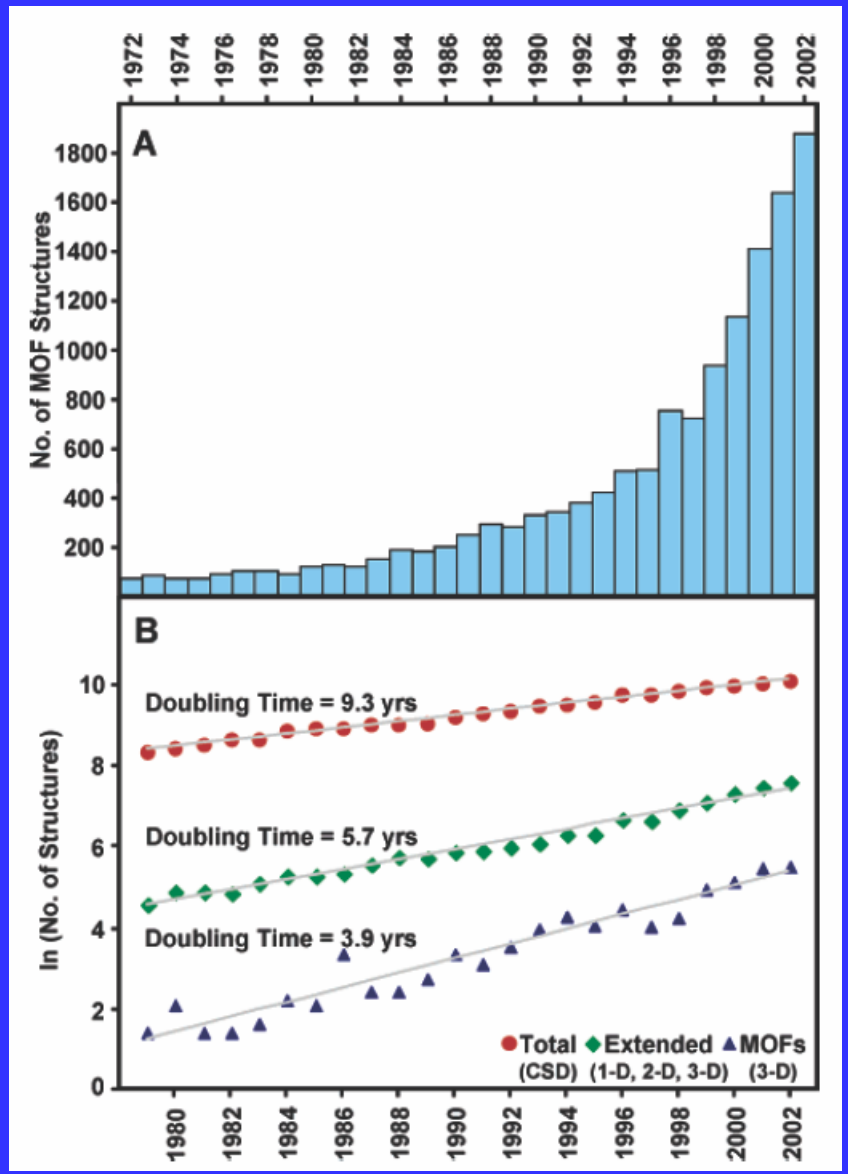
ΜΕΤΑΛΛΟ-ΟΡΓΑΝΙΚΟΙ ΣΚΕΛΕΤΟΙ ΓΙΑ ΕΦΑΡΜΟΓΕΣ ΑΠΟΘΗΚΕΥΣΗΣ ΑΕΡΙΩΝ

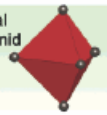
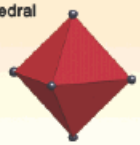
- Building units, design of MOF's
- Expansion, decoration, augmentation
- Gas absorption (methane, hydrogen, carbon dioxide)
-

Omar Yaghi et al.
Chem. Mater. 1999, 11, 2633, Acc. Chem. Res. 2005, 38, 176, Science 2005, 309, 1350, Science 2003, 300, 1127, JACS 2005, 127, 17998, Langmuir 2004, 20, 2683, JACS 2006, 128, 1304, Science 2002, 295, 469, Acc. Chem. Res. 2001, 34, 319.

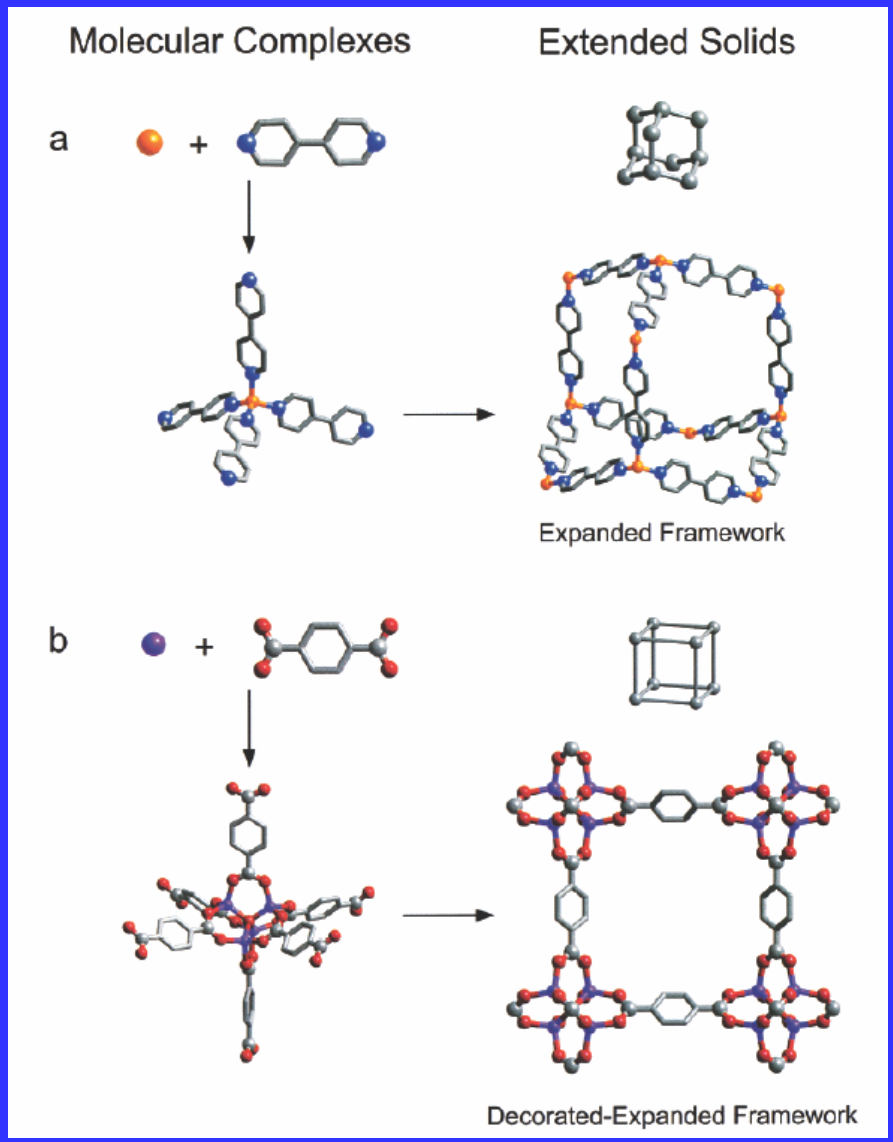
Progression of metal-organic framework (MOF) structures reported from 1972 through 2002 illustrating the dramatic increase in reports



Distribution of net types for each building block geometry

Building Blocks	CSD Refcode	Taxonomy Net	*No.*	*pq*
Trigonal (113) 	CAFRUX CDLGLU01 CDLGLU02 CDLGLU10 CDLGLU11 CECYOY CUFQOJ CUFROK CUFRUQ CUFSAX CUFSAX01 DAXXIJ DAXZIL DAYBAG FIGJIW GOGLUJ GOLRII GOLROO GOLRUU GUNFAW GUNFAW01 GUSNEN HEYTIO HEYTOU HEYTUA HUCKEV HUWHIQ HUYJOA HUYJUG HUYKAN HUYKER HUYKIV HUYKOB UYKUH IFUGIZ KEBRAK LIRFIB MOFQAZ MUBJOI MUBQIJ PAQDEQ PAQDEQ01 PIMYUF PUTYAE PUTYEI QAFGAG QITHAC QITHEG QUSWIK RADWOF RIZXUT TASFAU TASHUQ TIRHIL TUNFAJ VUWHAW YUWHAW01 WETSET WEMYOC WEMYOC01 WEMYUJ WOHSIV WOHSOB YAPFAG YINFEQ YUNVIM ZIWTII ZUQVAI ZUQVEM ZUQVIQ ZUQVOW ZUQVUC	srs	72	11
	AENCSE10 DULYAK GUBVUU HUNBEX KIRFIA LAQKIX LUDTUZ LUDVAH LUDVEL LUDVIP LUDYOV LUDYUB NOLYOC NUJXEV OBEDEE QETQIP QIVJAG QIYXIF QONVEU SEVQEW ZABQIC ZIBRAD ZIGGUU ZIGGUU01	ths	24	12
	CABQEB ROSCEH YUXMUZ	utd	3	12
	LOMFEY LOMFIC PEWJUW	etb	3	12
	QOJTUE QOJVAM	noe	2	23
	RIMXUG XEHXOX	nej	2	23
	RAJRUL	nob	1	22
	LIVTIT	nod	1	23
	DIPGAK	nob	1	24
	GOQWOY	noe	1	24
	AGAYOW	noe-a	1	34
	LUVNAU	noe	1	35
	OGOJOJ	nos	1	610
Tetrahedral (335) 	ACENIF ACOHIJ01 ADINCU AFENEE BACMOH BACMOH10 BAHGUN BOHGOU BONKUK BONLIZ CAWXAZ CEWNIB CICLOP CIDNIM CONXEI01 COVHEA CUGLTM CUGLTM01 CVPYCU10 DAHRJR DEQFOU DOCROC DOFREV DOFREV10 DOQFOE DOQGEV DUSTOA11 ECIWAO ECIWIW ECOGEI EDIKEH EDKIJ EFIMAH EFUWUX ENCUCC10 ENICCD EYCUCY10 FADWIR FAGHOE FAGHUL FAPYEA FAPYEA02 FAPYEA04 FAPYEA05 FAPYEA08 FAPYEA09 FAPYEA10 FAPYEA21 FAZWOS FOBQUO FOTPEJ FUGMOJ GAHKIJ02 GAHKIJ10 GEHUJV GEHNAI GISZUD GLALCU10 GMETCU GORQAF HEPHEP HIBSUG HODXIH HOGWAB HOQEAU HUJVOX HURNON HUXDO1 HUYLAO IDOGIR IGUFAR JARMEU JARMEU10 JIVXUH JUKVEQ JUKXIW JUKXIW01 KARPIC KARPOI KARPO01 KARRAW KARREA KARRIE KEGZOL KEGZOL01 KEJBOQ KEJBIQ KUNZED LAFJAR LEIVUB LOLVAJ LORNEL LOTRER LUMDEC LUMDIO MISCAR MASMIC MANFIA MAZYER MEHPAQ MIGMEJ MIGZUX MIHHIU MIHHOA MIHHUG MIJFIU MILTAC MOBBIO MTGLCU MUTGUD MUYNID NEYROY NHBZZN10 NIDXAZ NIGLUK NOGXUC NULROB NULRUH OBEDAA OBONUO ODUZOQ OGAWAU PAZXUJ PAZXUJ01 POQNUE PUWCAI PUWCEP PUWCII QAGTOH QAKDAH QALWUV QASLIF QEOGUE QEGHIP QEMYEM QOJKAB QOZDOT RAFNIV RAFNUH RAFNUH01 RASGAI REGIWW RENWEM RINPEJ ROMGAB RONZID RULVUP SARAW10 SCNTAC10 SEYDAB SUYFEX TACTAX TIFDOB TILVAI TILVEP TILVFI TILVOZ TILVUE TILWAM TILWEQ TIMKOP TIZVED TIZVED01 TIZVIH TIZVIH01 TMSNCM TONWUO TONWUO01 TUFWUM UFATEA UGEPEB UGOSOV UGUTOF UGUXAV VABJIS VABJUE VABKAL VABKEP VABLIU VABLUG VABMAN VABMER VIHTEL VIHWEO VIHWIS VOCKUT VOCQAF VODYIW WABVIF WALVOU WETQOB WIFFO WIFQUE WOFWE1 WOHIO WOJZOK WOJZOK01 WOVHEU WOXRAC WOXREG WUHXEC XANXUF XAPYAO XASGON XAYMUF XEBNEX XEFKOI XISNAY XISNEO XISXIG XISXOM XOTGUJ XOTHAP YEFNIG YEFPAA YEFPII YEFPUU YEYLUJ YEYMEU ZIHFEB ZIHFIF ZIHFUR ZIHFUR01 ZIMMEN ZITRUP ZNONAC ZOZJED ZUDRUL ZULFER ZULFIV ZUQPOQ	cia	233	11
	AHEFAU BISPAU DAQFAC ECUWOC EGUBET GEBQAL GEBQOZ GUXQEV HICVAQ HUPTER IDIWIB IDIWOH IDIWUN IDIXAU IDUDOA IFABIA IFABIA01 JOWRJW LEJBIX MALRUM MINVUO MINVUO01 MINVUA MINVUA01 MODWUX MODWUX01 PUWCOZ QOPHEI RUVCIU WEXNIW ZAYBEG	sra	31	13
	ACDMAL BEUJIL CUBMDZ01 QEFNAQ QQQGTA02 WABVOL WABVUR WABWAY WABWEC	sod	9	11
	CAGLIF GIPDUE IFUDAO IFUDES LAJDUV01 LAJDUV02 LAJDUV03 OHETIE VACFUB	cjz	9	11
	HGCNCO KEXFOI KEXFOI10 LOECUC NUBNAZ TENQOS WIBNOK XECJAQ YARVUL	crb	9	12
	LITHUR TCENCD10 WIWQOI WIWQUO ZENDAX ZENDEB	gis	6	12
	CERFAG DEHFUR FUCTAY IDUQUT LIYLEK YIQBAB	fou	6	12
	EGUHOD HEWHEA IDAKAZ MIMRAB MIMRAB01	irl	5	13
	HOKGUJ WURMUR WUKNAY	pcb	5	12
	FEFZOF FEYXEM	mmt	2	13
	IMIDZB IMIDZB01	zni	2	13
	IFEYIB PUWCUF	cng	2	14
	HUFZEB RUXWEM	noc	2	37
	AFDXAO AFIXES	nog	2	510
	ZUYWAR	gei	1	12
	TIDKA8	ieh	1	12
	JITQEI	qzd	1	12
	NUSMOX	uzh	1	12
	RIDKOE	pcl	1	14
	QAVDEW	bbf	1	22
	IDEBO1	nocs	1	22
	XAYNAM	bbm	1	24
	LATCIS	noq	1	24
	LATCEO	noc	1	24
	WILRIS	now	1	24
	XASDUQ	coe	1	25
	FALLOT	nol	1	28
	VEZXED	noa	1	32
Square (47) 	CAYSIE CAYSOK CAYYEG FAFMAA FAFMEE FAMSUH FAMTAO HOLVAF HUKZES HULCEW LIPJUP01	nbo	21	11
	QAFDOQ RAMSUT TIPRIT TIPRIT01 TIPROZ WUKWII WUKWII01 YIXBIQ YOVTIM YOVTOS	eds	18	12
	AGAYIQ ECUTAX FEVVIM IDEYOF NERNON ODAHIK PEBNEP POTWUQ POTXAX QAYTAL QIWQES SOBTUY			
	TUSAG TOPRAR TUSGOD UGIENUP VUGBOO ZURROI			
	AZPYCD JISGOH MEGFIN MIMVEJ UFUQIV VIWXUU XENCAU ZNACEU	lvt	8	11
(67) 	BIMDEF BIMDII CONGPY ENCDBZ01 JEJFAF JOKFIY MODPOK NINHOH NIQBUK PIZJAJ PIZJEN PUWDAM RANYOU RANZAH ROJNEJ SUDHOI UGUQOC WAWGOQ WAZCAB WIXJIW WIXJIW01 YAKKOK YARVEV ZEZGOA ZUWMIN	gts	25	21
	JOKXAI JOKXAT10 JOKXEM JOKXEM10 JOKXOW JOKXOW10 JOKXUC JOKXUC10 JOKYAJ JOKYAJ10 JOKYEN JOKYEN10 JOKYIR JOKYIR10 JOKYOX JOKYOX10 KEXFIC KEXFIC10 LAMFEK LAMFIO LAMFOU LAMGUB LAMHAI NUJCEA NUJCIE SEGMEW XAMLUS YIZWIN	gtl	28	32
	CUIMDZ03 HEGCEB HODWUS IMIDFE IMIDFE01 IMIDZA KECRAL KECRAL10 KECRAL11 KECRAL12 LEMPIC MIGKOC MIGKUI	tmg	13	22
	EGIFUV	asv	1	23
Trigonal Bipyramid (60) 	BUKLOJ BUKLOJ01 CILXIE DOSYAL GUGWOU01 GUXQAR JOSNAG JOSNAG01 KEXTAI KEXTEM LESBIU MINBEQ QAPWIN QAYTOZ QILAW QOZJOE QUHVEX01 QUPZAC QUPZIK QUPZOQ SIVIAI TUNEJ WOPXEE WUQMAI XAFNOH XAFNOH01 XEHFUL02 XIYEDA	bun	28	12
	AFEJOK BALFAV01 DAQSOD MABNEJ NIGHOA NIVFUT NIVFUT01 QUJVEW TUTLEZ WOPXAA WOPXAA01	sqp	18	12
	XAGTEE XANZUH XAPBAR XAPBEV XIPHIN XUHSOI YEQGIK			
	MABJOP MABJUV MABJUV01 MABKEG MABKIK MABKIK01	nok	6	26
	ACUBOP ACUBOP01 XIZPIF	noo	3	13
	WUGSUM WUGSUM01	nov	2	13
	QIBTAW QIBTEA	noy	2	13
	COYYOE	noz	1	13
Octahedral (152) 	ABUWOJ ACEPON AFEHUO AFEKAX BUKEW01 BUWAF BUWAF01 BUWAF02 BUKBUF CAHMON CAHMUT CAZGOZ CICSOW CICSOW01 CICSOW02 CSCNCA01 CSCNCC02 CUCTID DEFKUU DEPJIR DEPJIR01 DOMPUQ DOMPUQ10 DOQRUW DOYSIT DUCHIS ECOWOI EDUSIF EDUSOI EDUSUR EDUTAY EDUTEC EDUTIG EDUTOM EDUTUS EDUVAA EDUVEE EDUVII EDUVOO EDUVUU EDUWAB EFUFEQ FEVTEF GIDQOZ GIDQOZ01 GIDQOZ02 GIDQOZ03 GIDQOZ04 GIVHIC GLYCEA GOKKIA GORWUF GUJVAI HEBROL HIXDOH HIXDOH01 HOBBEF HOFXOP HOFXUV HUKQEZ HUKRAG HUKREK HUKRIO HUWSUN IBOTOI IBUTEE IDAJUS KEXFAU LINGAQ LINGEU LINJEX LINJOH LISKUT LISKUT01 LOTXEX LOTXOH LUMZUO LUNBAX LUNBEB LUVWUU MABLAD MACUFR MEBFAA MEZSAL MIHBAG MIJNAU MITXIW MIZQOB MOLLII MUHJEE MUHJEE01 MURREW MUSPAR MUSWOM NEXGOM NEYYIZ NEYYOF NEYZAS NICZAA NICZAA01 NOBLOF NOBLUI NOBMAS NOLQUA ODQPUY OFUWIV01 OFUWIV02 OXCFOR PURSOK PUWDEQ QAMXIL QATDEU QEBJOW QEBJOW01 QEQCIY QIQWOC REVSOA RIFPEB SUPZUY TEHQIG TOGCUN TUXNEF UHAXUW VADWON VINROZ VOVVUL VOJWAS WILWOD XEZMUK XJGWUF XILSEQ XOFFUT XOHVAR XOYCET XUDSIV XUDSUK XUVHEB YFORMD02 YIQBEF YUTGEZ ZESFUY ZIBFUL ZOXZIV ZOZJAZ ZUTBAR	pcu	145	11
	JETNIF JETNOL QUSBIP VARREL VARRIP ZUVTEP	nia	6	21
	EGOZAB	stz	1	12

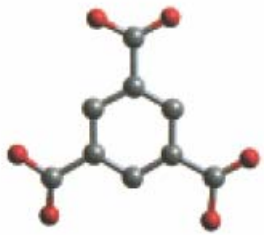
Assembly of MOFs by “copolymerization” of metal ions and linkers



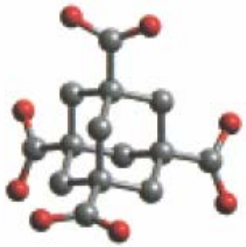
Polytopic organic linkers

1,4-benzenedicarboxylate
(BDC)

1,4-azodibenzoate
(ADB)

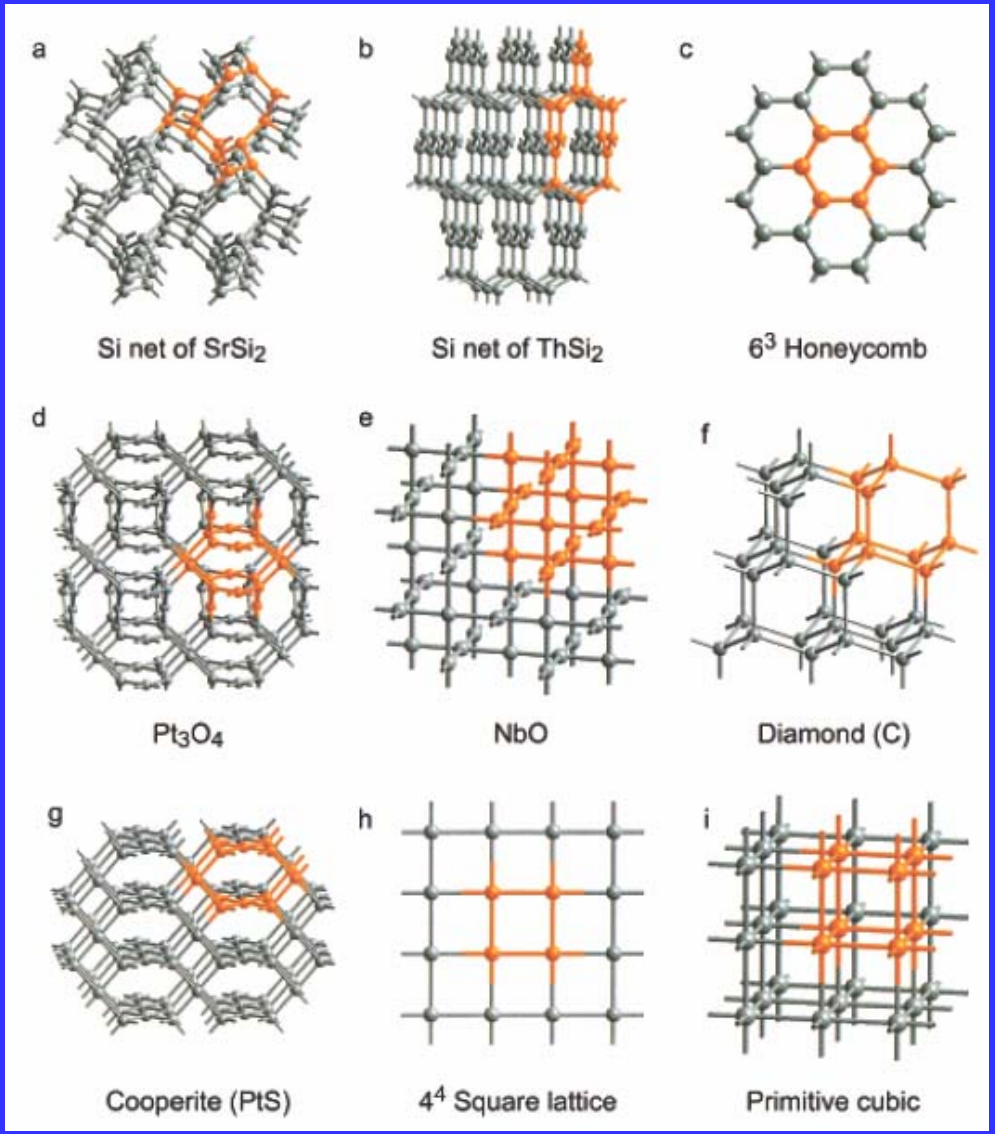


1,3,5-benzenetricarboxylate
(BTC)

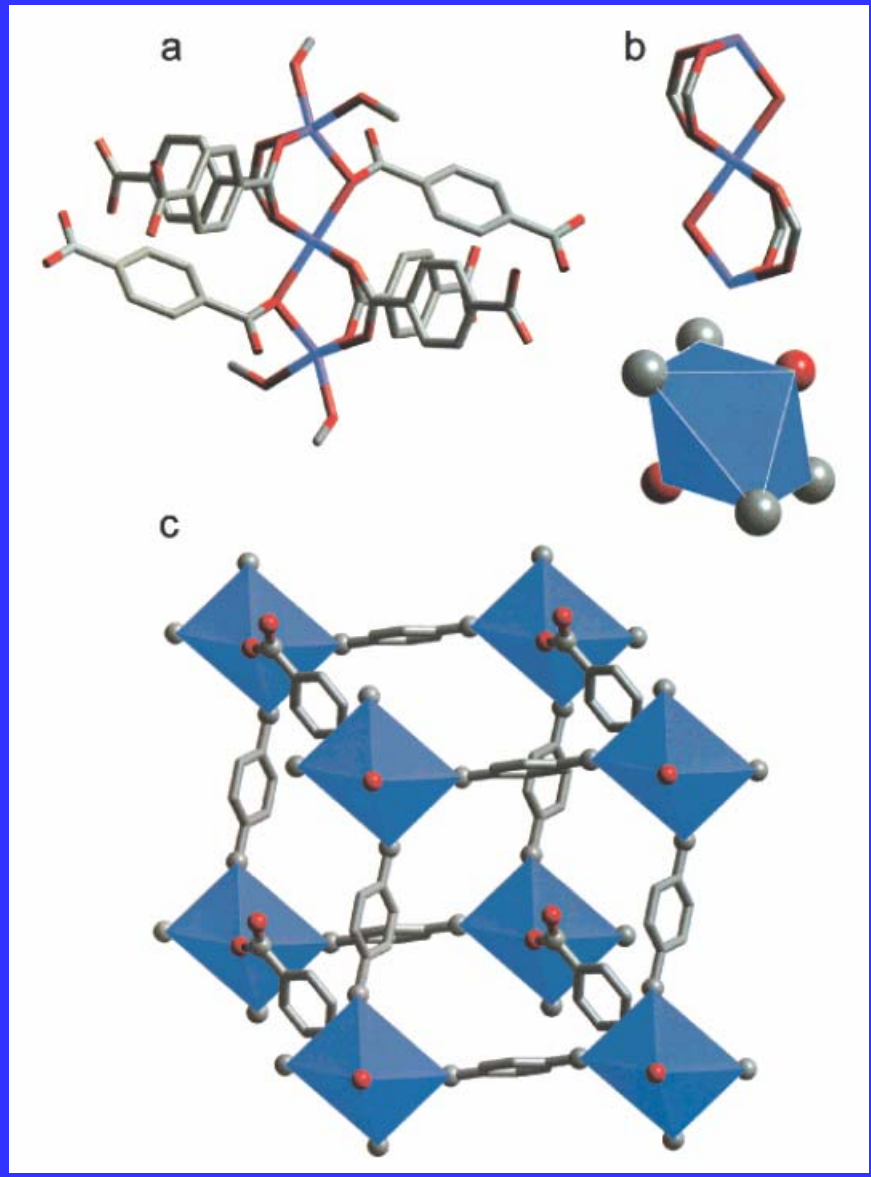


1,3,5,7-adamantanetetracarboxylate
(ATC)

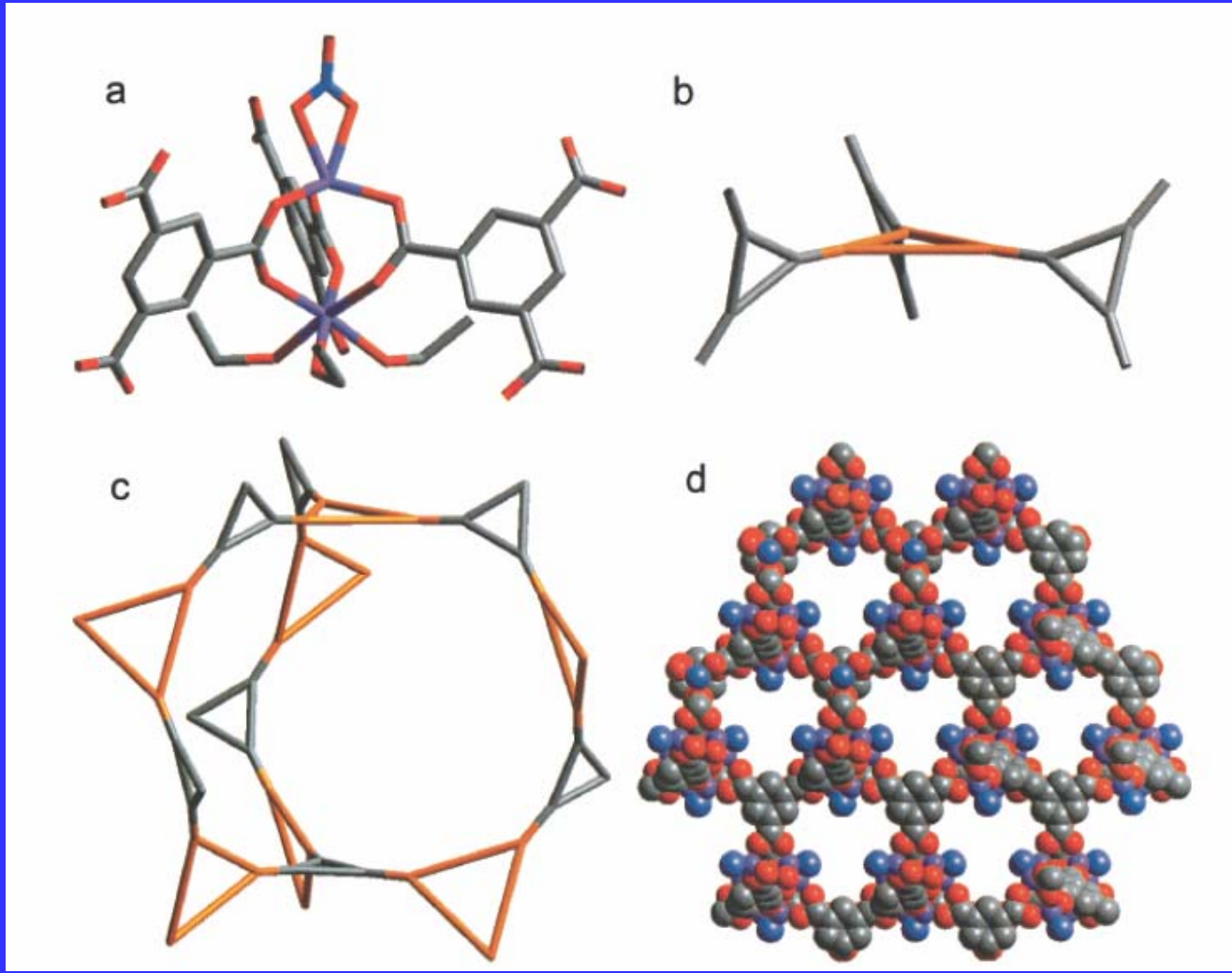
Common structural nets



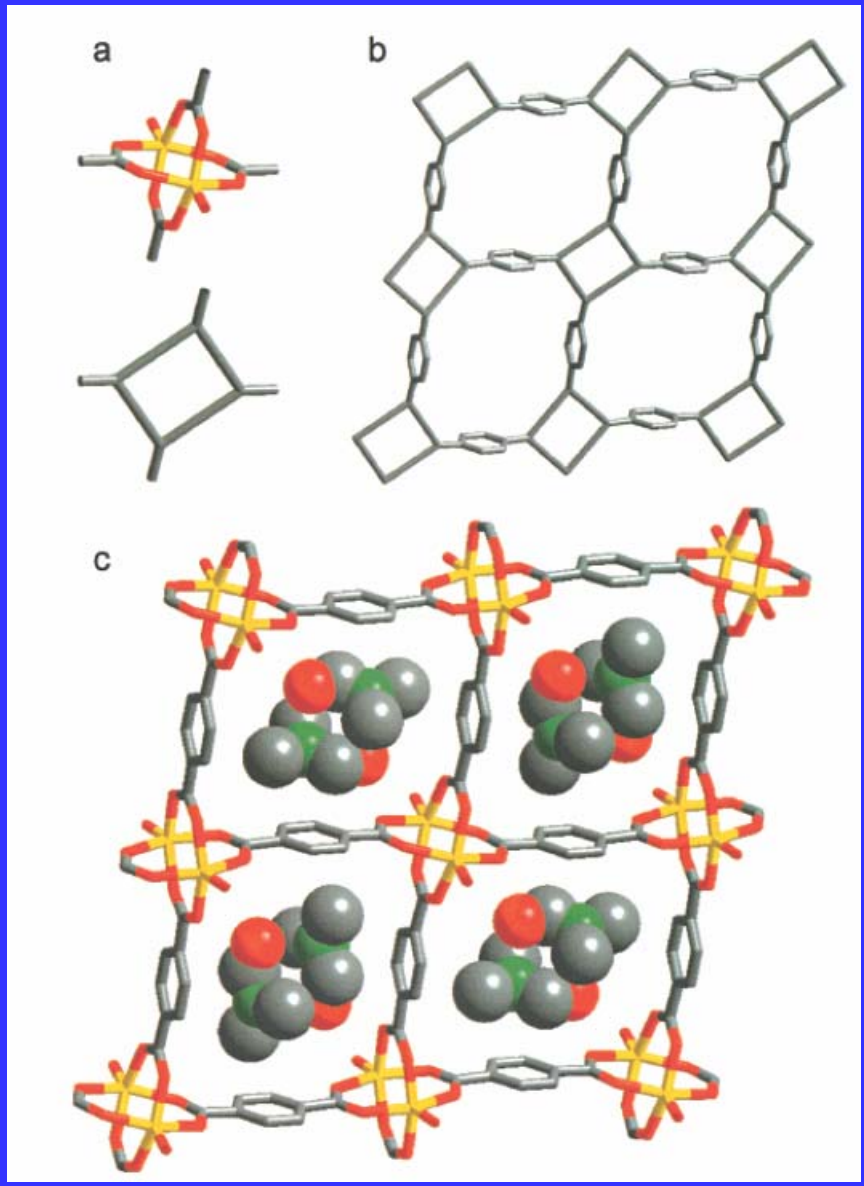
Building unit in the crystal structure of Zn3(BDC)3x6CH3OH (MOF-3)
BDC = benzenedicarboxylate



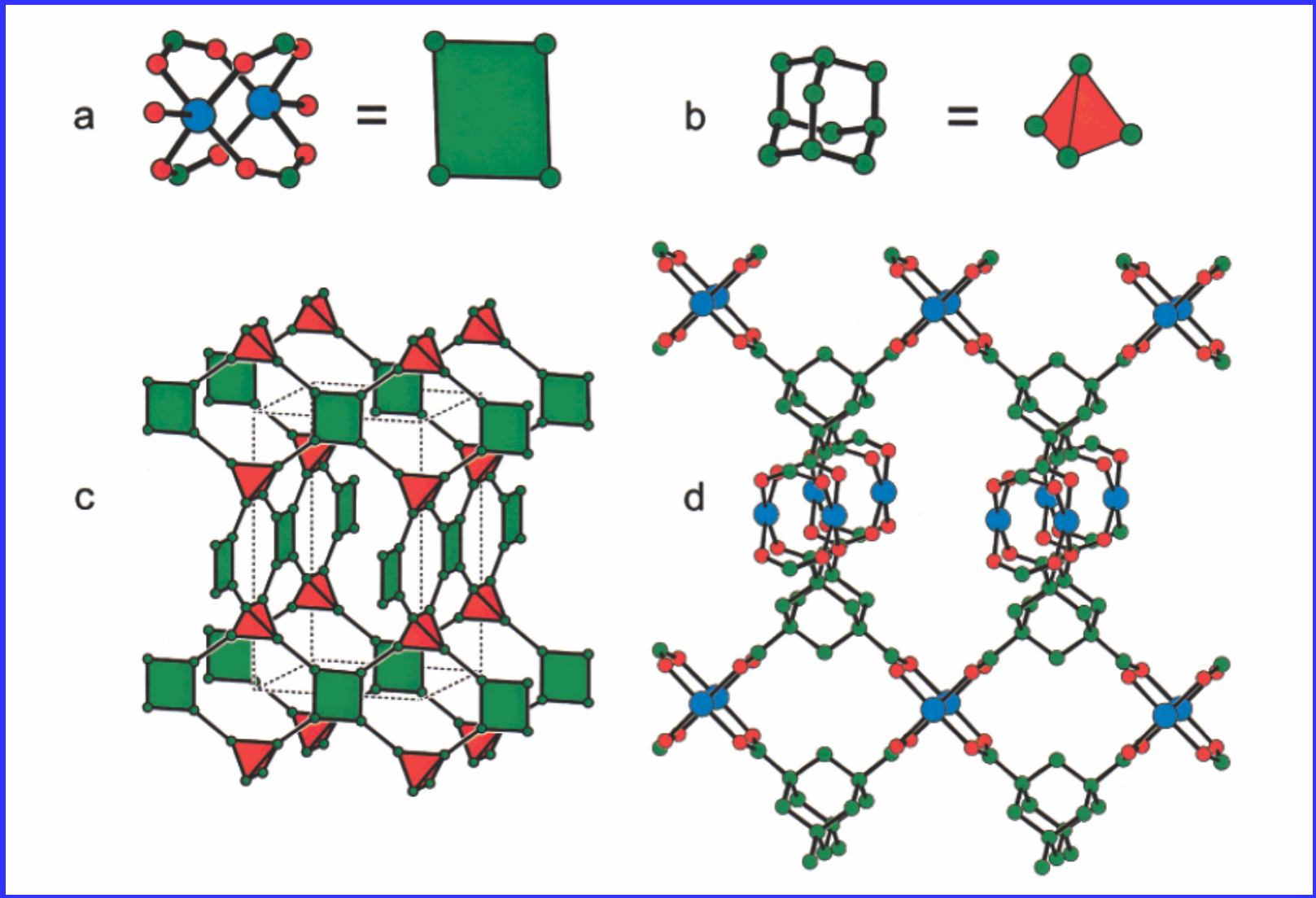
Building unit in the crystal structure of Zn2(BTC)(NO3)x(C2H5OH)5(H2O) (MOF-4)
BTC = benzene-tricarboxylate



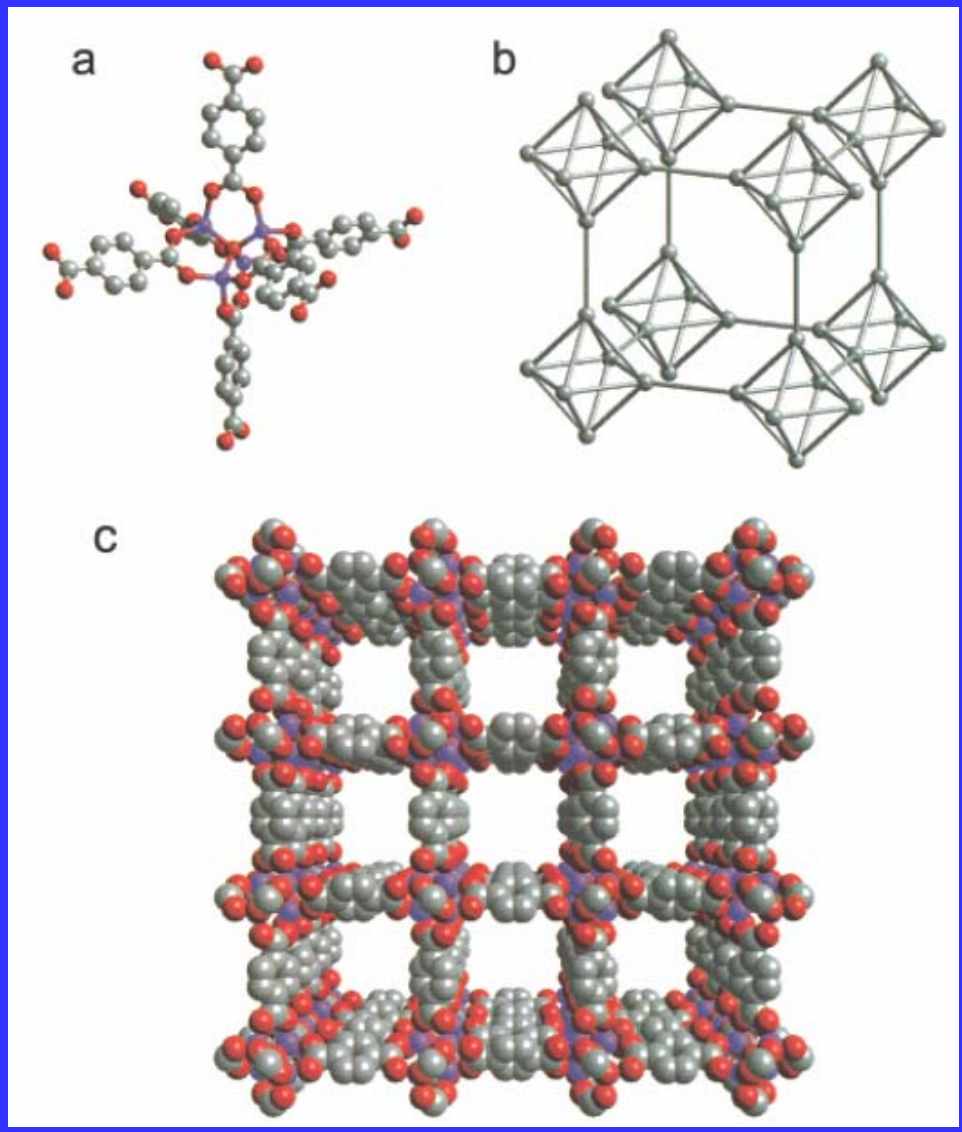
Paddle-wheel cluster, a square SBU, which is the building unit in the crystal structure of Zn(BDC)(H2O)x(DMF) (MOF-2)



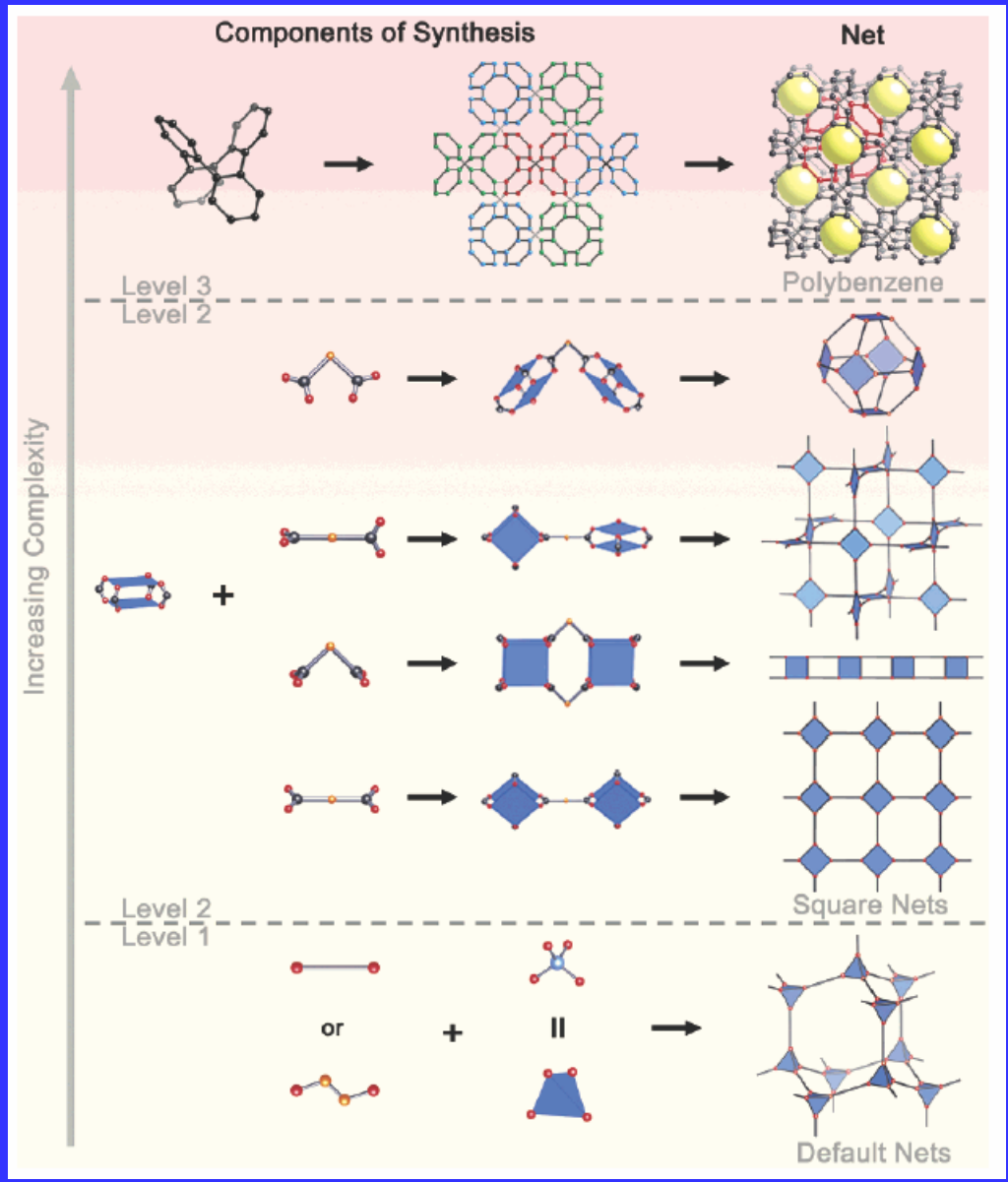
Paddle-wheel Cu2(OCO)4 SBU (Cu, blue; C, green; O, red) of square geometry (green) and (b) adamantane SBU (C, green) of tetrahedral geometry (red).



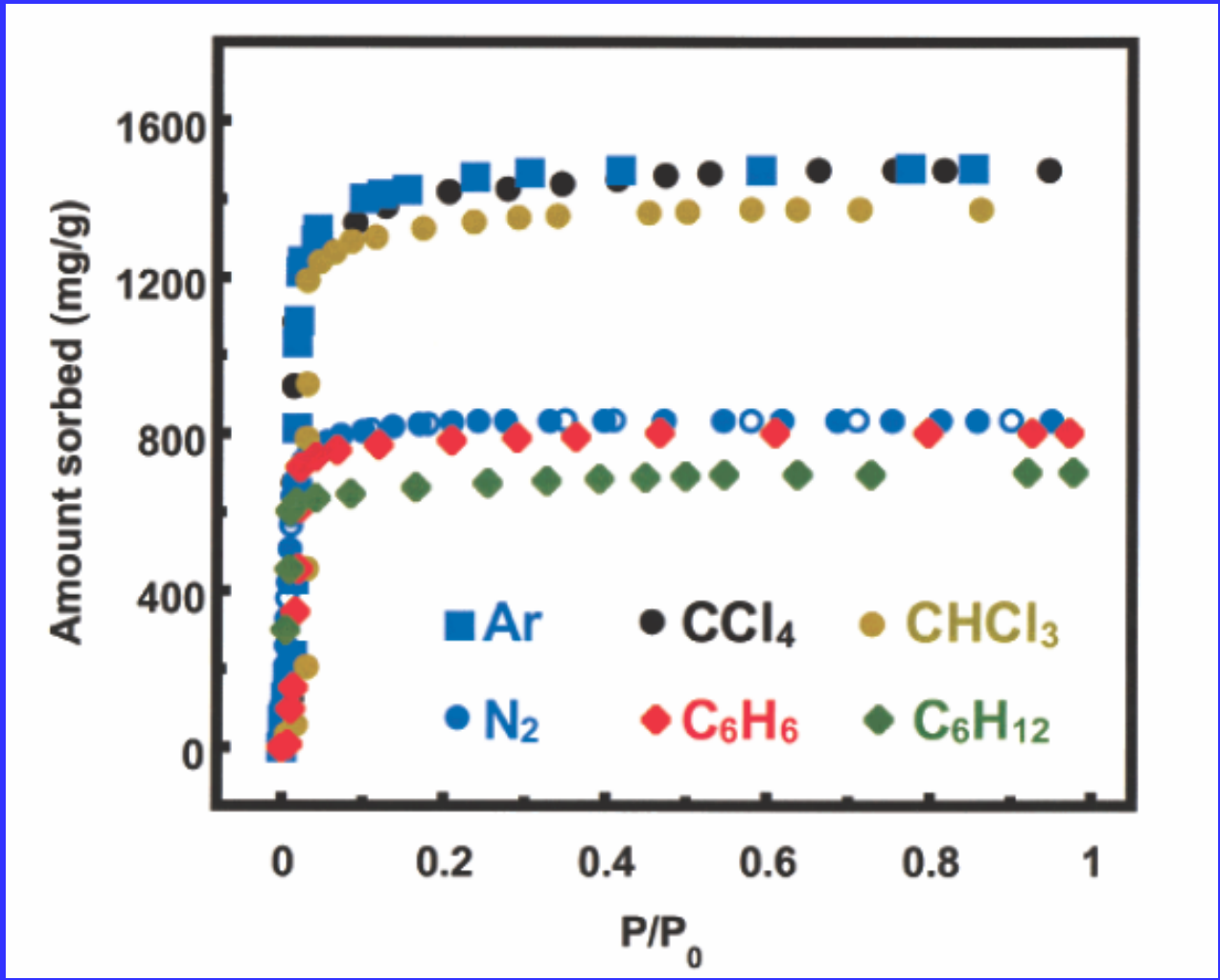
Building unit present in crystals of Zn4O(BDC)3x(DMF)8(C6H5Cl) (MOF-5)



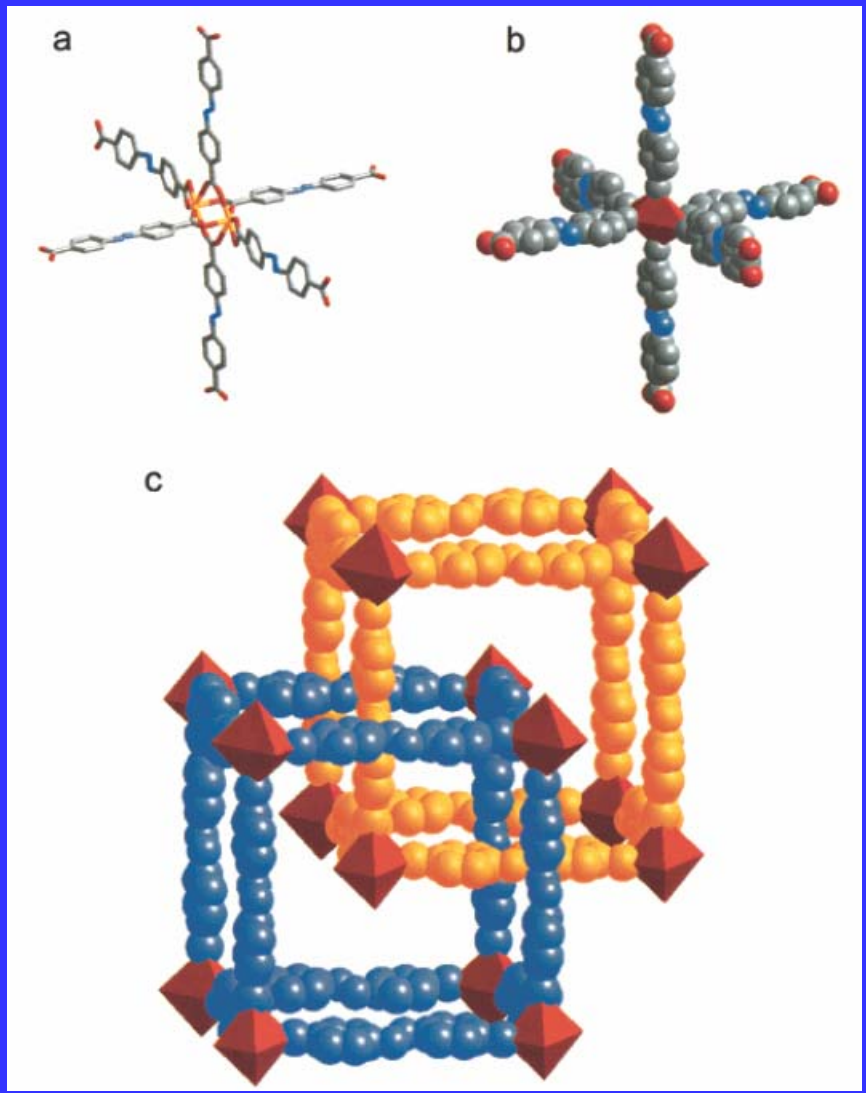
Complexity of MOF structures by varying the topology of the organic linkers



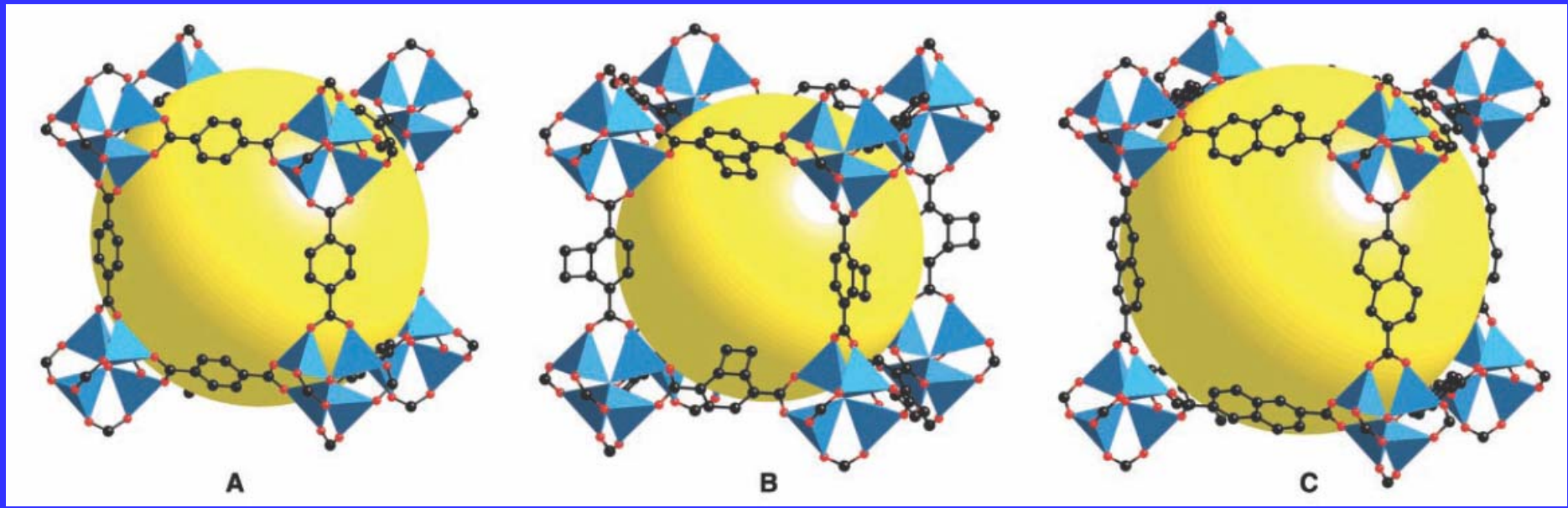
Typical gas sorption isotherms for MOFs, shown here for MOF-5.



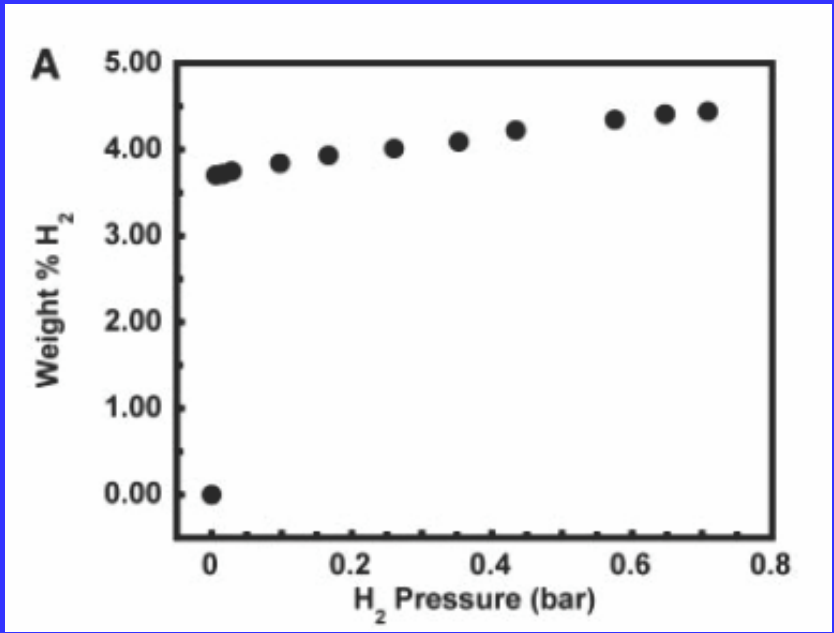
Crystal structure of MOF-9 approximately octahedral Tb2(ADB)3-(DMSO)4 building units (Tb, orange; O, red; C, gray; N, blue)

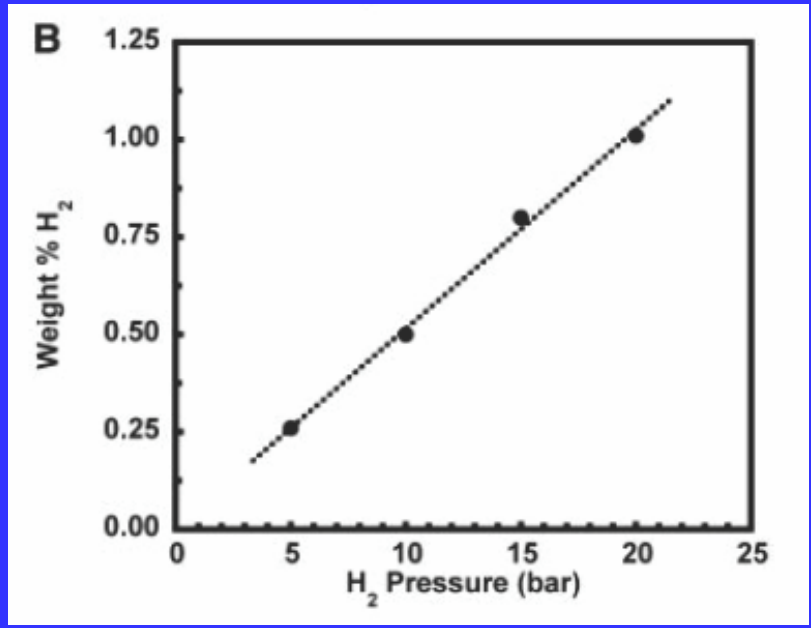


Single-crystal x-ray structures of MOF-5 (A), IRMOF-6 (B), and IRMOF-8 (C)

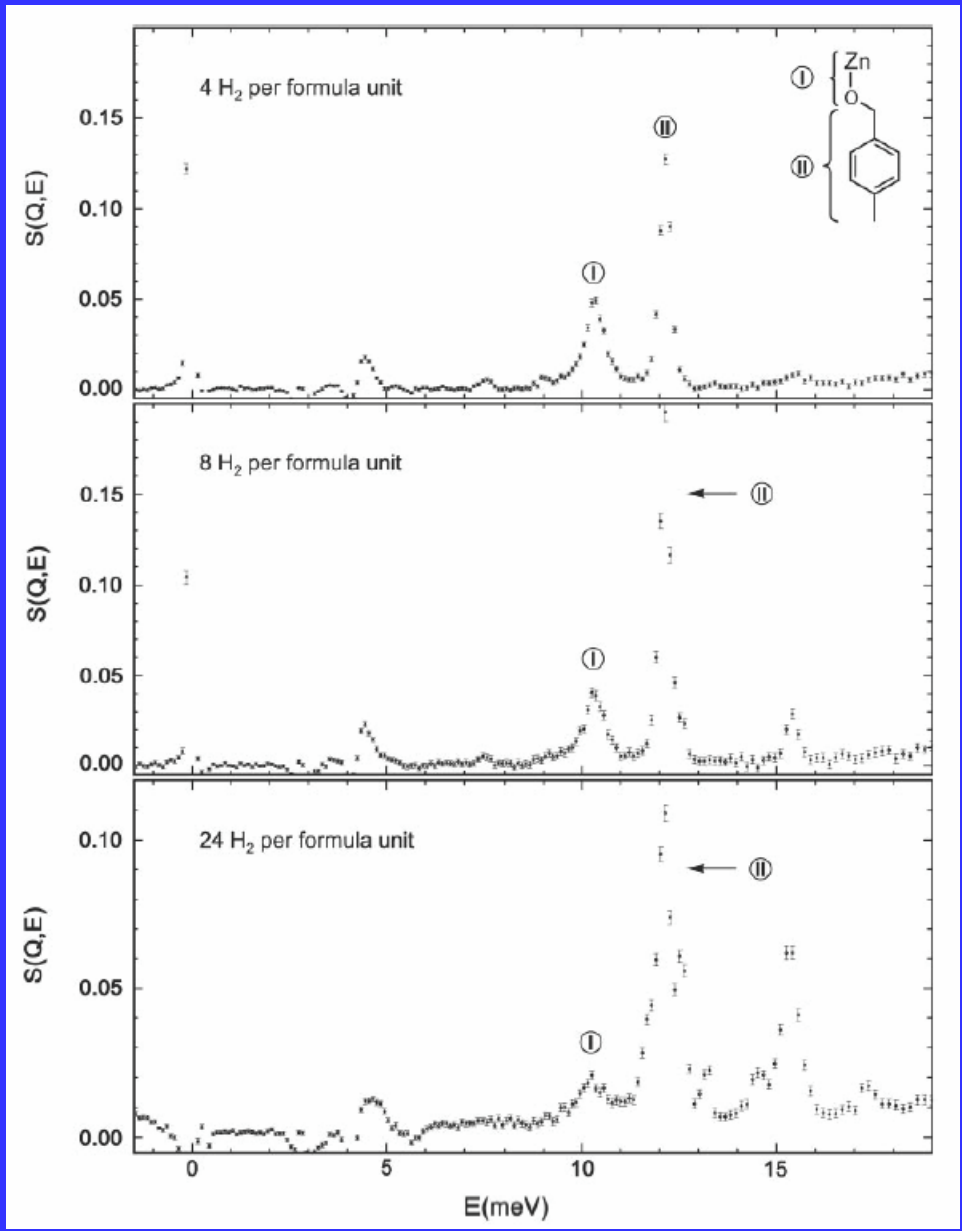


Hydrogen gas sorption isotherm for MOF-5 at (A) 78 K and (B) 298 K.

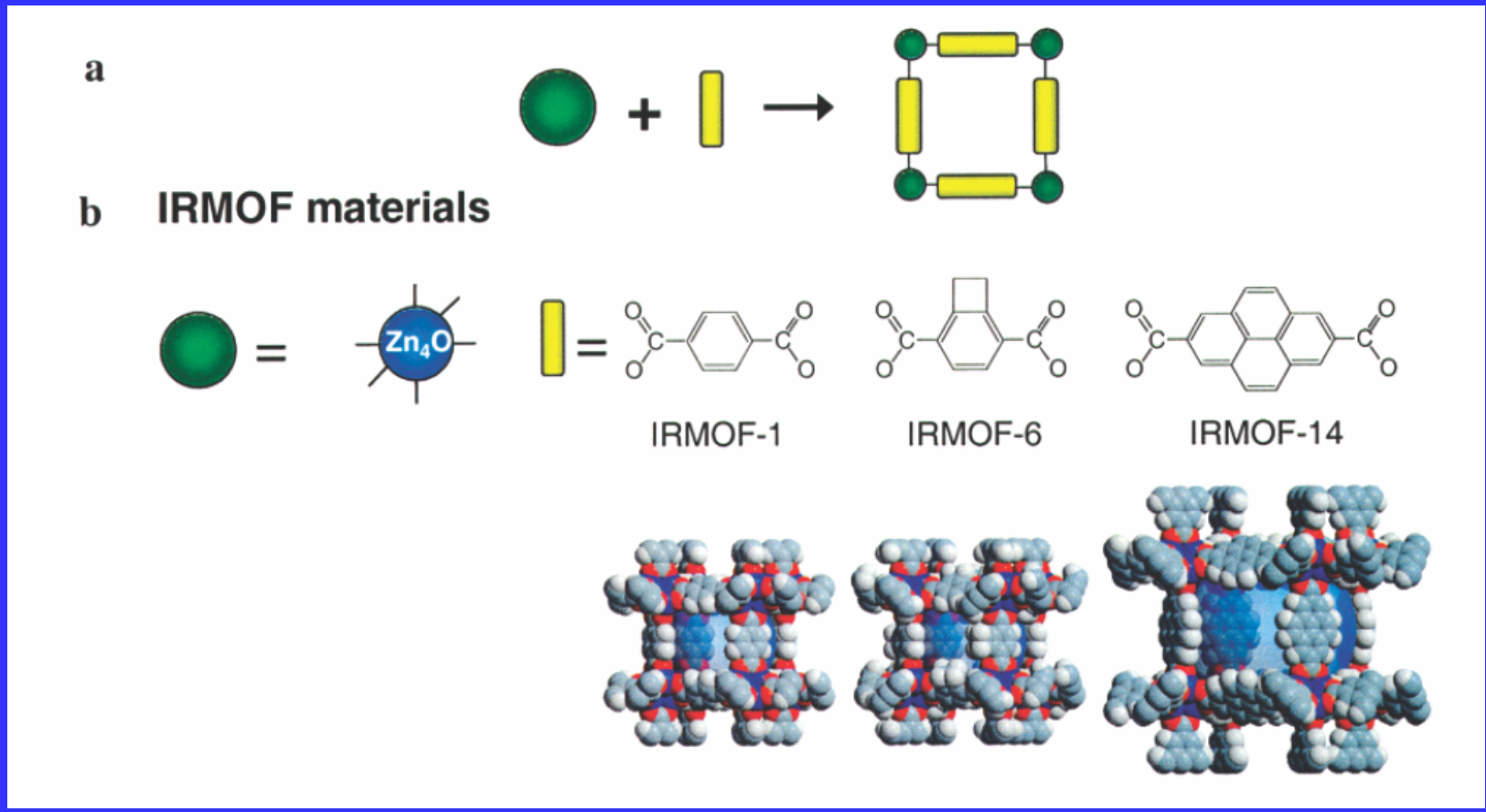




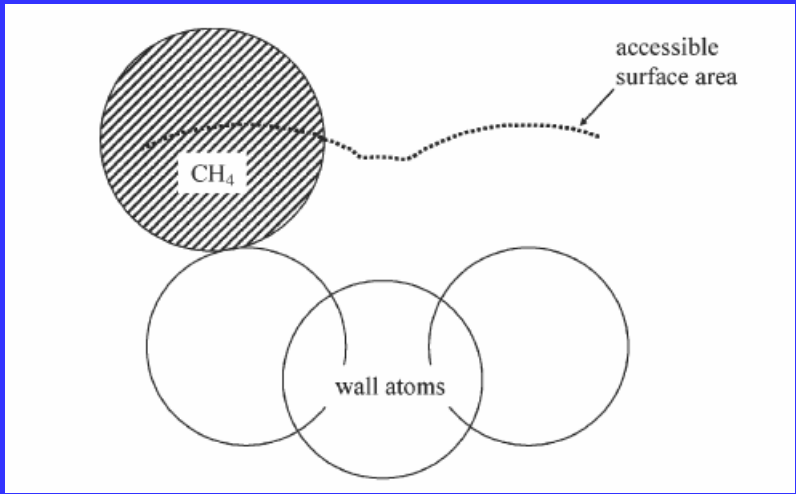
INS spectra (T = 10 K) for H2 adsorbed in MOF-5 with loadings of 4 H2 (top), 8 H2 (middle), and 24 H2 (bottom) per formula unit [Zn4O(BDC)3]

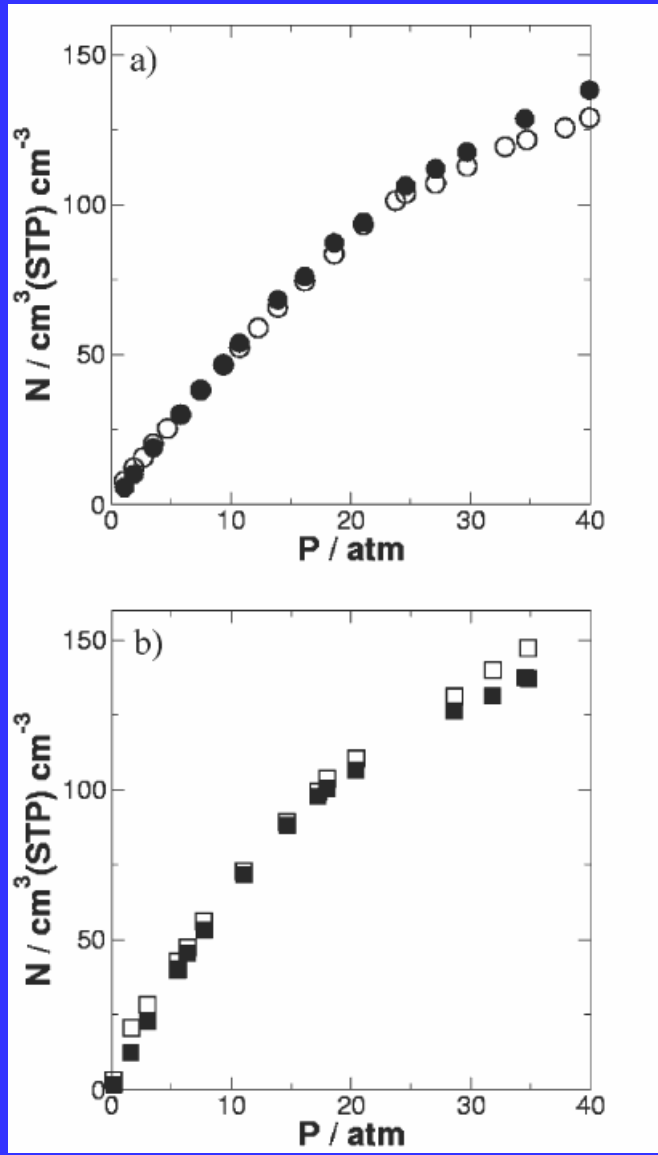


Examples of ligand-bridged metal-organic materials synthesized in a self-assembly process for methane storage applications



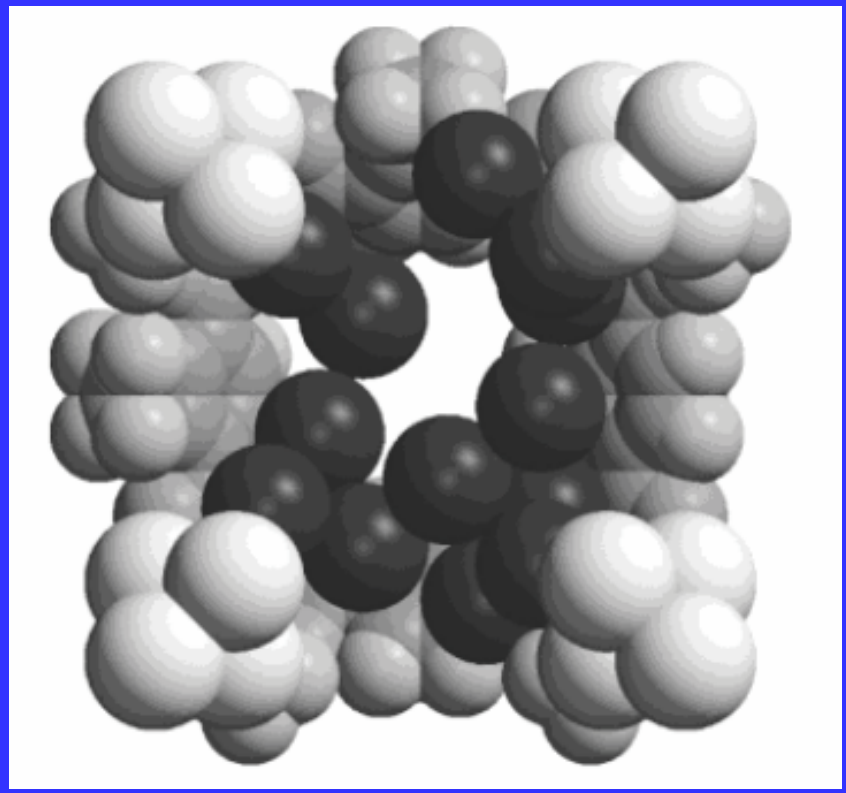
Definition of the accessible surface area



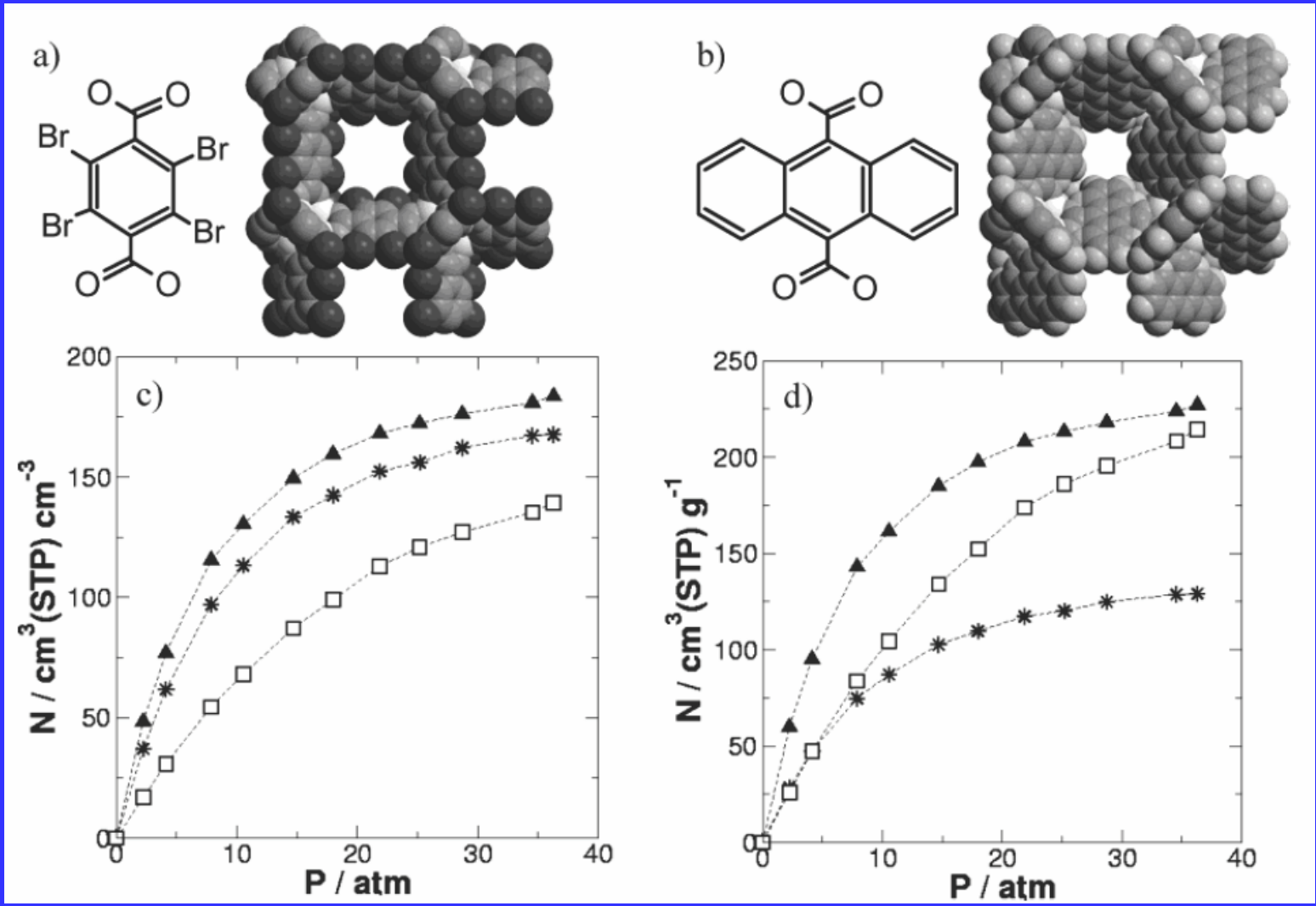


Experimental and simulated methane adsorption isotherms at 298 K: (a) IRMOF-1 and (b) IRMOF-6 (open symbols, experimental results; closed symbols, simulation results)

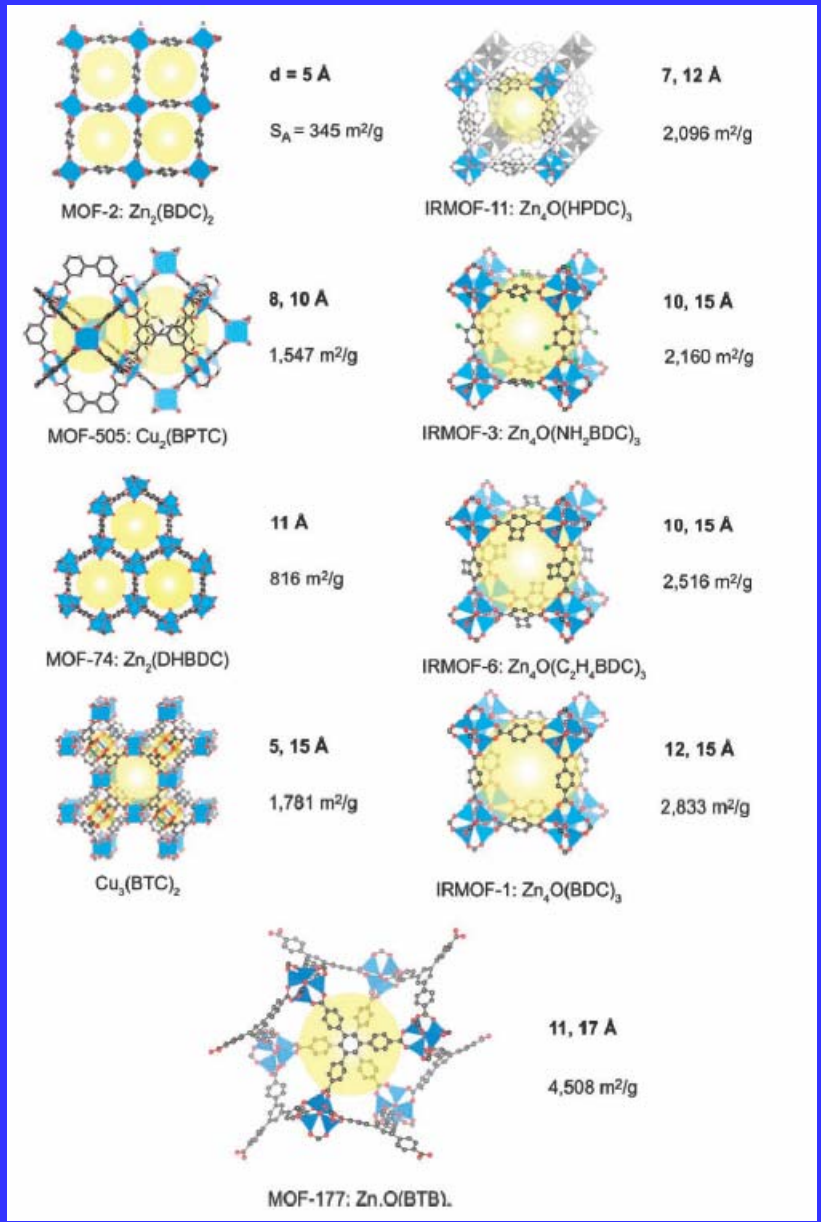
Snapshot of methane molecules (dark gray spheres) adsorbed in IRMOF-6 (gray framework) at 35 bar.



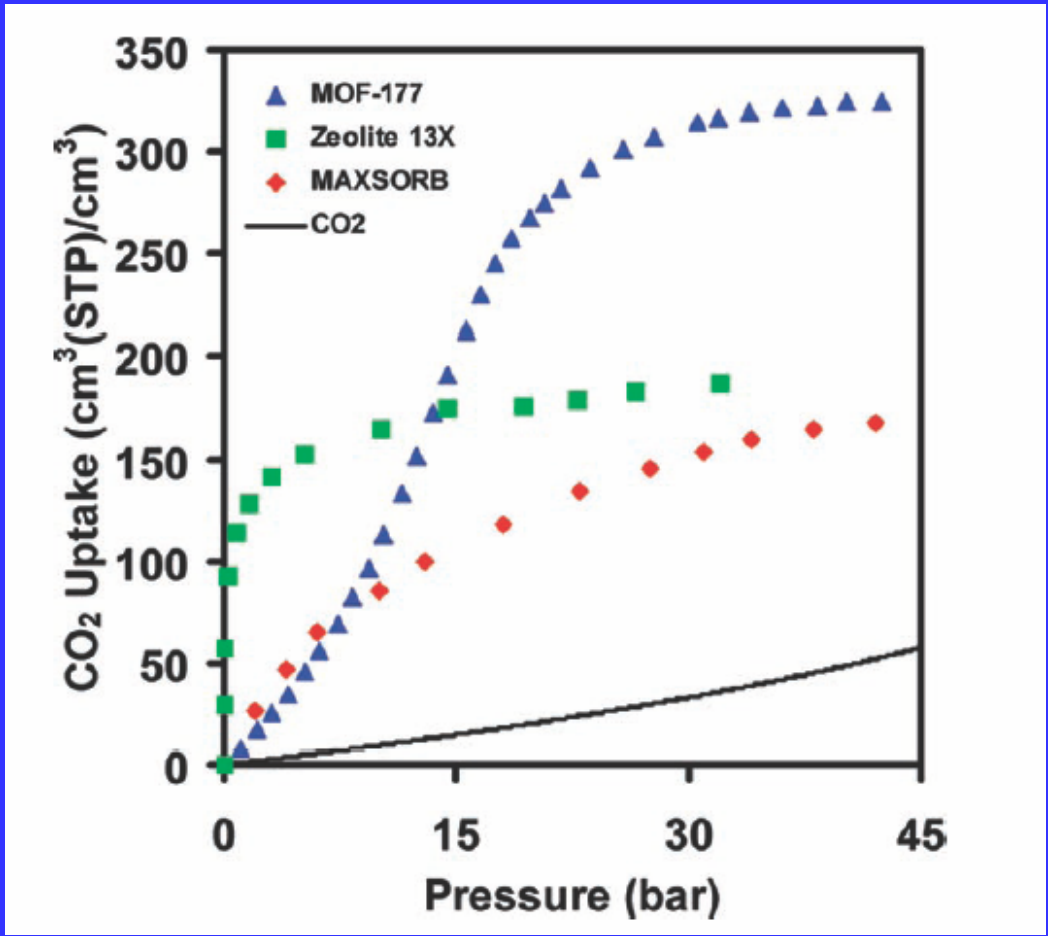
Molecularly designed IRMOF materials and the predicted adsorption isotherms



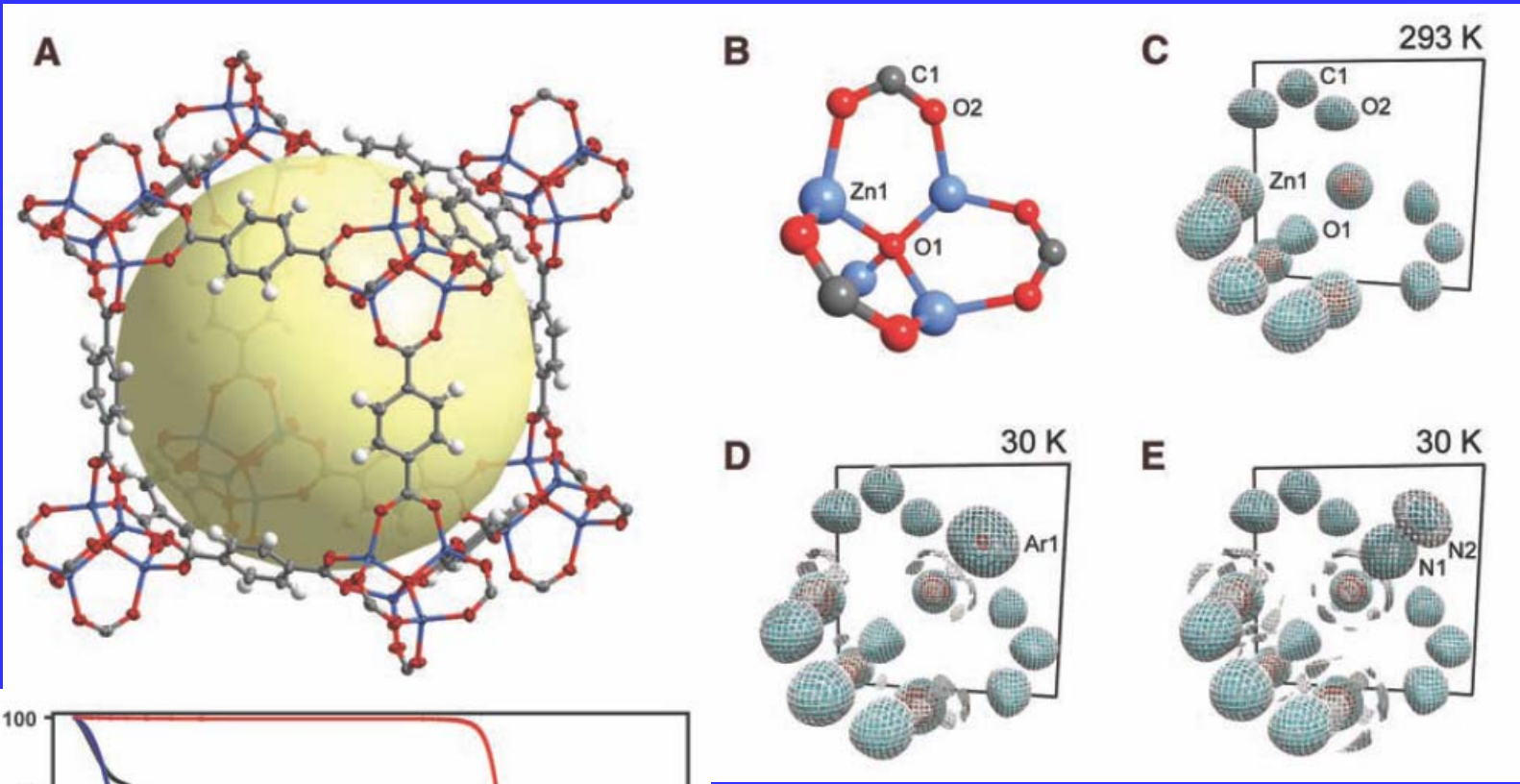
Crystal structures of MOFs examined for CO2 storage capacity at room temperature.

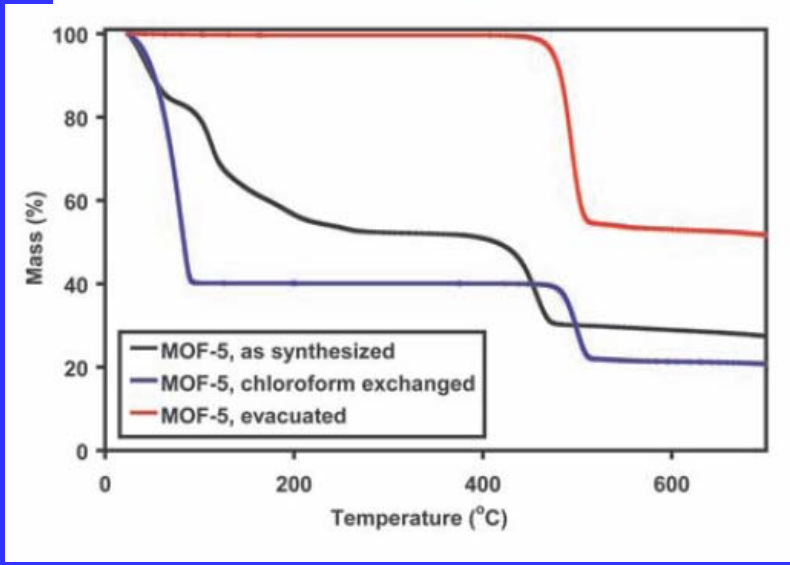


Comparison of the volumetric CO2 capacity of crystalline MOF-177 relative to zeolite 13X pellets, MAXSORB carbon powder, and pressurized CO2.



Gas adsorption sites in MOF-5





Argon gas adsorption sites in MOF-5