Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

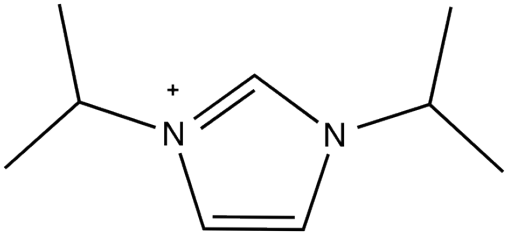
for

Synthesis and structural characterization of Zn-containing DAF-1

by

Ana B. Pinar, Lynne B. McCusker,* Christian Baerlocher, Son-Jong Hwang, Dan Xie, Annabelle Benin and Stacey I. Zones

N,N'-di-isopropyl-imidazolium



^{13}C CPMAS NMR

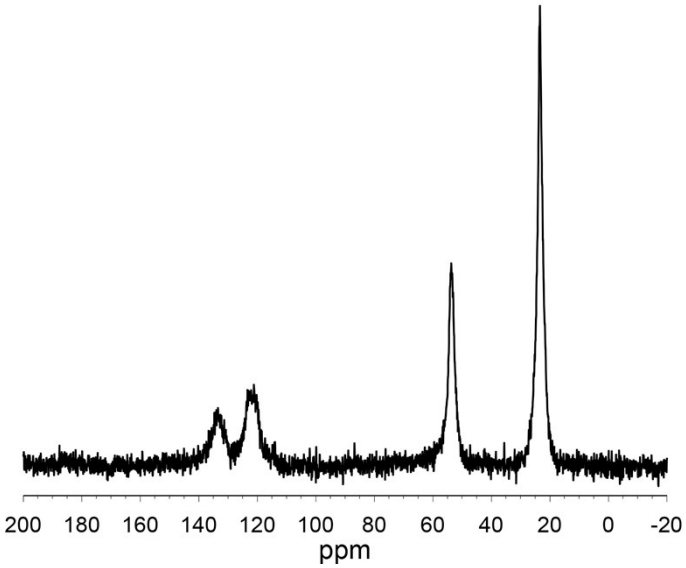


Fig. S1. $^{13}C\{^{1}H\}$ CPMAS spectrum of Zn-DAF-1 (ω_r = 8 kHz). The signals at 133 and 122 ppm correspond to carbons in the imidazolium ring, and those at 53 and 23 ppm to the isopropyl carbons.

^{19}F MAS NMR

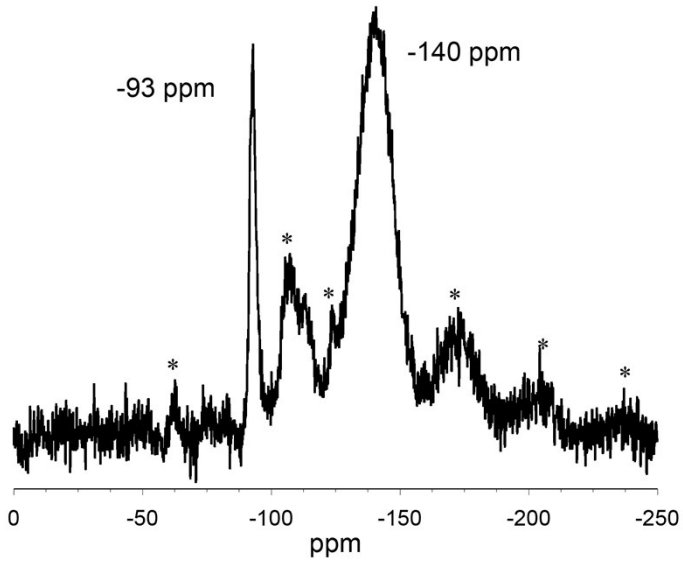


Fig. S2. ^{19}F MAS spectrum of Zn-DAF-1 (ω_r = 14.5 kHz). Spinning sidebands are indicated with asterisks.

^{27}Al {19F} CPMAS NMR

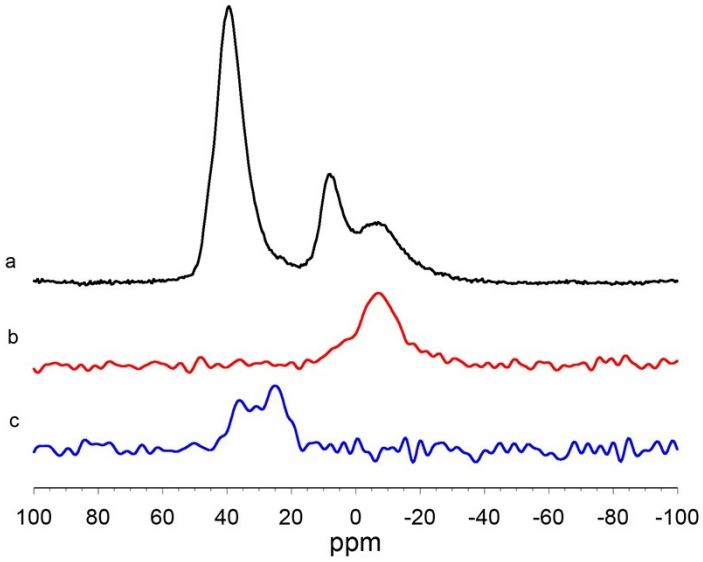


Fig. S3. (a) ^{27}Al MAS spectrum of Zn-DAF-1 with ^{1}H decoupling alone.
(b) ^{27}Al{^{19}F} CPMAS signal with irradiation of ^{19}F resonance at -140 ppm, and (c) at -93 ppm.
ω_r = 14 kHz.

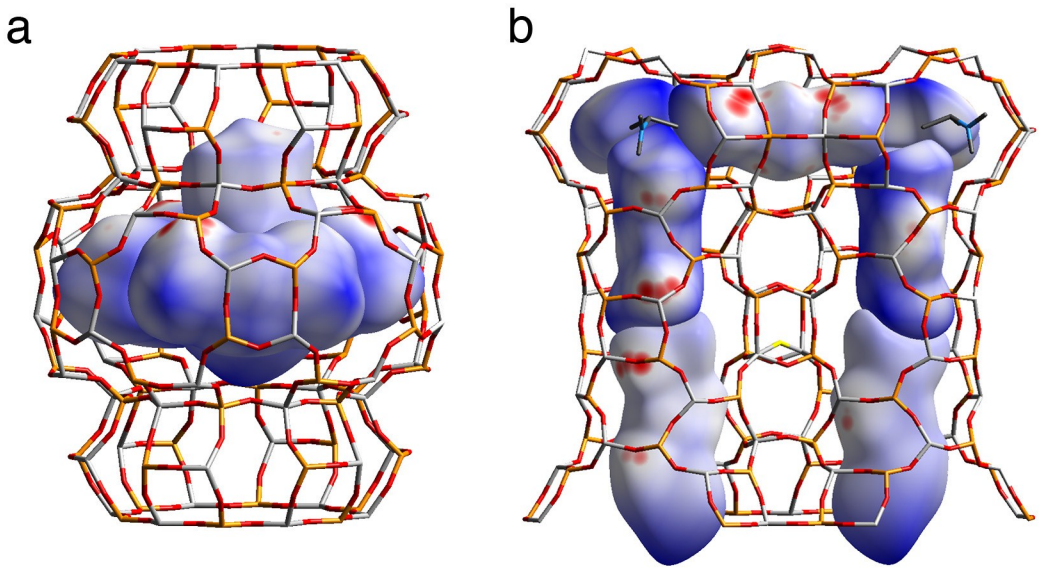


Fig. S4. Hirshfeld surfaces calculated using CrystalExplorer [26] for the four crystallographically distinct DIPI cations in Zn-DAF-1 showing how their arrangement fills the channels and cavities of the **DFO**-type framework. (a) DIPI-1 and DIPI-2 in the large cavity of channel B. (b) DIPI-3 in channel A and DIPI-4 in the aperture between neighboring channels A. A contact distance normalized by the van der Waals radii of the atoms involved (*dnorm*) has been used. Red areas represent intermolecular contacts shorter than the sum of the van der Waals radii of the atoms. Distances around the sum of van der Waals radii are white and longer contacts are blue.

[26] J. J. McKinnon, D. Jayatilaka and M. A. Spackman, *Chem. Commun*. 2007, 3814.

Crystallographic Information File (cif) for Zn-DAF-1

No estimated standard deviations are given for the non-framework atoms, because they were heavily constrained and restrained (more or less as rigid bodies) and were not refined to convergence.

```
data_Zn-DAF-1
_cell_length_a                   22.2244(1)
_cell_length_b                   22.2244(1)
_cell_length_c                   42.3293(3)
_cell_angle_alpha                90.0
_cell_angle_beta                 90.0
_cell_angle_gamma               120.0

_symmetry_space_group_name_H-M     'P 6/m c c'
_symmetry_Int_Tables_number         192
_symmetry_cell_setting             hexagonal
loop_
_symmetry_equiv_pos_as_xyz
'+x,+y,+z'
'-y,+x-y,+z'
'-x+y,-x,+z'
'-x,-y,+z'
'+y,-x+y,+z'
'+x-y,+x,+z'
'+y,+x,1/2+z'
'+x-y,-y,1/2+z'
'-x,-x+y,1/2+z'
'-y,-x,1/2+z'
'-x+y,+y,1/2+z'
'+x,+x-y,1/2+z'
'-x,-y,-z'
'+y,-x+y,-z'
'+x-y,+x,-z'
'+x,+y,-z'
'-y,+x-y,-z'
'-x+y,-x,-z'
'-y,-x,1/2-z'
'-x+y,+y,1/2-z'
'+x,+x-y,1/2-z'
'+y,+x,1/2-z'
'+x-y,-y,1/2-z'
'-x,-x+y,1/2-z'

_pd_proc_ls_prof_wR_factor        0.113
_pd_proc_ls_prof_wR_expected      0.050
_refine_ls_R-factor               0.144

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
Al1    Al   1.000      0.2139(5)   0.2927(4)   0.1283(2)    0.010
Al2    Al   1.000      0.1463(5)   0.4304(5)   0.1578(2)    0.010
```

Al3	Al	1.000	0.3900(4)	0.4715(5)	0.1014(2)	0.010
Al4	Al	1.000	0.3907(4)	0.4695(4)	0.2141(2)	0.010
Al5	Al	0.746(6)	0.1212(5)	0.3783(4)	0.0647(1)	0.010
Zn5	Zn	0.254	0.1212	0.3783	0.0647	0.010
Al6	Al	1.000	0.2176(6)	0.2969(5)	0.0	0.010
P1	P	1.000	0.0756(5)	0.2877(3)	0.1290(2)	0.010
P2	P	1.000	0.2904(4)	0.4333(4)	0.1599(2)	0.010
P3	P	1.000	0.0868(4)	0.4728(5)	0.0997(2)	0.010
P4	P	1.000	0.0823(4)	0.4683(4)	0.2130(2)	0.010
P5	P	1.000	0.2608(5)	0.3821(4)	0.0643(1)	0.010
P6	P	1.000	0.0763(7)	0.2930(4)	0.0	0.010
O1	O	1.000	0.1253(6)	0.2606(7)	0.1325(4)	0.010
O2	O	1.000	0.2405(9)	0.3283(6)	0.0905(2)	0.010
O3	O	1.000	0.2284(6)	0.2245(6)	0.1337(3)	0.010
O4	O	1.000	0.2583(9)	0.3556(5)	0.1570(3)	0.010
O5	O	1.000	0.0835(9)	0.3190(6)	0.0960(2)	0.010
O6	O	1.000	0.0924(9)	0.3416(5)	0.1544(3)	0.010
O7	O	1.000	0.2341(6)	0.4529(8)	0.1548(3)	0.010
O8	O	1.000	0.3194(5)	0.4538(7)	0.1924(2)	0.010
O9	O	1.000	0.3468(6)	0.4686(8)	0.1359(3)	0.010
O10	O	1.000	0.1263(8)	0.4704(8)	0.1282(3)	0.010
O11	O	1.000	0.1312(6)	0.4549(7)	0.1941(2)	0.010
O12	O	1.000	0.3334(5)	0.4421(6)	0.0693(2)	0.020
O13	O	1.000	0.4531(6)	0.5572(6)	0.0944(3)	0.020
O14	O	1.000	0.4295(9)	0.421(1)	0.1057(3)	0.020
O15	O	1.000	0.1072(8)	0.4474(6)	0.0704(2)	0.020
O16	O	1.000	0.422(1)	0.414(1)	0.2023(4)	0.020
O17	O	1.000	0.4561(6)	0.5567(6)	0.2094(5)	0.020
O18	O	1.000	0.3646(6)	0.454(1)	0.2530(2)	0.020
O19	O	1.000	0.2107(6)	0.4101(7)	0.0640(4)	0.020
O20	O	1.000	0.2559(8)	0.3470(5)	0.0332(1)	0.020
O21	O	1.000	0.0862(9)	0.3367(5)	0.0291(1)	0.020
O22	O	1.000	0.2296(7)	0.2255(8)	0.0	0.020
O23	O	1.000	0.1296(7)	0.2696(9)	0.0	0.020
N11	N	0.207	0.2717	0.2157	0.2544	0.030
N12	N	0.207	0.2157	0.2717	0.2544	0.030
C11	C	0.242	0.2566	0.2214	0.2237	0.030
C12	C	0.242	0.2214	0.2566	0.2237	0.030
C13	C	0.242	0.2564	0.2564	0.2717	0.030
C14	C	0.242	0.2953	0.1671	0.2666	0.030
C15	C	0.311	0.2374	0.0910	0.2634	0.030
C16	C	0.311	0.3584	0.1763	0.2480	0.030
C17	C	0.242	0.1671	0.2953	0.2666	0.030
C18	C	0.311	0.0910	0.2374	0.2634	0.030
C19	C	0.311	0.1763	0.3584	0.2480	0.030
N21	N	0.083	0.9405	0.9319	0.7969	0.030
N22	N	0.083	0.9405	0.9319	0.7455	0.030
C21	C	0.097	0.9143	0.9730	0.7872	0.030
C22	C	0.097	0.9143	0.9730	0.7552	0.030
C23	C	0.097	0.9592	0.9104	0.7712	0.030
C24	C	0.097	0.9557	0.9220	0.8305	0.030
C25	C	0.125	1.0343	0.9519	0.8347	0.030
C26	C	0.125	0.9311	0.9601	0.8526	0.030
C27	C	0.097	0.9557	0.9220	0.7118	0.030
C28	C	0.125	1.0343	0.9519	0.7072	0.030
C29	C	0.125	0.9311	0.9601	0.6899	0.030
N31	N	0.281	0.3290	0.6379	0.1188	0.030
N32	N	0.281	0.3290	0.6379	0.1707	0.030

C31	C	0.327	0.3914	0.6464	0.1287	0.030
C32	C	0.327	0.3914	0.6464	0.1607	0.030
C33	C	0.327	0.2936	0.6378	0.1447	0.030
C34	C	0.327	0.3145	0.6492	0.0851	0.030
C35	C	0.421	0.2793	0.5792	0.0666	0.030
C36	C	0.421	0.2691	0.6845	0.0839	0.030
C37	C	0.327	0.3145	0.6492	0.2044	0.030
C38	C	0.421	0.2793	0.5792	0.2219	0.030
C39	C	0.421	0.2691	0.6845	0.2058	0.030
N41	N	0.146	0.5682	0.5114	1.0015	0.030
N42	N	0.146	0.5114	0.5682	1.0015	0.030
C41	C	0.170	0.5399	0.5046	0.9720	0.030
C42	C	0.170	0.5046	0.5399	0.9720	0.030
C43	C	0.170	0.5537	0.5537	1.0185	0.030
C44	C	0.170	0.6079	0.4767	1.0122	0.030
C45	C	0.218	0.5733	0.4019	1.0	0.030
C46	C	0.218	0.6825	0.5170	1.0	0.030
C47	C	0.170	0.4767	0.6079	1.0122	0.030
C48	C	0.218	0.4019	0.5733	1.0	0.030
C49	C	0.218	0.5170	0.6825	1.0	0.030
F1	F	0.330	0.5	0.0	0.2674	0.030
O101	O	1.000	0.9086	0.8724	0.9487	0.013
O102	O	0.317	0.6667	0.3333	0.0	0.030
O103	O	0.201	0.7490	0.2510	0.0	0.030
O104	O	1.000	0.0	0.0	0.5	0.013