Supporting Information

Design of 3D 1,3,5,7-tetraphenyladamantane based covalent organic frameworks as hydrogen storage materials

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The supporting information provides the space group symmetries and coordinates of four designed adm-ACOF frameworks.

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Name
adm-ACOF-1

Space group symmetry
I-43m
a = b = c = 33.1972
alpha = beta = gamma = 90º

Atom	x	y	z
C1	0.45404	0.27800	0.62482
C2	0.46159	0.24097	0.65326
B3	0.42746	0.48854	0.46721
O4	0.43399	0.45503	0.49422
C5	0.51435	0.33711	0.54165
C6	0.50905	0.37002	0.51550
C7	0.48417	0.32487	0.56949
C8	0.47322	0.39277	0.51638
C9	0.44305	0.38172	0.54413
C10	0.44840	0.34846	0.56983
H11	0.44725	0.30446	0.64319
H12	0.42741	0.27185	0.60633
H13	0.54109	0.32201	0.53983
H14	0.53175	0.37720	0.49592
H15	0.41665	0.39758	0.54576
H16	0.42513	0.34205	0.58880
H17	0.52591	0.25497	0.55085
C18	0.50000	0.25000	0.57056

Name
adm-ACOF-2

Space group symmetry
P-43m
a = b = c = 21.581
alpha = beta = gamma = 90º

Atom	x	y	z
H1	0.88782	0.47393	0.96875
C2	0.13844	0.61429	0.05959
C3	0.17088	0.66084	0.09170
H4	0.15768	0.59998	0.01902
H5	0.21151	0.67703	0.07337
C6	0.95752	0.54452	0.95752
C7	0.08116	0.58972	0.08116
C8	0.14711	0.68584	0.14711
C9	0.91780	0.50000	0.00000
C10	0.00000	0.58487	0.00000
H11	0.02888	0.61509	0.97112
C12	0.73946	0.82211	0.82211
C13	0.76732	0.76732	0.84872

Name
adm-ACOF-3

Space group symmetry
I-43m
a = b = c = 49.2532
alpha = beta = gamma = 90º

Atom	x	y	z
B1	0.36960	0.53342	0.47722
O2	0.38754	0.53358	0.45408
C3	0.58735	0.46443	0.31568
C4	0.56912	0.50939	0.30902
C5	0.55162	0.50574	0.33129
C6	0.55194	0.48129	0.34609
C7	0.57007	0.46068	0.33812
H8	0.59981	0.44860	0.31095
H9	0.57082	0.44268	0.34848
H10	0.56809	0.52758	0.29913
H11	0.53871	0.52115	0.33658
O12	0.37810	0.51233	0.49566
C13	0.43745	0.46881	0.47621
C14	0.44490	0.48360	0.45215
C15	0.39978	0.50079	0.48348
C16	0.40554	0.51353	0.45910
C17	0.42767	0.50527	0.44342
C18	0.41541	0.47880	0.49225
H19	0.43045	0.51552	0.42571
H20	0.41005	0.47066	0.51045
C21	0.58752	0.48889	0.30031
C22	0.49368	0.27581	0.60592
C23	0.46884	0.26853	0.62482
H24	0.21403	0.61291	0.46362
H25	0.20096	0.63765	0.48588
H26	0.49644	0.26742	0.67502
C27	0.50000	0.25000	0.66174

Name
adm-ACOF-4

Space group symmetry
P-43m
a = b = c = 32.1251
alpha = beta = gamma = 90º

Atom	x	y	z
O1	0.32419	0.16077	0.89088
C2	0.16964	0.20135	0.76713
C3	0.16784	0.29392	0.86258
C4	0.19974	0.26445	0.86178
H5	0.22081	0.26707	0.88517
H6	0.14356	0.61694	0.05081
H7	0.10596	0.56711	0.01279
C8	0.11601	0.60629	0.06277
C9	0.09338	0.57621	0.04039
H10	0.92468	0.48248	0.97901
C11	0.10058	0.62212	0.10058
C12	0.05468	0.56002	0.05468
C13	0.97148	0.52995	0.97148
B14	0.34392	0.12285	0.87715
C15	0.94483	0.50000	0.00000
C16	0.00000	0.55710	0.00000
H17	0.98060	0.57739	0.01940