.56	0.31	6.67	3.57
TDpolymer-5-A	947	TDpolymer-5-A	2D	hcb	-	-	2779	0.15	89.2	0.28	0.08	0.89	2.56	0.30	6.66	3.56
NKCOF-21	948	NKCOF-21	3D	bcu	-	-	5652	0.34	16.2	0.57	0.17	0.16	4.70	4.74	3.62	7.00
NKCOF-22	949	NKCOF-22	3D	bcu	-	-	6733	0.25	17.5	0.67	0.13	0.18	5.88	5.55	2.85	7.59

NKCOF-23	950	NKCOF-23	3D	bcu	-	-	7493	0.21	19.8	0.75	0.10	0.20	6.72	6.01	2.25	7.95
NUST-5	951	NUST-5	3D	pcb	-	-	6384	0.22	23.2	0.64	0.11	0.23	5.69	4.90	3.22	7.28
NUST-6	952	NUST-6	3D	pcb	-	-	6094	0.22	21.2	0.61	0.11	0.21	5.41	4.80	3.47	7.19
HFPB−TABPB	953	HFPB−TABPB	2D	kgd	-	-	1683	0.75	10.4	0.17	0.38	0.10	1.05	1.51	5.19	4.78
HFPB−TAPA	954	HFPB−TAPA	2D	kgd	-	-	1037	0.99	5.9	0.10	0.49	0.06	0.52	0.98	4.53	4.35
HFPB−TAPT	955	HFPB−TAPT	2D	kgd	-	-	363	0.92	4.8	0.04	0.46	0.05	0.20	0.35	5.20	4.12
TPB-TFB-COF	956	TPB-TFB-COF	2D	hcb	-	-	1723	0.69	12.3	0.17	0.35	0.12	1.13	1.51	5.41	4.80
TPB-TFB-COF-AA	957	the AA-stacking mode of TPB-TFB-COF	2D	hcb	AA	-	1728	0.69	12.3	0.17	0.35	0.12	1.13	1.51	5.41	4.80
TPB-TFB-COF-AB	958	the AB-stacking mode of TPB-TFB-COF	2D	hcb	AB	-	2552	0.69	6.4	0.26	0.35	0.06	1.67	2.39	4.87	5.39
PT-COF	959	PT-COF	2D	hcb	-	-	1633	0.71	20.2	0.16	0.35	0.20	1.05	1.30	5.40	4.50
TPE-Ph_COF	544	TPE-Ph COF	2D	kgm	-	-	2948	0.42	27.2	0.29	0.21	0.27	2.32	2.15	5.56	5.23
sonoCOF-A3	961	sonoCOF-A3	2D	sql	-	-	2042	0.63	13.5	0.20	0.31	0.14	1.40	1.77	5.46	4.99
sonoCOF-A4	962	sonoCOF-A4	2D	sql	-	-	0	0.82	4.8	0.00	0.41	0.05	0.00	0.00	5.90	4.03
sonoCOF-A7	963	sonoCOF-A7	2D	hcb	-	-	2700	0.44	21.2	0.27	0.22	0.21	2.10	2.13	5.68	5.27
sonoCOF-B1	964	sonoCOF-B1	2D	hcb	-	-	2196	0.42	29.7	0.22	0.21	0.30	1.73	1.54	6.16	4.78
TPE-Ph-COF	545	TPE-Ph COF	2D	kgm	-	-	1889	0.60	23.8	0.19	0.30	0.24	1.33	1.44	5.69	4.63
sonoCOF-B2	966	sonoCOF-B2	2D	hcb	-	-	2293	0.41	29.3	0.23	0.21	0.29	1.82	1.62	6.13	4.86
sonoCOF-B4	967	sonoCOF-B4	2D	sql	-	-	4285	0.40	13.7	0.43	0.20	0.14	3.43	3.70	4.57	6.33
sonoCOF-B7	968	sonoCOF-B7	2D	hcb	-	-	3916	0.61	6.4	0.39	0.31	0.06	2.71	3.67	4.21	6.15
sonoCOF-C1	969	sonoCOF-C1	2D	hcb	-	-	2312	0.41	29.0	0.23	0.20	0.29	1.84	1.64	6.13	4.88
sonoCOF-C2	970	sonoCOF-C2	2D	hcb	-	-	2556	0.37	30.0	0.26	0.18	0.30	2.09	1.79	6.08	5.01
sonoCOF-C3	971	sonoCOF-C3	2D	sql	-	-	1996	0.61	15.9	0.20	0.30	0.16	1.39	1.68	5.57	4.91
sonoCOF-D1	972	sonoCOF-D1	2D	hcb	-	-	2589	0.34	32.2	0.26	0.17	0.32	2.15	1.76	6.14	4.99
sonoCOF-D2	973	sonoCOF-D2	2D	hcb	-	-	2327	0.39	30.8	0.23	0.19	0.31	1.88	1.61	6.18	4.85
sonoCOF-D3	974	sonoCOF-D3	2D	sql	-	-	1887	0.62	16.3	0.19	0.31	0.16	1.30	1.58	5.58	4.83
sonoCOF-E1	975	sonoCOF-E1	2D	hcb	-	-	2476	0.32	37.9	0.25	0.16	0.38	2.08	1.54	6.31	4.78
COF-TPDA-PDA	766	COFTPDA-PDA	2D	kgm	-	-	2191	0.52	26.1	0.22	0.26	0.26	1.62	1.62	5.76	4.79
sonoCOF-E2	977	sonoCOF-E2	2D	hcb	-	-	2688	0.30	37.4	0.27	0.15	0.37	2.28	1.68	6.20	4.92

sonoCOF-E3	978	sonoCOF-E3	2D	sql	-	-	1498	0.67	21.8	0.15	0.33	0.22	1.00	1.17	5.65	4.43
sonoCOF-F11	979	sonoCOF-F11	2D	mtf	-	-	2008	0.70	8.6	0.20	0.35	0.09	1.31	1.84	5.21	5.05
sonoCOF-F3	980	sonoCOF-F3	2D	mtf	-	-	1502	0.81	10.6	0.15	0.41	0.11	0.89	1.34	5.05	4.62
sonoCOF-F5	981	sonoCOF-F5	2D	hcb	-	-	2209	0.58	15.9	0.22	0.29	0.16	1.57	1.86	5.53	5.05
sonoCOF-F6	982	sonoCOF-F6.	2D	hcb	-	-	2674	0.39	25.4	0.27	0.19	0.25	2.15	1.99	5.90	5.18
sonoCOF-F7	983	sonoCOF-F7	2D	hcb	-	-	2506	0.54	11.7	0.25	0.27	0.12	1.83	2.21	5.46	5.36
sonoCOF-F8	984	sonoCOF-F8	2D	hcb	-	-	1888	0.73	10.4	0.19	0.36	0.10	1.20	1.69	5.15	4.90
COF-DHTA	875	COF-DHTA	2D	kgm	-	-	2563	0.48	25.9	0.26	0.24	0.26	1.95	1.90	5.66	5.03
sonoCOF-G2	986	sonoCOF-G2	2D	hcb	-	-	1962	0.57	18.6	0.20	0.29	0.19	1.40	1.60	5.73	4.85
DHP-COF-AA	936	AA-stacking mode of DHP-COF	2D	kgm	-	-	2838	0.45	26.8	0.28	0.22	0.27	2.21	2.08	5.57	5.17
sonoCOF-G6	988	sonoCOF-G6	2D	hcb	-	-	2422	0.33	36.6	0.24	0.17	0.37	2.02	1.53	6.32	4.78
sonoCOF-G7	989	sonoCOF-G7	2D	hcb	-	-	2245	0.54	16.8	0.22	0.27	0.17	1.64	1.87	5.67	5.08
sonoCOF-G8	990	sonoCOF-G8	2D	hcb	-	-	2207	0.48	23.1	0.22	0.24	0.23	1.68	1.70	5.93	4.93
sonoCOF-H1	991	sonoCOF-H1	2D	hcb	-	-	2206	0.54	18.0	0.22	0.27	0.18	1.62	1.81	5.71	5.03
sonoCOF-A11	960	sonoCOF-A11	2D	kgm	-	-	2476	0.56	21.9	0.25	0.28	0.22	1.79	1.93	5.43	5.02
sonoCOF-H7	993	sonoCOF-H7	2D	hcb	-	-	2338	0.53	15.9	0.23	0.27	0.16	1.71	1.97	5.61	5.16
sonoCOF-I1	994	sonoCOF-I1	2D	hcb	-	-	1657	0.70	12.4	0.17	0.35	0.12	1.08	1.45	5.42	4.75
sonoCOF-I10	995	sonoCOF-I10	2D	hcb	-	-	1830	0.65	15.0	0.18	0.32	0.15	1.24	1.56	5.52	4.82
sonoCOF-I2	996	sonoCOF-I2	2D	hcb	-	-	1483	0.81	11.5	0.15	0.40	0.12	0.88	1.31	5.08	4.59
sonoCOF-I5	997	sonoCOF-I5	2D	hcb	-	-	1768	0.66	16.7	0.18	0.33	0.17	1.18	1.47	5.51	4.72
sonoCOF-I6	998	sonoCOF-I6	2D	hcb	-	-	1962	0.51	24.0	0.20	0.25	0.24	1.46	1.49	5.99	4.75
sonoCOF-I8	999	sonoCOF-I8	2D	hcb	-	-	1078	1.08	9.7	0.11	0.54	0.10	0.50	0.97	4.11	4.17
sonoCOF-I9	1000	sonoCOF-I9	2D	hcb	-	-	1794	0.68	14.4	0.18	0.34	0.14	1.19	1.54	5.43	4.79
sonoCOF-J1	1001	sonoCOF-J1	2D	hcb	-	-	2639	0.55	13.0	0.26	0.28	0.13	1.91	2.30	5.34	5.38
sonoCOF-J11	1002	sonoCOF-J11	2D	sql	-	-	176	1.42	5.0	0.02	0.71	0.05	0.05	0.17	2.85	3.52
sonoCOF-J2	1003	sonoCOF-J2	2D	hcb	-	-	2033	0.61	15.1	0.20	0.30	0.15	1.41	1.73	5.55	4.95
sonoCOF-J3	1004	sonoCOF-J3	2D	sql	-	-	325	1.66	7.3	0.03	0.83	0.07	0.06	0.30	1.66	3.29
sonoCOF-J4	1005	sonoCOF-J4	2D	sql	-	-	0	1.20	3.9	0.00	0.60	0.04	0.00	0.00	3.98	3.68
sonoCOF-K1	1006	sonoCOF-K1	2D	hcb	-	-	2656	0.55	13.1	0.27	0.27	0.13	1.93	2.31	5.33	5.39
sonoCOF-K11	1007	sonoCOF-K11	2D	sql	-	-	249	1.16	5.3	0.02	0.58	0.05	0.10	0.24	4.07	3.80

sonoCOF-K2	1008	sonoCOF-K2	2D	hcb	-	-	3956	0.50	12.9	0.40	0.25	0.13	2.97	3.45	4.53	6.09
sonoCOF-K3	1009	sonoCOF-K3	2D	sql	-	-	582	1.03	9.0	0.06	0.51	0.09	0.28	0.53	4.58	3.99
sonoCOF-K4	1010	sonoCOF-K4	2D	sql	-	-	0	1.15	3.9	0.00	0.57	0.04	0.00	0.00	4.27	3.74
Am-COF-BFTPD-MDA-AA	1011	Am-COF-BFTPD-MDA with AA stacking	2D	sql	-	-	2194	0.65	10.7	0.22	0.32	0.11	1.48	1.96	5.27	5.13
Am-COF-BTCA-TATTA-AA	1012	Am-COF-BTCA-TATTA with AA stacking	2D	hcb	-	-	1432	0.84	11.9	0.14	0.42	0.12	0.83	1.26	4.98	4.52
sonoCOF-B11	965	sonoCOF-B11	2D	kgm	-	-	2937	0.40	28.1	0.29	0.20	0.28	2.35	2.11	5.66	5.23
Am-COF-PTTA-TPA-AA	1014	Am-COF-PTTA-TPA with AA stacking	2D	sql	-	-	2492	0.49	18.4	0.25	0.24	0.18	1.88	2.03	5.67	5.20
sonoCOF-E11	976	sonoCOF-E11	2D	kgm	-	-	3667	0.32	33.3	0.37	0.16	0.33	3.08	2.45	5.31	5.51
Am-COF-TFPPy-BD-AA	1016	Am-COF-TFPPy-BD with AA stacking	2D	sql	-	-	2204	0.51	20.4	0.22	0.26	0.20	1.64	1.76	5.80	4.98
Am-COF-TFPPy-PDA-AA	1017	Am-COF-TFPPy-PDA with AA stacking	2D	sql	-	-	3391	0.37	20.6	0.34	0.18	0.21	2.77	2.69	5.39	5.71
Im-COF-BFTPD-MDA-AA	1018	Im-COF-BFTPD-MDA with AA stacking	2D	sql	-	-	2233	0.62	11.1	0.22	0.31	0.11	1.54	1.98	5.35	5.16
Im-COF-BTCA-TATTA-AA	1019	Im-COF-BTCA-TATTA with AA stacking	2D	hcb	-	-	1564	0.78	11.6	0.16	0.39	0.12	0.95	1.38	5.13	4.65
Am-COF-ETTA-TPA-AA	1013	Am-COF-ETTA-TPA with AA stacking	2D	kgm	-	-	2383	0.49	27.7	0.24	0.24	0.28	1.80	1.72	5.76	4.87
Am-COF-QPTA-PDA-AA	1015	Am-COF-QPTA-PDA with AA stacking	2D	kgm	-	-	1612	0.70	21.2	0.16	0.35	0.21	1.05	1.27	5.47	4.47

Im-COF-TFPPy-BD-AA	1022	Im-COF-TFPPy-BD with AA stackin	2D	sql	-	-	2399	0.48	20.2	0.24	0.24	0.20	1.82	1.91	5.78	5.11
Im-COF-TFPPy-PDA-AA	1023	Im-COF-TFPPy-PDA with AA stacking	2D	sql	-	-	3722	0.34	20.5	0.37	0.17	0.21	3.09	2.96	5.21	5.90
V-2D-COF-NO1	1024	v-2D-COF-NO1 with serrated stacking mode	2D	hcb	-	-	2059	0.56	20.7	0.21	0.28	0.21	1.49	1.63	5.73	4.85
V-2D-COF-NO2	1025	v-2D-COF-NO2 with serrated stacking mode	2D	hcb	-	-	2064	0.55	20.6	0.21	0.28	0.21	1.49	1.64	5.74	4.86
COF-38	1026	COF-38	2D	sql	-	-	6950	0.25	22.4	0.69	0.12	0.22	6.09	5.40	2.68	7.56
COF-39	1027	COF-39	2D	sql	-	-	6685	0.22	25.4	0.67	0.11	0.25	5.94	4.99	2.95	7.36
Im-COF-ETTA-TPA-AA	1020	Im-COF-ETTA-TPA with AA stacking	2D	kgm	-	-	2618	0.46	25.9	0.26	0.23	0.26	2.02	1.94	5.70	5.08
Im-COF-QPTA-PDA-AA	1021	Im-COF-QPTA-PDA with AA stacking	2D	kgm	-	-	1850	0.63	22.0	0.19	0.31	0.22	1.27	1.44	5.59	4.64
Py-Bde-COF	1030	Py-Bde-COF	2D	kgm	-	-	2232	0.45	36.9	0.22	0.22	0.37	1.73	1.41	6.02	4.56
LZU-191-AA	1031	the unit cell of LZU-191 AA stacking	2D	hcb	-	-	1903	0.49	28.0	0.19	0.24	0.28	1.44	1.37	6.12	4.62
TAPB-OMeTA-AA	1032	TAPB-OMeTA COF in AA stacking structure.	2D	hcb	-	-	2402	0.41	27.7	0.24	0.21	0.28	1.91	1.74	6.04	4.96
TA-Por-sp2-COF	1033	TA-Por-sp2-COF	2D	hcb	-	-	6780	0.25	17.5	0.68	0.13	0.17	5.93	5.59	2.81	7.61
COF-TPDA-PMDA	1034	COF TPDA-PMDA	2D	kgm	-	-	1997	0.59	26.1	0.20	0.30	0.26	1.40	1.48	5.62	4.62
COF-Py-BPTA-AA	1035	COFPy-BPTA with AA stacking	2D	sql	-	-	1950	0.69	13.2	0.20	0.35	0.13	1.28	1.69	5.27	4.89

CQ-COF-Py-BPTA-AA	1036	CQ-COFPy-BPTA with AA stacking	2D	sql	-	-	1732	0.71	14.4	0.17	0.36	0.14	1.12	1.48	5.33	4.72
CQ-COF-TAPB-BPTA-AA	1037	CQ-COFTAPB-BPTA with AA stacking	2D	hcb	-	-	1742	0.55	26.8	0.17	0.28	0.27	1.26	1.28	5.97	4.51
NiPc-NH-CoPcF8-AA	1038	AA-stacking mode of NiPc-NH-CoPcF8 via Pawley	2D	sql	-	-	628	1.41	8.8	0.06	0.71	0.09	0.18	0.57	2.75	3.64
NiPc-NH-CuPcF8-AA	1039	AA-stacking mode of NiPc-NH-CuPcF8 via Pawley	2D	sql	-	-	626	1.42	8.8	0.06	0.71	0.09	0.18	0.57	2.73	3.63
N-TAPB-MeTA-AA	1040	AA stacking N-TAPB-MeTA	2D	hcb	-	-	2297	0.41	28.6	0.23	0.20	0.29	1.83	1.64	6.14	4.88
N-TAPB-OMeTA-AA	1041	AA stacking N-TAPB-OMeTA	2D	hcb	-	-	2294	0.45	26.6	0.23	0.23	0.27	1.78	1.68	5.97	4.90
TAPB-MeTA-AA	1042	AA stacking TAPB-MeTA	2D	hcb	-	-	2365	0.39	28.7	0.24	0.20	0.29	1.90	1.69	6.13	4.93
TAPB-OMeTA-H-AB	1043	quasi-AB stacking TAPB-OMeTA-H in CDCl3	2D	hcb	-	-	2309	0.56	11.8	0.23	0.28	0.12	1.67	2.04	5.55	5.24
COF-BPDA	1044	COF-BPDA	2D	sql	-	-	1796	0.74	12.1	0.18	0.37	0.12	1.13	1.58	5.17	4.79
COF-DFB	1045	COF-DFB	2D	sql	-	-	1395	0.82	10.0	0.14	0.41	0.10	0.82	1.26	5.08	4.58
COF-904-30d	1046	COF-904-30d	3D	hcb	-	-	0	1.15	2.4	0.00	0.57	0.02	0.00	0.00	3.97	4.12
JUC-640-Co	1047	JUC-640-Co based on the stp net.	3D	stp	-	-	6873	0.11	49.5	0.69	0.06	0.49	6.49	3.47	2.95	6.84
JUC-640-Ni	1048	JUC-640-Ni based on the stp net.	3D	stp	-	-	6859	0.11	49.4	0.69	0.06	0.49	6.48	3.47	2.97	6.83

BDF-COF-A2-AA	1049	BDF-COF-A2-Eclipsed	2D	hcb	-	-	1234	1.00	14.9	0.12	0.50	0.15	0.62	1.05	4.39	4.17
BDF-COF-A4-AA	1050	BDF-COF-A4-Eclipsed	2D	hcb	AA	-	593	1.13	10.8	0.06	0.56	0.11	0.26	0.53	4.10	3.84
BDF-COF-A4-AB	1051	BDF-COF-A4-Staggered	2D	hcb	AB	-	0	1.13	3.9	0.00	0.56	0.04	0.00	0.00	4.36	3.75
BDF-COF-A6-AA	1052	BDF-COF-A6-Eclipsed	2D	hcb	-	-	97	1.27	5.8	0.01	0.63	0.06	0.04	0.09	3.62	3.61
JNU-3	1053	JNU-3	2D	hcb	-	-	1911	0.57	23.2	0.19	0.28	0.23	1.37	1.47	5.79	4.69
JNU-4	1054	JNU-4	2D	hcb	-	-	2127	0.43	31.9	0.21	0.22	0.32	1.67	1.45	6.17	4.67
NKCOF-14	1055	NKCOF-14	3D	dia	-	-	7273	0.33	14.0	0.73	0.17	0.14	6.06	6.26	2.27	7.88
NKCOF-14-4	1056	NKCOF-14 calculated based on 4-fold interpenetrated dia net	3D	dia	-	-	6435	0.38	13.1	0.64	0.19	0.13	5.22	5.59	2.89	7.45
NKCOF-15-AA	1057	NKCOF-15calculated based on the AA-stacking mode	2D	sql	-	-	1956	0.64	13.9	0.20	0.32	0.14	1.33	1.69	5.48	4.93
COF-NUST-31	1058	COF-NUST-31	2D	hcb	-	-	1623	0.67	17.1	0.16	0.34	0.17	1.08	1.35	5.56	4.63
COF-NUST-32	1059	COF-NUST-32	2D	hcb	-	-	1703	0.67	16.4	0.17	0.34	0.16	1.13	1.42	5.50	4.69
COF-NUST-33	1060	COF-NUST-33	2D	hcb	-	-	1878	0.67	13.9	0.19	0.34	0.14	1.24	1.62	5.38	4.85
DhaTph-COOH	1061	DhaTph-COOH	2D	sql	-	-	1381	0.73	18.6	0.14	0.37	0.19	0.88	1.12	5.46	4.40
TJU-1	1062	TJU-1	2D	hcb	-	-	2813	0.60	9.0	0.28	0.30	0.09	1.97	2.56	5.03	5.54
F-TBT-COF	1063	F-TBT-COF	2D	hcb	-	-	2172	0.60	16.4	0.22	0.30	0.16	1.52	1.82	5.47	4.99
MeO-TBT-COF	1064	MeO-TBT-COF	2D	hcb	-	-	2201	0.64	13.6	0.22	0.32	0.14	1.50	1.90	5.31	5.05
TBT-COF	1065	TBT-COF	2D	hcb	-	-	2329	0.55	16.2	0.23	0.27	0.16	1.69	1.95	5.57	5.13
TT-COF	1066	TT-COF	3D	dia	-	-	7633	0.18	34.6	0.76	0.09	0.35	6.96	4.99	2.16	7.60
TAB-TFB-COF-AA	1067	the AA-stacking mode of TAB-TFB-COF	2D	hcb	AA	-	1211	1.01	10.9	0.12	0.51	0.11	0.60	1.08	4.34	4.27

TAB-TFB-COF-AB	1068	the AB-stacking mode of TAB-TFB-COF	2D	hcb	AB	-	0	0.98	4.8	0.00	0.49	0.05	0.00	0.00	5.08	3.87
TAB-TFP-COF-AA	1069	the AA-stacking mode of TAB-TFP-COF	2D	hcb	AA	-	1016	1.13	10.4	0.10	0.57	0.10	0.44	0.91	3.89	4.06
TAB-TFP-COF-AB	1070	AB-stacking mode of TAB-TFP-COF	2D	hcb	AB	-	0	1.09	4.7	0.00	0.54	0.05	0.00	0.00	4.55	3.77
COF3	1071	COF3	2D	hcb	-	-	2446	0.33	38.1	0.24	0.16	0.38	2.04	1.51	6.31	4.75
CZ-DHZ-COF-AA	1072	the AA-stacking mode of CZ-DHZ-COF	2D	hcb	-	-	1630	0.73	10.0	0.16	0.37	0.10	1.03	1.47	5.30	4.78
Me3TFB_Me2BD-AA	1073	Me3TFB_Me2BD-eclipsed	2D	hcb	AA	-	1874	0.54	21.3	0.19	0.27	0.21	1.37	1.48	5.94	4.76
Me3TFB_Me2BD-AB	1074	Me3TFB_Me2BD-staggered	2D	hcb	AB	-	3015	0.58	7.4	0.30	0.29	0.07	2.14	2.79	4.96	5.70
Me3TFB_Me2PA-AA	1075	Me3TFB_Me2PA-eclipsed	2D	hcb	AA	-	1402	0.76	5.2	0.14	0.38	0.05	0.87	1.33	5.33	4.79
Me3TFB_Me2PA-AB	1076	Me3TFB_Me2PA-staggered	2D	hcb	AB	-	1522	0.70	14.0	0.15	0.35	0.14	0.99	1.31	5.49	4.64
Me3TFB_Me4BD-AA	1077	Me3TFB_Me4BD-eclipsed	2D	hcb	AA	-	1710	0.57	21.6	0.17	0.29	0.22	1.22	1.34	5.92	4.64
Me3TFB_Me4BD-AB	1078	Me3TFB_Me4BD-staggered	2D	hcb	AB	-	3905	0.60	7.6	0.39	0.30	0.08	2.74	3.61	4.27	6.13
Me3TFB_Me4PA-AA	1079	Me3TFB_Me4PA-eclipsed	2D	hcb	AA	-	1330	0.78	14.0	0.13	0.39	0.14	0.81	1.14	5.28	4.46
Me3TFB_Me4PA-AB	1080	Me3TFB_Me4PA-staggered	2D	hcb	AB	-	1338	0.83	5.1	0.13	0.41	0.05	0.78	1.27	5.08	4.69
TFB_Me2BD-AA	1081	TFB_Me2BD-eclipsed	2D	hcb	AA	-	2300	0.49	21.1	0.23	0.24	0.21	1.74	1.81	5.82	5.03
TFB_Me2BD-AB	1082	TFB_Me2BD-staggered	2D	hcb	AB	-	5166	0.51	7.8	0.52	0.25	0.08	3.85	4.76	3.61	6.84

TFB_Me2PA-AA	1083	TFB_Me2PA-eclipsed	2D	hcb	AA	-	2088	0.62	14.3	0.21	0.31	0.14	1.45	1.79	5.48	5.00
TFB_Me2PA-AB	1084	TFB_Me2PA-staggered	2D	hcb	AB	-	1889	0.69	5.7	0.19	0.34	0.06	1.24	1.78	5.32	5.08
TFB_Me4BD-AA	1085	TFB_Me4BD-eclipsed	2D	hcb	AA	-	2026	0.52	21.7	0.20	0.26	0.22	1.50	1.59	5.89	4.84
TFB_Me4BD-AB	1086	TFB_Me4BD-staggered	2D	hcb	AB	-	4618	0.55	7.5	0.46	0.28	0.08	3.35	4.27	3.90	6.53
TFB_Me4PA-AA	1087	TFB_Me4PA-eclipsed	2D	hcb	AA	-	1485	0.70	14.1	0.15	0.35	0.14	0.97	1.28	5.55	4.62
TFB_Me4PA-AB	1088	TFB_Me4PA-staggered	2D	hcb	AB	-	1790	0.76	5.3	0.18	0.38	0.05	1.11	1.70	5.11	4.98
COF-TAPA-BTPA-AA	1089	COFTAPA-BTPA AA stacking model	2D	hcb	AA	-	2238	0.54	16.8	0.22	0.27	0.17	1.64	1.86	5.67	5.08
COF-TAPA-BTPA-AB	1090	COFTAPA-BTPA AB stacking model (Staggered)	2D	hcb	AB	-	4007	0.56	7.5	0.40	0.28	0.07	2.88	3.71	4.31	6.22
COF-TAPB-BTPA-AA	1091	COFTAPA-BTPA AA stacking	2D	hcb	AA	-	2082	0.56	18.3	0.21	0.28	0.18	1.50	1.70	5.71	4.94
COF-TAPB-BTPA-AB	1092	COF-TAPB-BTPA AB stacking model (Staggered)	2D	hcb	AB	-	3094	0.59	8.5	0.31	0.29	0.08	2.19	2.83	4.88	5.71
COF-TTA-BTPA-AA	1093	COFTTA-BTPA AA stacking model (Eclipsed)	2D	hcb	AA	-	4835	0.33	18.2	0.48	0.16	0.18	4.04	3.96	4.32	6.54
COF-TTA-BTPA-AB	1094	COFTTA-BTPA AB stacking model (Staggered)	2D	hcb	AB	-	2483	0.66	7.7	0.25	0.33	0.08	1.67	2.29	5.04	5.35
JUC-505	1095	JUC-505	2D	hcb	-	-	1416	0.91	14.0	0.14	0.45	0.14	0.77	1.22	4.69	4.38

JUC-505-COOH	1096	JUC-505-COOH	2D	hcb	-	-	1187	1.01	13.9	0.12	0.50	0.14	0.59	1.02	4.37	4.17
JUC-505-H	1097	JUC-505-H	2D	hcb	-	-	1373	0.77	17.7	0.14	0.39	0.18	0.84	1.13	5.30	4.38
COF2-AA	1098	COF 2 with AA stacking.	2D	hcb	-	-	2018	0.50	24.9	0.20	0.25	0.25	1.52	1.52	6.00	4.77
COF3-AA	1099	COF 3 with AA stacking.	2D	hcb	-	-	1984	0.53	21.5	0.20	0.26	0.21	1.46	1.56	5.90	4.82
NAHA-Tp-AA	1100	NAHA-Tp	2D	hcb	-	-	1440	0.74	18.0	0.14	0.37	0.18	0.91	1.18	5.39	4.44
3D-TAPPy-TFPA	1101	3D TAPPy-TFPA with non-interpenetrated-fjh topology	3D	fih	-	-	7964	0.13	26.2	0.80	0.06	0.26	7.46	5.88	1.91	8.07
3D-TAPPy-TFPA-1	1102	3D TAPPy-TFPA with interpenetrated fjh topology	3D	fjh	-	-	5502	0.27	22.1	0.55	0.13	0.22	4.76	4.29	3.89	6.82
Tf-DHzOH	1103	Tf-DHzOH	2D	hcb	-	-	2469	0.47	21.6	0.25	0.24	0.22	1.88	1.94	5.75	5.11
TpBpy	1104	TpBpy	2D	hcb	-	-	5405	0.32	21.7	0.54	0.16	0.22	4.53	4.23	3.85	6.73
TpPy	1105	TpPy	2D	hcb	-	-	1958	0.24	21.2	0.20	0.12	0.21	1.72	1.54	7.08	5.10
COF-SQ	1106	COF-SQ	2D	hcb	-	-	2011	0.47	27.4	0.20	0.23	0.27	1.54	1.46	6.12	4.72
COF-SQ-Ph	1107	COF-SQ-Ph	2D	hcb	-	-	1208	0.70	23.9	0.12	0.35	0.24	0.78	0.92	5.70	4.18
Tp-BDOH	1108	Tp-BDOH	2D	hcb	-	-	1869	0.57	21.9	0.19	0.28	0.22	1.34	1.46	5.83	4.71
TAPT-DMTP-COF-AA	1109	TAPT-DMTP-COF (AA-stacking mode)	2D	hcb	AA	-	2206	0.46	26.4	0.22	0.23	0.26	1.69	1.62	5.99	4.85
TAPT-DMTP-COF-AB	1110	TAPT-DMTP-COF (AB-stacking mode)	2D	hcb	AB	-	3074	0.53	12.4	0.31	0.26	0.12	2.27	2.69	5.10	5.64
COF-CN-AA	1111	COF-CN with AA packing	2D	hcb	-	-	1736	0.67	15.4	0.17	0.34	0.15	1.15	1.47	5.49	4.73
COF-NH2-AA	1112	COF-NH2 with AA packing	2D	hcb	-	-	2165	0.54	15.7	0.22	0.27	0.16	1.58	1.82	5.72	5.07
APCOF-1	1113	APCOF-1	2D	sql	-	-	1897	0.75	12.2	0.19	0.38	0.12	1.18	1.67	5.06	4.83

TB-DA-COF-AA	1114	TB-DA COF with AA stacking mode	2D	hcb	AA	-	2176	0.45	26.1	0.22	0.23	0.26	1.69	1.61	6.06	4.85
TB-DA-COF-AB	1115	TB-DA COF with AB stacking mode	2D	hcb	AB	-	3926	0.41	14.2	0.39	0.21	0.14	3.11	3.37	4.82	6.12
Dpy-TFPB	1116	Dpy-TFPB	2D	kgd	-	-	1820	0.65	15.2	0.18	0.33	0.15	1.23	1.54	5.51	4.80
Bpda-BthCOF-AA	1117	Bpda-BthCOF-AA	2D	hcb	AA	-	2266	0.40	29.7	0.23	0.20	0.30	1.81	1.59	6.19	4.84
Bpda-BthCOF-AB	1118	Bpda-BthCOF-AB	2D	hcb	AB	-	4138	0.43	13.0	0.41	0.21	0.13	3.25	3.60	4.60	6.25
3D-TPB-COF-OMe	1119	3D-TPB-COF-OMe	3D	pts	-	-	355	1.01	4.9	0.04	0.50	0.05	0.18	0.34	4.79	4.02
3D-TPB-COF-Ph	1120	3D-TPB-COF-Ph	3D	ljh	-	-	2357	0.72	8.1	0.24	0.36	0.08	1.51	2.17	4.89	5.21
T-COF-CF3-AA	1121	the unit cell of T-COF-CF3 with AA stacking	2D	hcb	-	-	2277	0.38	34.3	0.23	0.19	0.34	1.84	1.50	6.24	4.73
T-COF-CH3-AA	1122	the unit cell of T-COF-CH3 with AA stacking	2D	hcb	-	-	2403	0.34	35.8	0.24	0.17	0.36	1.99	1.54	6.29	4.78
T-COF-H-AA	1123	the unit cell of T-COF-H with AA stacking	2D	hcb	-	-	2404	0.33	38.4	0.24	0.17	0.38	2.00	1.48	6.33	4.72
TPB-DPPA-COF	1124	TPB-DPPA-COF	2D	hcb	-	-	2879	0.55	17.3	0.29	0.27	0.17	2.09	2.38	5.17	5.37
TFPPer-TAPPer-COF-AA	1125	the AA-stacking mode of TFPPer-TAPPer-COF	2D	sql	-	-	1502	0.76	13.6	0.15	0.38	0.14	0.93	1.30	5.26	4.58
PICOF-1-AA	1126	PICOF-1 eclipsed conformation	2D	sql	-	-	1638	0.71	16.3	0.16	0.36	0.16	1.05	1.37	5.37	4.62
PICOF-1-AB	1127	PICOF-1 staggered conformation.	2D	sql	-	-	1012	0.91	6.6	0.10	0.46	0.07	0.55	0.94	4.90	4.40

BPTD-COF	1128	BPTD-COF	2D	triangular	-	-	1686	0.75	11.1	0.17	0.38	0.11	1.05	1.50	5.19	4.76
TAPT-DHNDA	1129	TAPT-DHNDA	2D	hcb	-	-	2018	0.45	29.4	0.20	0.23	0.29	1.56	1.42	6.19	4.68
Dpy-Bt-COF	1130	Dpy-Bt-COF	2D	hcb	-	-	3546	0.33	23.3	0.35	0.17	0.23	2.96	2.72	5.39	5.74
COF-TFPB-DB	1131	COF-TFPB-DB	2D	kgm	-	-	3023	0.40	27.8	0.30	0.20	0.28	2.42	2.18	5.59	5.28
Pyaph-COF-AA	1132	Pyaph-COF with AA-stacking.	2D	sql	-	-	2233	0.52	19.1	0.22	0.26	0.19	1.65	1.81	5.75	5.02
Pythz-COF-AA	1133	Pythz-COF with AA-stacking.	2D	sql	-	-	2199	0.50	22.3	0.22	0.25	0.22	1.65	1.71	5.86	4.94
TFPT-HZ-COF	1134	TFPT-HZ-COF	2D	hcb	-	-	2116	0.49	23.1	0.21	0.24	0.23	1.60	1.63	5.97	4.88
TFT-HZ-COF	1135	TFT-HZ-COF	2D	hcb	-	-	2738	0.40	26.7	0.27	0.20	0.27	2.19	2.01	5.82	5.17
Azo-COF-AA	1136	AA stacking mode of Azo-COF	2D	sql	-	-	2438	0.44	23.6	0.24	0.22	0.24	1.91	1.86	5.92	5.08
Tp-COF-AA	1137	AA stacking mode of Tp-COF	2D	sql	-	-	2374	0.42	26.1	0.24	0.21	0.26	1.88	1.75	6.04	4.99
BHU-1-AA	1138	simulated AA stacking crystal structure of BHU-1	2D	hcb	AA	-	1339	0.68	15.6	0.13	0.34	0.16	0.88	1.13	5.72	4.52
BHU-1-AB	1139	simulated AB stacking crystal structure of BHU-1	2D	hcb	AB	-	3494	0.45	12.8	0.35	0.23	0.13	2.70	3.04	5.03	5.91
NKPOM-OF-1(Co)	1140	NKPOM-OF-1(Co)	2D	sql	-	-	2596	0.93	12.8	0.26	0.47	0.13	1.39	2.26	3.96	4.98
NKPOM-OF-1(Mn)	1141	NKPOM-OF-1(Mn)	2D	sql	-	-	2604	0.93	12.8	0.26	0.46	0.13	1.40	2.27	3.96	4.99
NKPOM-OF-2(Co)	1142	NKPOM-OF-2(Co)	2D	sql	-	-	2315	0.95	11.6	0.23	0.48	0.12	1.21	2.05	4.03	4.86
NKPOM-OF-2(Mn)	1143	NKPOM-OF-2(Mn)	2D	sql	-	-	2322	0.95	11.6	0.23	0.47	0.12	1.22	2.05	4.04	4.87

ND-COF-1-AA	1144	ND-COF-1 in eclipsed AA model	2D	hcb	AA	-	3041	0.36	25.2	0.30	0.18	0.25	2.49	2.27	5.69	5.40
ND-COF-1-AB	1145	ND-COF-1 in staggered AB model	2D	hcb	AB	-	5139	0.44	11.0	0.51	0.22	0.11	4.01	4.57	3.79	6.80
ND-COF-1-ABC	1146	ND-COF-1 in ABC stacking model	2D	hcb	-	-	4225	0.54	7.6	0.42	0.27	0.08	3.07	3.90	4.20	6.34
ND-COF-2-AA	1147	ND-COF-2 in eclipsed AA	2D	hcb	-	-	2816	0.40	24.6	0.28	0.20	0.25	2.25	2.12	5.75	5.27
ND-COF-2-AB	1148	ND-COF-2 in staggered AB	2D	hcb	AA	-	4998	0.45	10.8	0.50	0.23	0.11	3.87	4.46	3.88	6.73
ND-COF-2-ABC	1149	ND-COF-2 in ABC stacking model	2D	hcb	AB	-	3603	0.58	7.6	0.36	0.29	0.08	2.55	3.33	4.54	5.99
3D-Sp-COF-1	1150	3D-Sp-COF based on the 1-fold-interpenetrated dia topology	3D	dia	-	1	9056	0.04	44.1	0.91	0.02	0.44	8.85	5.06	0.92	8.16
3D-Sp-COF-2	1151	3D-Sp-COF based on the 2-fold-interpenetrated dia topology	3D	dia	-	2	9163	0.09	20.7	0.92	0.04	0.21	8.76	7.26	0.80	8.87

3D-Sp-COF-3	1152	3D-Sp-COF based on the 3-fold-interpenetrated dia topology	3D	dia	-	3	9238	0.13	17.8	0.92	0.07	0.18	8.62	7.59	0.71	8.95
3D-Sp-COF-4	1153	3D-Sp-COF based on the 4-fold-interpenetrated dia topology	3D	dia	-	4	8720	0.18	16.0	0.87	0.09	0.16	7.94	7.32	1.16	8.70
3D-Sp-COF-5	1154	3D-Sp-COF based on the 5-fold-interpenetrated dia topology	3D	dia	-	5	8600	0.22	17.3	0.86	0.11	0.17	7.64	7.12	1.24	8.56
3D-Sp-COF-6	1155	3D-Sp-COF based on the 6-fold-interpenetrated dia topology	3D	dia	-	6	6989	0.28	16.4	0.70	0.14	0.16	6.02	5.84	2.59	7.72

3D-Sp-COF-7	1156	3D-Sp-COF based on the 7-fold-interpenetrated dia topology staggered AB-stacking (b) model of QL-COF-1	3D	dia	-	7	3863	0.41	14.7	0.39	0.20	0.15	3.08	3.30	4.89	6.08
QL-COF-1-AA	1157	staggered AB-stacking (e) model of QL-COF-2	2D	hcb	AA	-	1812	0.52	27.8	0.18	0.26	0.28	1.34	1.31	6.07	4.56
QL-COF-2-AB	1158	Azo-COF-1 with AA stacking	2D	hcb	AB	-	796	1.02	10.0	0.08	0.51	0.10	0.39	0.72	4.51	4.08
Azo-COF-1	1159	Azo-COF-2 with AA stacking	2D	kgm	-	-	2422	0.51	25.0	0.24	0.25	0.25	1.81	1.82	5.66	4.96
Azo-COF-2	1160	Im-COF-1with AA stacking.	2D	sql	-	-	2165	0.57	17.8	0.22	0.29	0.18	1.55	1.78	5.60	4.98
Im-COF-1	1161	Im-COF-2 with AA stacking	2D	kgm	-	-	2618	0.46	25.9	0.26	0.23	0.26	2.02	1.94	5.70	5.08
Im-COF-2	1162	COF-TAPB	2D	sql	-	-	2117	0.56	18.1	0.21	0.28	0.18	1.52	1.73	5.67	4.95
COF-TAPB	1163	COF-TAPT	2D	hcb	-	-	1995	0.59	17.0	0.20	0.30	0.17	1.41	1.66	5.64	4.90
COF-TAPT	1164	TAPB-TA-COF	2D	hcb	-	-	1978	0.60	16.9	0.20	0.30	0.17	1.38	1.64	5.61	4.88
TAPB-TA-COF	1165	Ec-COF-1	2D	sql	-	-	2036	0.59	16.8	0.20	0.29	0.17	1.44	1.69	5.62	4.93
Ec-COF-1	1166	TpBpy-AA optimized by using DFT	2D	sql	-	-	2418	0.56	14.9	0.24	0.28	0.15	1.74	2.06	5.46	5.20
TpBpy-AA	1167	TpBpy-AB optimized by using DFT	2D	hcb	-	-	4418	0.31	22.5	0.44	0.15	0.23	3.74	3.42	4.72	6.23
TpBpy-AB	1168		2D	hcb	-	-	2568	0.62	9.3	0.26	0.31	0.09	1.78	2.33	5.15	5.39

CYANO-COF-AA	1169	CYANO-COF(AA stacking)	2D	hcb	AA	-	1819	0.65	18.3	0.18	0.33	0.18	1.22	1.49	5.51	4.71
CYANO-COF-AB	1170	CYANO-COF(AB stacking)	2D	hcb	AB	-	4053	0.65	6.1	0.41	0.33	0.06	2.73	3.81	4.00	6.19
PY-BPY-COF	1171	PY-BPY-COF	2D	sql	-	-	2200	0.50	20.4	0.22	0.25	0.20	1.65	1.75	5.85	4.99
PY-DHBD-COF	1172	PY-DHBD-COF	2D	sql	-	-	2034	0.52	21.2	0.20	0.26	0.21	1.50	1.60	5.88	4.86
PyTTA-BPDA-COF-AA	1173	the AA-stacking mode of PyTTA-BPDA COF	2D	sql	-	-	2430	0.44	21.6	0.24	0.22	0.22	1.89	1.90	5.89	5.12
PyTTA-BPyDCA-COF-AA	1174	the AA-stacking mode of PyTTA-BPyDCA COF	2D	sql	-	-	2447	0.44	21.6	0.24	0.22	0.22	1.90	1.92	5.88	5.13
PyTTA-TPA-COF-AA	1175	the AA-stacking mode of PyTTA-TPA COF	2D	sql	-	-	2376	0.50	18.3	0.24	0.25	0.18	1.78	1.94	5.72	5.14
TFPM-PZI	1176	TFPM-PZI calculated based on the 5-fold interpenetrated dia net	3D	dia	-	-	3046	0.52	8.0	0.30	0.26	0.08	2.25	2.80	5.14	5.76
DPP-3D-COF	1177	the simulated dia-c5 interpenetrated DPP-3D-COF	3D	dia	-	-	7203	0.28	17.4	0.72	0.14	0.17	6.18	5.95	2.40	7.79
dynaCOF-330	1178	dynaCOF-330	3D	dia	-	-	0	1.17	3.7	0.00	0.59	0.04	0.00	0.00	4.14	3.72
dynaCOF-330I	1179	dynaCOF-330I	3D	dia	-	-	0	1.31	3.3	0.00	0.65	0.03	0.00	0.00	3.46	3.59
dynaCOF-330IV	1180	dynaCOF-330IV	3D	dia	-	-	0	1.25	2.9	0.00	0.63	0.03	0.00	0.00	3.74	3.66
Zn-Pz-DHTP-COF-AA	1181	the AA-stacking mode of Zn-Pz-DHTP-COF	2D	sql	-	-	2295	0.51	18.5	0.23	0.25	0.18	1.71	1.87	5.74	5.08

Zn-Pz-PEO-COF-AA	1182	he AA-stacking mode of Zn-Pz-PEO-COF	2D	sql	-	-	2494	0.64	10.4	0.25	0.32	0.10	1.70	2.23	5.12	5.30
Zn-Salen-COF-SDU113	1183	Zn-Salen-COF-SDU113	2D	hcb	-	-	4670	0.25	31.2	0.47	0.12	0.31	4.10	3.21	4.68	6.15
BDA-DCTP-AA	1184	BDA-DCTP-AA	2D	hcb	-	-	2078	0.51	23.2	0.21	0.25	0.23	1.55	1.60	5.91	4.83
BDA-TMT-AA	1185	BDA-TMT-AA	2D	hcb	-	-	2323	0.46	24.0	0.23	0.23	0.24	1.79	1.77	5.91	4.98
BTTA-DCTP-AA	1186	BTTA-DCTP-AA	2D	hcb	-	-	2170	0.57	16.2	0.22	0.29	0.16	1.55	1.82	5.59	5.03
BTTA-TMT-AA	1187	BTTA-TMT-AA	2D	hcb	-	-	2448	0.54	16.4	0.24	0.27	0.16	1.79	2.05	5.51	5.19
DAFB-DCTP-AA	1188	DAFB-DCTP-AA	2D	hcb	-	-	1925	0.56	19.3	0.19	0.28	0.19	1.38	1.55	5.80	4.82
EDA-DCTP-AA	1189	EDA-DCTP-AA	2D	hcb	-	-	2365	0.42	28.0	0.24	0.21	0.28	1.87	1.70	6.05	4.93
TDA-DCTP-AA	1190	TDA-DCTP-AA	2D	hcb	-	-	2238	0.40	31.1	0.22	0.20	0.31	1.79	1.54	6.22	4.79
TDA-TMT-AA	1191	TDA-TMT-AA	2D	hcb	-	-	2430	0.38	31.6	0.24	0.19	0.32	1.97	1.66	6.12	4.89
TFPB-DCTP-AA	1192	TFPB-DCTP-AA	2D	hcb	-	-	1493	0.76	11.5	0.15	0.38	0.11	0.93	1.32	5.27	4.64
TFPB-TMT-AA	1193	TFPB-TMT-AA	2D	hcb	-	-	1690	0.71	12.2	0.17	0.35	0.12	1.09	1.48	5.38	4.77
TFPT-DCTP-AA	1194	TFPT-DCTP-AA	2D	hcb	-	-	1478	0.79	11.2	0.15	0.39	0.11	0.90	1.31	5.17	4.62
TFPT-TMT-AA	1195	TFPT-TMT-AA	2D	hcb	-	-	1669	0.73	11.9	0.17	0.36	0.12	1.06	1.47	5.29	4.75
TPA-DCTP-AA	1196	TPA-DCTP-AA	2D	hcb	-	-	1328	0.85	9.4	0.13	0.42	0.09	0.77	1.20	5.00	4.54
TPA-TMT-AA	1197	TPA-TMT-AA	2D	hcb	-	-	1563	0.78	10.3	0.16	0.39	0.10	0.96	1.40	5.16	4.69
2D-t-COF	1198	2D-t-COF	2D	hcb	-	-	8220	0.15	20.9	0.82	0.07	0.21	7.61	6.51	1.65	8.33
b-COF	1199	b-COF	2D	hcb	-	-	8563	0.13	22.3	0.86	0.06	0.22	8.02	6.66	1.35	8.49
t-COF	1200	t-COF	2D	hcb	-	-	8286	0.14	21.4	0.83	0.07	0.21	7.70	6.51	1.59	8.36
TpBd-SO3H-AA	1201	TpBd-SO3H calculated based on P6/M(AA)	2D	hcb	-	-	2428	0.58	12.7	0.24	0.29	0.13	1.72	2.12	5.36	5.25
TpPa-SO3H(2)-AA	1202	TpPa-SO3H(2) calculated based on P6/M group(AA)	2D	hcb	-	-	1474	0.71	13.4	0.15	0.36	0.13	0.95	1.28	5.48	4.62
TpPa-SO3H-AA	1203	TpPa-SO3H calculated	2D	hcb	-	-	1318	0.34	21.5	0.13	0.17	0.21	1.09	1.04	7.20	4.67

		based on P6/M group（AA)														
BT-COF-AA	1204	BT-COF-AA	2D	hcb	-	-	1898	0.48	26.5	0.19	0.24	0.26	1.44	1.40	6.14	4.67
BT-COF-AB	1205	BT-COF-AB	2D	hcb	-	-	2998	0.55	12.3	0.30	0.27	0.12	2.17	2.63	5.08	5.58
COF-805	1206	COF-805	3D	bor	-	-	2071	0.78	8.1	0.21	0.39	0.08	1.27	1.90	4.85	5.02
COF-806	1207	COF-806	3D	bor	-	-	2702	0.66	9.8	0.27	0.33	0.10	1.81	2.44	4.88	5.39
COF-807	1208	COF-807	3D	bor	-	-	2837	0.62	14.1	0.28	0.31	0.14	1.96	2.44	4.96	5.38
Zn-COF	1209	Zn-COF	3D	dia	-	-	2150	0.64	13.6	0.22	0.32	0.14	1.47	1.86	5.35	5.03
TpTta-AA	1210	AA stacking arrangement of TpTta	2D	hcb	AA	-	1492	0.85	11.2	0.15	0.42	0.11	0.86	1.32	4.90	4.56
TpTta-AB	1211	AB stacking arrangement of TpTta	2D	hcb	AB	-	3209	0.62	6.2	0.32	0.31	0.06	2.21	3.01	4.68	5.80
NHC-AuCl-COF-AA	1212	NHC-AuCl-COF with AA Space	2D	hcb	AA	-	5191	0.21	43.7	0.52	0.10	0.44	4.66	2.92	4.31	6.08
NHC-AuCl-COF-AB	1213	NHC-AuCl-COF with AB Space	2D	hcb	AB	-	4221	0.43	20.1	0.42	0.21	0.20	3.31	3.37	4.54	6.08
NHC-AuCl-COF-re-AA	1214	NHC-AuCl-COF with AA Space Reversed AA Space	2D	hcb	-	-	2781	0.33	36.9	0.28	0.17	0.37	2.32	1.75	6.01	4.95
0N-COF	1215	0N-COF	2D	hcb	-	-	6751	0.18	19.0	0.68	0.09	0.19	6.16	5.47	2.96	7.63
1N-COF	1216	1N-COF	2D	hcb	-	-	6636	0.18	19.0	0.66	0.09	0.19	6.03	5.38	3.06	7.57
2N-COF	1217	2N-COF	2D	hcb	-	-	6506	0.18	18.9	0.65	0.09	0.19	5.91	5.28	3.17	7.50
3N-COF	1218	3N-COF	2D	hcb	-	-	6415	0.19	18.9	0.64	0.09	0.19	5.82	5.20	3.25	7.45
paiOF	1219	πOF	3D		-	-	1183	0.85	9.7	0.12	0.43	0.10	0.68	1.07	5.06	4.45
AA-K-COF	1220	the eclipsed Kagome (AA-K) mode of the COF	2D	kgm	-	-	1612	0.59	36.3	0.16	0.29	0.36	1.14	1.03	5.91	4.13

Zn-Por-TT-COF-AA	1221	AA-stacking mode of Zn-Por-TT COF	2D	sql	-	-	1825	0.58	20.7	0.18	0.29	0.21	1.30	1.45	5.82	4.72
TAPT-2,3-NA(OH)2-COF-AA	1222	TAPT-2,3-NA(OH)2COFwith A–A	2D	hcb	-	-	892	0.35	33.7	0.09	0.18	0.34	0.74	0.59	7.51	4.08
TpFH	1223	TpFH	2D	hcb	-	-	1062	1.07	9.5	0.11	0.54	0.09	0.49	0.96	4.15	4.18
TADP-COF	1224	TADP-COF	2D	sql	-	-	1782	0.66	16.4	0.18	0.33	0.16	1.20	1.49	5.51	4.74
PS-COF-1-AA	1225	PS-COF-1 with AA stacking	2D	hcb	-	-	2447	0.26	52.8	0.24	0.13	0.53	2.13	1.16	6.56	4.38
TFPM-PDAN	1226	TFPM-PDAN	3D	dia	-	-	1019	0.82	5.3	0.10	0.41	0.05	0.60	0.97	5.29	4.53
COFTab-Dva	1227	COFTab-Dva	2D	hcb	-	-	2225	0.44	26.3	0.22	0.22	0.26	1.73	1.64	6.05	4.88
BPD-COF	1228	BPD-COF	2D	hcb	-	-	2151	0.49	23.6	0.22	0.24	0.24	1.63	1.64	5.94	4.88
TpPa-2	1229	TpPa-2	2D	hcb	-	-	1518	0.78	13.8	0.15	0.39	0.14	0.92	1.31	5.17	4.56
COF1-AA	1230	the AA-stacking mode of COF1	2D	hcb	-	-	1880	0.64	14.7	0.19	0.32	0.15	1.28	1.60	5.52	4.86
COF2-AA	1231	the AA-stacking mode of COF2	2D	hcb	-	-	2050	0.54	22.1	0.21	0.27	0.22	1.50	1.60	5.81	4.82
COF-TPDD-AA	1232	COF-TPDD with AA packing	2D	hcb	-	-	2037	0.50	28.5	0.20	0.25	0.28	1.53	1.46	5.98	4.67
CFD-DBD-AA	1233	the eclipsed AA-stacking unit cell of COF-DBD	2D	hcb	-	-	1771	0.60	20.9	0.18	0.30	0.21	1.24	1.40	5.76	4.66
COF-p-NEU1	1234	COF-p-NEU1.	2D	hcb	-	-	2373	0.34	36.7	0.24	0.17	0.37	1.97	1.50	6.34	4.75
COF-p-NEU2	1235	COF-p-NEU2	2D	hcb	-	-	2209	0.37	35.8	0.22	0.19	0.36	1.80	1.42	6.34	4.66
COF-1	1236	COF	3D	sqc	-	-	7372	0.38	8.2	0.74	0.19	0.08	5.95	6.77	2.12	8.06
COF-2	1237	COF	3D	sqc	-	-	7426	0.38	8.2	0.74	0.19	0.08	6.01	6.82	2.08	8.09
COF-3	1238	COF	3D	sqc	-	-	1392	0.82	6.8	0.14	0.41	0.07	0.82	1.30	5.06	4.67
COF-318-AB	1239	COF-318-AB	2D	hcb	-	-	1733	0.86	7.2	0.17	0.43	0.07	0.99	1.61	4.70	4.79
DCTMP-DMTP-COF-AB	1240	the AB-stacking mode of DCTMP-DMTP-COF	2D	hcb	-	-	2621	0.58	6.7	0.26	0.29	0.07	1.86	2.44	5.23	5.53

COF-1-AA	1241	eclipsed (AA) stacking unit cell of COF-1	2D	hcb	-	-	1896	0.66	15.3	0.19	0.33	0.15	1.27	1.61	5.41	4.82
JNU-2	1242	JNU-2	2D	sql	-	-	1845	0.69	14.6	0.18	0.35	0.15	1.20	1.57	5.32	4.79