

Table 2. Correspondences of OSDAs and tiles in real zeolites.

OSDA	$V_{OSDA}, \text{\AA}^3$	Zeolite	Tile	$V_{tile}, \text{\AA}^3$	Number of OSDAs in the cage	$\frac{V_{OSDA}}{V_{tile}}$
methylamine	33.74	MTN	<i>t-mtn</i> 28/16:[5 ¹² .6 ⁴]	139.84	2	0.48
dimethylamine	48.48	ASV	<i>t-sty</i> 24/10:[4 ⁴ .6 ⁴ .12 ²]	77.03	1	0.63
dimethylammonium	48.48	BSV	<i>t-gie-1</i> 24/8:[4 ³ .6 ² .12 ³]	94.87	1	0.51
ethylenediamine	58.99	GIS	<i>t-gsm</i> 20/10:[4 ⁶ .8 ⁴]	73.91	1	0.80
ethylenediamine	58.99	GIS	<i>t-gsm</i> 20/10:[4 ⁶ .8 ⁴]	69.33	1	0.85
trimethylamine	63.6	SWY	<i>t-gme</i> 24/14:[4 ⁹ .6 ² .8 ³]	121.9	1	0.52
pyrrolidine	68.28	FER	<i>t-fer</i> 36/20:[5 ¹⁶ .6 ² .8 ²]	124.24	1	0.55
pyridine	70.51	FER	<i>t-fer</i> 36/20:[5 ¹⁶ .6 ² .8 ²]	138.39	1	0.51
1,3-propanediamine	73.29	THO	<i>t-krr</i> 20/6:[8 ⁶]	94.26	1	0.78
piperazine	78.29	BOF	<i>t-bof</i> 22/10:[4 ³ .52.6 ³ .10 ²]	116.38	1	0.67
tetramethylammonium	80.13	ATT	<i>t-gsm</i> 20/10:[4 ⁶ .8 ⁴]	112.66	1	0.71

tetramethylammonium	80.13	AWO	<i>t-awo</i> 26/14:[4 ⁷ .6 ⁴ .8 ³]	85.33	1	0.94
tetramethylammonium	80.13	MTN	<i>t-mtn</i> 28/16:[5 ¹² .6 ⁴]	134.18	1	0.60
1,3-dimethylimidazolium	87.54	ITW	<i>t-itw</i> 32/16:[4 ⁴ .5 ⁴ .64.8 ⁴]	160.51	1	0.54
1,3- dimethylimidazolium	87.75	CHA	<i>t-cha</i> 36/20:[4 ¹² .6 ² .8 ⁶]	302.48	2	0.59
N-methylpiperazine	93.43	JSW	<i>t-jsw</i> 38/20:[4 ⁶ .6 ¹² .8 ²]	183.33	1	0.51
1,2,3-trimethylimidazolium	102.03	ITW	<i>t-itw</i> 32/16:[4 ⁴ .5 ⁴ .64.8 ⁴]	174.31	1	0.59
1,3,4-trimethylimidazolium	102.08	ITW	<i>t-itw</i> 32/16:[4 ⁴ .5 ⁴ .64.8 ⁴]	167.66	1	0.61
quinuclidine	102.47	AST	<i>t-trd</i> 32/18:[4 ⁶ .6 ¹²]	194.07	1	0.53
P-chlorotoluene	103.58	MFI	<i>t-mfi-2</i> 22/6:[6 ² .10 ⁴]	142.07	1	0.73
diethylentriammonium	105.66	OWE	<i>t-owe</i> 24/10:[4 ⁴ .8 ⁶]	148.95	1	0.71
P-dichlorobenzene	106.28	MFI	<i>t-mfi-2</i> 22/6:[6 ² .10 ⁴]	142.19	1	0.75
P-dibromobenzene	112.43	MFI	<i>t-mfi-2</i> 22/6:[6 ² .10 ⁴]	142.3	1	0.79
1- ethyl-2,3-dimethylimidazolium	118.1	ITW	<i>t-itw</i> 32/16:[4 ⁴ .5 ⁴ .64.8 ⁴]	163.88	1	0.72

3-azabicyclo(3.2.2)nonan	120.35	SGT	<i>t-sgw</i> 36/20:[5 ¹² .6 ⁸]	246.45	1	0.49
2-Ethyl-1,3,4-trimethylimidazolium	147.19	STW	<i>t-stw</i> 34/18:[4 ⁶ .5 ⁸ .8 ² .10 ²]	231.4	1	0.64
N-cyclopentyl diazabicyclooctane	176.3	EEI	<i>t-eei-2</i> 66/34:[5 ¹² .6 ²⁰ .8 ²]	568.13	2	0.62
tetrapropylammonium	195.19	AFR	<i>t-afr</i> 40/20:[4 ¹⁰ .6 ⁶ .8 ² .12 ²]	411.34	1	0.47
1,6-hexanebis(trimethylammonium)	209.15	UOZ	<i>t-uoz</i> 52/30:[4 ¹⁰ .6 ²⁰]	360.93	1	0.58
1,4,7,10,13,16-hexaoxacyclooctadecane	217.44	MSO	<i>t-znl</i> 48/26:[4 ⁶ .6 ²⁰]	343.54	1	0.63
18-crown-6	217.44	RHO	<i>t-grc</i> 48/26:[4 ¹² .6 ⁸ .8 ⁶]	456.36	1	0.48
hexamethylene bisdiazabicyclooctane	292.57	SWY	<i>t-swy</i> 60:32/[4 ¹⁵ .6 ⁸ .8 ⁹]	551.63	1	0.53

Table 3 Suitable OSDAs for stuffing tiles of promising hypothetical zeolites.

Hypothetical zeolite	$V_{tile}, \text{\AA}^3$	OSDA	$V_{OSDA}, \text{\AA}^3$	Number of OSDAs	$\frac{V_{OSDA}}{V_{tile}} \cdot 100\%$
166_3_8908 194_5_3713581	544.22	hexamethylene bisdiazabicyclooctane	292.57	1	53.76
194_3_1140 PCOD8327034 PCOD8330642	548.95	hexamethylene bisdiazabicyclooctane	292.57	1	53.30
194_3_867 PCOD8327143 PCOD8327146 PCOD8330668	371.67	1,6-hexanebis(trimethylammonium)	209.15	1	56.27
194_4_80618 194_5_3722034 PCOD8321510	208.56	N-cyclopentylidiazabicyclooctane	176.3	1	84.53
194_5_3713587	488.34	N-cyclopentylidiazabicyclooctane	176.3	2	36.10
194_5_3722023	620.36	hexamethylene bisdiazabicyclooctane	292.57	2	47.16
194_5_3920375 PCOD8327036	296.86	2-Ethyl-1,3,4-trimethylimidazolium	147.19	1	49.58
194_5_3920376 PCOD8327038	647.37	hexamethylene bisdiazabicyclooctane	292.57	2	45.19
194_5_3920386	837.12	hexamethylene bisdiazabicyclooctane	292.57	2	34.95
227_3_593	136.83	tetramethylammonium	80.13	1	58.56
227_3_593	37.83	methylamine	33.74	1	89.19
PCOD8327068	700.22	hexamethylene bisdiazabicyclooctane	292.57	2	41.78
PCOD8327180	495.75	1,6-hexanebis(trimethylammonium)	209.15	2	42.19
194_5_1577965	906.94	hexamethylene bisdiazabicyclooctane	292.57	2	32.26
166_3_6806 194_5_3713591 194_5_3713592	425.44	N-cyclopentylidiazabicyclooctane	176.3	2	41.44

166_3_8899 194_5_3722022 194_5_3920380 194_5_3920382 PCOD8327040 PCOD8327041	230.71	2-ethyl-1,3,4-trimethylimidazolium	147.19	1	63.80
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