

Supporting Information

Machine learning boosted Design of Ionic Liquid-based Deep Eutectic Solvents for CO₂ Capture

Ruina Zhang,^[a] Guokai Cui,^{*[a]} Guoxiong Zhan,^[b] Mengyi Ma,^[a] Xiaochun Zhang,^[b] Xiangping Zhang,^{*[b,c]} and Hanfeng Lu^{*[a]}

^[a] Innovation Team of Air Pollution Control, Institute of Catalytic Reaction Engineering, Zhejiang Key Laboratory of Surface and Interface Science and Engineering for Catalysts, State Key Laboratory of Green Chemical Synthesis and Conversion, College of Chemical Engineering, Zhejiang University of Technology, Hangzhou 310014, China.

^[b] Center of Ionic Liquids and Green Energy, Beijing Key Laboratory of Solid State Battery and Energy Storage Process, State Key Laboratory of Mesoscience and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China

^[c] State Key Laboratory of Heavy Oil Processing, College of Chemical Engineering and Environment, China University of Petroleum (Beijing), Beijing 102249, China

* Correspondence: chemcgk@163.com (G Cui); xpzhang@ipe.ac.cn (X Zhang); luhf@zjut.edu.cn (H Lu).

ORCID: <https://orcid.org/0000-0002-7223-2869> (G Cui)

Table S1. Databank of abbreviations of ILs, full name of HBDs, molar ratios of HBD to IL, temperature (in K), partial pressure (in kPa), and CO₂ absorption capacity (in g/kg) for DESs.

Entry	Type	IL	HBD	HBD:IL ratio	molar	<i>T</i> (K)	<i>P</i> (kPa)	CO ₂ capacity (g/kg)	Ref.
1	ammonium	[ACh][Cl]	1,2,4-Triazole	1		303~333	56.3~593.2	0.6~9.6	1
2	ammonium	[ACh][Cl]	Guaiacol	3~5		293~323	48.6~558.6	0.5~8.6	2
3	ammonium	[ACh][Cl]	Imidazole	1.5~3		303~333	26.3~594	0.3~12.9	1
4	ammonium	[ACh][Cl]	Levulinic acid	3		303~333	65.7~576.4	1.1~13.2	3
5	ammonium	[BHDE][Cl]	Acetic acid	2		298	210~2026	2.8~37.1	4
6	ammonium	[BHDE][Cl]	Lactic acid	2		298	283~2086	0.7~21.9	4
7	ammonium	[BTEA][Cl]	2-Ethylaminoethanol	4		303~323	103.832~1829.42	40.3~123.1	5
8	ammonium	[BTEA][Cl]	2-Methylaminoethanol	4		303~323	377.537~1337.62	64.3~106.7	5
9	ammonium	[BTEA][Cl]	Acetic acid	2		298	325~2054	5.6~42.9	4
10	ammonium	[BTMA][Cl]	Acetic acid	2		298	219~2037	3.4~64.0	4
11	ammonium	[BTMA][Cl]	Glycerol	2		298	394~2026	1.6~11.4	4
12	ammonium	[Ch][Cl]	Diethanolamine	4		303	100	147.5	6
13	ammonium	[Ch][Cl]	Ethanolamine	2~6		303	100	137.1~252.5	6
14	ammonium	[Ch][Cl]	Methyldiethanolamine	4~5		303	100	38.4~42.9	6
15	ammonium	[Ch][Cl]	Triethanolamine	4~5		303	100	39.9~59.5	6
16	ammonium	[Ch][Cl]	1,2-Butanediol	4		303~333	371.3~3443.3	3.8~47.3	7

17	ammonium	[Ch][Cl]	1,2-Propanediol	3~4	293~323	104.4~525.6	0.9~8.3	8
18	ammonium	[Ch][Cl]	1,4-Butanediol	3~4	293~323	105.8~525.9	1.0~7.1	8
19	ammonium	[Ch][Cl]	2,3-Butanediol	3~4	293~323	107.1~528.8	1.1~8.4	8
20	ammonium	[Ch][Cl]	Diethanolamine	6	298~303	523.4~1000	13.3~40.8	9, 10
21	ammonium	[Ch][Cl]	Diethylene glycol	3~4	293~323	110.4~1119.7	0.9~14.6	10, 11
22	ammonium	[Ch][Cl]	Ethanolamine	2~7	298~328	182~4504	22.1~248.6	4, 9, 12
23	ammonium	[Ch][Cl]	Ethylene glycol	2~8	298~343	36~6323	0.4~137.6	9, 10
24	ammonium	[Ch][Cl]	Ethylenecyanohydrin	2~3	298~328	114.2~1414.8	1.9~62.2	13
25	ammonium	[Ch][Cl]	Furfuryl alcohol	3~5	303~333	65.2~586.4	0.7~10.0	14
26	ammonium	[Ch][Cl]	Glycerol	2~8	298~343	187~6347	2.4~162.5	9, 15
27	ammonium	[Ch][Cl]	Guaiacol	3~5	293~323	46.9~545.9	0.5~8.3	2
28	ammonium	[Ch][Cl]	Levulinic acid	3~5	303~333	60~587.4	0.9~12.6	14
29	ammonium	[Ch][Cl]	Methyldiethanolamine	6~7	303	445.6~1096	42.9~89.6	10
30	ammonium	[Ch][Cl]	Phenol	2~4	293~333	99~13300	1.0~176.4	11, 16
31	ammonium	[Ch][Cl]	Succinimide	1.7~6	313~333	293.834~1149.06	0.7~1.0	17
32	ammonium	[Ch][Cl]	Triethanolamine	4	298	1000	13.0	9
33	ammonium	[Ch][Cl]	Triethylene glycol	3~4	293~323	109.3~520.3	1.0~8.5	11
34	ammonium	[Ch][Cl]	Urea	1.5~4	298~343	40.5~12730	0.5~227.4	18

35	ammonium	[Ch][Pro]	Ethylene glycol	3~5	298	100	59.1~71.8	19
36	ammonium	[DEA][Cl]	Guaiacol	3~5	293~323	45.1~550.7	0.7~10.2	2
37	ammonium	[MOE-DEMA][1,2,3- Triz]	Ethylene glycol	2~4	298	100	75.1~100.1	20
38	ammonium	[MOE-DEMA][1,2,3- Triz]	Pinacol	2~4	298	100	19.2~28.3	20
39	ammonium	[TBA][1,2,3-Triz]	Ethylene glycol	2~4	298	100	63.0~81.0	21
40	ammonium	[TBA][Br]	2-Ethylaminoethanol	4	303~323	210.655~1425.19	32.6~88.2	5
41	ammonium	[TBA][Br]	2-Methylaminoethanol	4	303~323	101.488~1177.27	38.9~106.0	5
42	ammonium	[TBA][Br]	Acetic acid	2	298	388~2011	6.0~49.7	4
43	ammonium	[TBA][Br]	Decanoic acid	2	303~323	419~1138	7.8~29.9	22
44	ammonium	[TBA][Br]	Diethanolamine	6	298~303	610.5~1011.2	15.7~38.0	9, 10
45	ammonium	[TBA][Br]	Diethylene glycol	2~4	303	590~1392.5	8.6~29.0	10
46	ammonium	[TBA][Br]	Ethanolamine	5~7	298~303	100~2040	23.5~163.3	4, 6, 9
47	ammonium	[TBA][Br]	Ethylene glycol	2~4	303	412~1374.2	4.5~20.1	10
48	ammonium	[TBA][Br]	Hexanoic acid	2~4	303~323	444~1335	8.9~42.0	22
49	ammonium	[TBA][Br]	Levulinic acid	3	303~333	70.2~586.4	1.0~11.9	3
50	ammonium	[TBA][Br]	Methyldiethanolamine	2~4	303	423.2~1021	11.5~80.0	10
51	ammonium	[TBA][Br]	Triethanolamine	3~5	298~303	100~1000	20.7~26.2	6, 9
52	ammonium	[TBA][Cl]	Acetic acid	2	298	348~2002	8.1~62.1	4

53	ammonium	[TBA][Cl]	Decanoic acid	2	298~323	90~1990	1.8~66.7	23
54	ammonium	[TBA][Cl]	Ethanolamine	5	303	100	176.7	6
55	ammonium	[TBA][Cl]	Lactic acid	2	308~318	93~1992	1.6~42.0	24
56	ammonium	[TBA][Cl]	Levulinic acid	3	303~333	63.2~591.6	1.1~13.3	3
57	ammonium	[TEA][1,2,4-Triz]	Ethylene glycol	2	298	100	125.0	25
58	ammonium	[TEA][4-PyO]	Dimethyl sulfoxide	4	313~328	5~100	39.5~90.6	26
59	ammonium	[TEA][4-PyO]	Ethylene glycol	4	313~328	5~100	23.9~77.3	26
60	ammonium	[TEA][4-PyO]	Succinonitrile	4	313~328	5~100	25.0~71.8	26
61	ammonium	[TEA][Br]	Ethanolamine	5	303	100	192.5	6
62	ammonium	[TEA][Br]	Levulinic acid	3	303~333	68.7~587.8	0.9~10.6	3
63	ammonium	[TEA][Br]	Triethanolamine	5	303	100	34.9	6
64	ammonium	[TEA][CH(CN)2]	1-Ethylimidazole	1	303	0.001~1.3	7.5~137.3	27
65	ammonium	[TEA][CH(CN)2]	Dimethylaminoethoxyethanol	1	303	0.003~1.326	7.9~126.3	27
66	ammonium	[TEA][CH(CN)2]	Ethylene glycol	1	303	0.01~1.32	13.2~117.5	27
67	ammonium	[TEA][CH(CN)2]	Imidazole	1	303	0.021~1.3	7.0~101.2	27
68	ammonium	[TEA][CH(CN)2]	Tetramethylene sulfone	1	303	0.01~1.33	8.8~113.1	27
69	ammonium	[TEA][Car]	4-Methylimidazole	2	298~333	100	79.3~87.3	28
70	ammonium	[TEA][Car]	Ethylene glycol	2	298~333	100	87.2~94.8	28
71	ammonium	[TEA][Cl]	Acetic acid	2~3	298	281~2018	5.5~54.1	4
72	ammonium	[TEA][Cl]	Ethanolamine	2~6	303	100	173.6~218.4	6

73	ammonium	[TEA][Cl]	Hexanoic acid	2~4	303~323	388~1263	8.6~36.9	22
74	ammonium	[TEA][Cl]	Lactic acid	2	308~318	94~1993	1.2~29.9	24
75	ammonium	[TEA][Cl]	Levulinic acid	3	303~333	66.1~585.4	1.0~12.1	3
76	ammonium	[TEA][Cl]	Octanoic acid	3	298	353~2018	6.9~61.2	4
77	ammonium	[TEA][Cl]	Phenol	3	313	2120~11170	41.0~139.7	16
78	ammonium	[TEA][Im]	Ethylene glycol	2	298	100	129.0	25
79	ammonium	[TEA][Pyrz]	Ethylene glycol	1	293	0.042~5	120.0~160.0	29
80	ammonium	[TEA][Thy]	4-Methylimidazole	2	298	100	89.3	28
81	ammonium	[TEA][Thy]	Ethylene glycol	2	298	100	98.1	28
82	ammonium	[TEMA][Cl]	Acetic acid	2	298	198~1837	3.6~51.7	4
83	ammonium	[TEMA][Cl]	Ethylene glycol	2	298	138~1345	2.7~27.5	4
84	ammonium	[TEMA][Cl]	Glycerol	2	298	150~1648	0.7~19.1	4
85	ammonium	[TEMA][Cl]	Lactic acid	2	298	143~1863	2.1~23.4	4
86	ammonium	[TEMA][Cl]	Levulinic acid	2	298	136~1617	2.5~27.0	4
87	ammonium	[TEPA][Cl]	thymol	3~7	313~333	10.1~101.3	40.6~86.8	30
88	ammonium	[TETA][Cl]	Diethylene glycol	1~7	313	100	65.9~158.7	31
89	ammonium	[TETA][Cl]	Ethylene glycol	1~7	303~323	12~100	104.6~181.4	31
90	ammonium	[TETA][Cl]	N-Methyl pyrrolidone	7	313	100	41.0	31
91	ammonium	[TETA][Cl]	thymol	3~7	313~333	10.1~101.3	42.7~90.3	30
92	ammonium	[TMA][Cl]	Ethanolamine	2~6	303	100	78.5~245.6	6

93	ammonium	[TMA][Cl]	Acetic acid	4	298	294~2096	33.0~65.6	4
94	ammonium	[TMA][Cl]	Lactic acid	2	308~318	95~1993	1.1~28.5	24
95	ammonium	[TMA][Cl]	Phenol	3	313	2360~12170	36.2~136.4	16
96	ammonium	[TOA][Br]	Decanoic acid	2	298~323	90~1990	1.7~58.6	23
97	ammonium	[TOA][Cl]	Decanoic acid	1.5~2	298~323	90~1990	1.8~61.9	23
98	ammonium	[TOMA][Br]	Decanoic acid	2	298~323	90~1990	1.8~57.5	23
99	ammonium	[TOMA][Cl]	Decanoic acid	2	298~308	90~1990	2.0~59.5	23
100	ammonium	[TPA][Br]	Formic acid	1~2	298~318	168.308~3520.14	2.8~103.0	32
101	ammonium	[TPA][Cl]	Acetic acid	6	298	350~2030	11.0~75.7	4
102	ammonium	[TPA][Cl]	Ethanolamine	4~7	298	357~2019	14.9~155.1	4
103	Guanidinium	[Gua][Cl]	Ethanolamine	2	298	226~2025	13.5~73.2	4
104	imidazolium	[Bmim][Cl]	Ethanolamine	1~4	298	100	84.0~214.0	33
105	imidazolium	[Emim][1,2,4-Triz]	Ethylene glycol	2~4	298	100	97.8~134.9	34
106	imidazolium	[Emim][2-CNpyr]	Ethylene glycol	1~2	298	0.041~100	41.8~155.0	35
107	imidazolium	[Emmim][1,2,4-Triz]	Ethylene glycol	2~4	298	100	95.7~133.1	34
108	imidazolium	[lPim][1,2,4-Triz]	Ethylene glycol	3~5	298	100	81.9~103.7	36
109	phosphonium	[ATPP][Br]	Diethylene glycol	4~16	303	156~1954	8.7~320.7	37
110	phosphonium	[ATPP][Br]	Phenol	4~6	313~333	159.9~1387.3	6.0~78.7	38
111	phosphonium	[ATPP][Br]	Triethylene glycol	4~16	303	142~1957	6.3~282.7	37
112	phosphonium	[BTPP][Cl]	Glycerol	12	298	1000	20.6	9

113	phosphonium	[n-BTPP][Br]	Ethylene glycol	12	298	1000	26.3	9
114	phosphonium	[MTPP][Br]	1,2-Propanediol	4	298	220~2026	1.0~24.2	4
115	phosphonium	[MTPP][Br]	Acetic acid	4	298	173~2014	3.2~133.0	4
116	phosphonium	[MTPP][Br]	Ethanolamine	6~8	298	1000	63.2~71.6	9
117	phosphonium	[MTPP][Br]	Ethylene glycol	3	298	192~2018	2.0~15.5	4
118	phosphonium	[MTPP][Br]	Glycerol	4	298	161~2026	0.4~12.7	4
119	phosphonium	[MTPP][Br]	Levulinic acid	3	298	301~2068	1.1~30.3	4
120	phosphonium	[MTPP][Br]	Methyldiethanolamine	7	313	101.325	18.0	39
121	phosphonium	[P4,4,4,2COOH][Br]	Diethylene glycol	2	303~333	325.7~2462.8	14.5~266.0	40
122	phosphonium	[P4,4,4,2COOH][Br]	Ethylene glycol	2	303~333	202.4~2191	9.6~191.5	40
123	phosphonium	[P4,4,4,2NH2][Br]	Diethylene glycol	4	303~333	223.6~2256.4	8.5~157.8	40
124	phosphonium	[P4,4,4,2NH2][Br]	Ethylene glycol	4	303~333	249~2302.4	9.2~153.6	40
125	phosphonium	[P4,4,4,2OH][Br]	Diethylene glycol	2	303~333	202.3~2472.7	9.0~584.7	40
126	phosphonium	[P4,4,4,2OH][Br]	Ethylene glycol	2	303~333	146.7~2293.5	6.7~176.0	40
127	phosphonium	[P4,4,4,2][Br]	Diethylene glycol	2	303~333	176.8~2551	6.8~187.0	40
128	phosphonium	[P4,4,4,2][Br]	Ethylene glycol	2	303~333	147.5~2477.4	4.6~152.6	40
129	phosphonium	[TBP][Br]	Diethylene glycol	4	313~333	94.4~1398.1	3.8~77.6	38
130	phosphonium	[TBP][Br]	Phenol	4	313~333	163.8~1578.5	5.8~79.2	38
131	phosphonium	[TEP][1,2,4-Triz]	Ethylene glycol	2	298	100	118.0	25
132	phosphonium	[TEP][Im]	Ethylene glycol	2	298	100	118.0	25

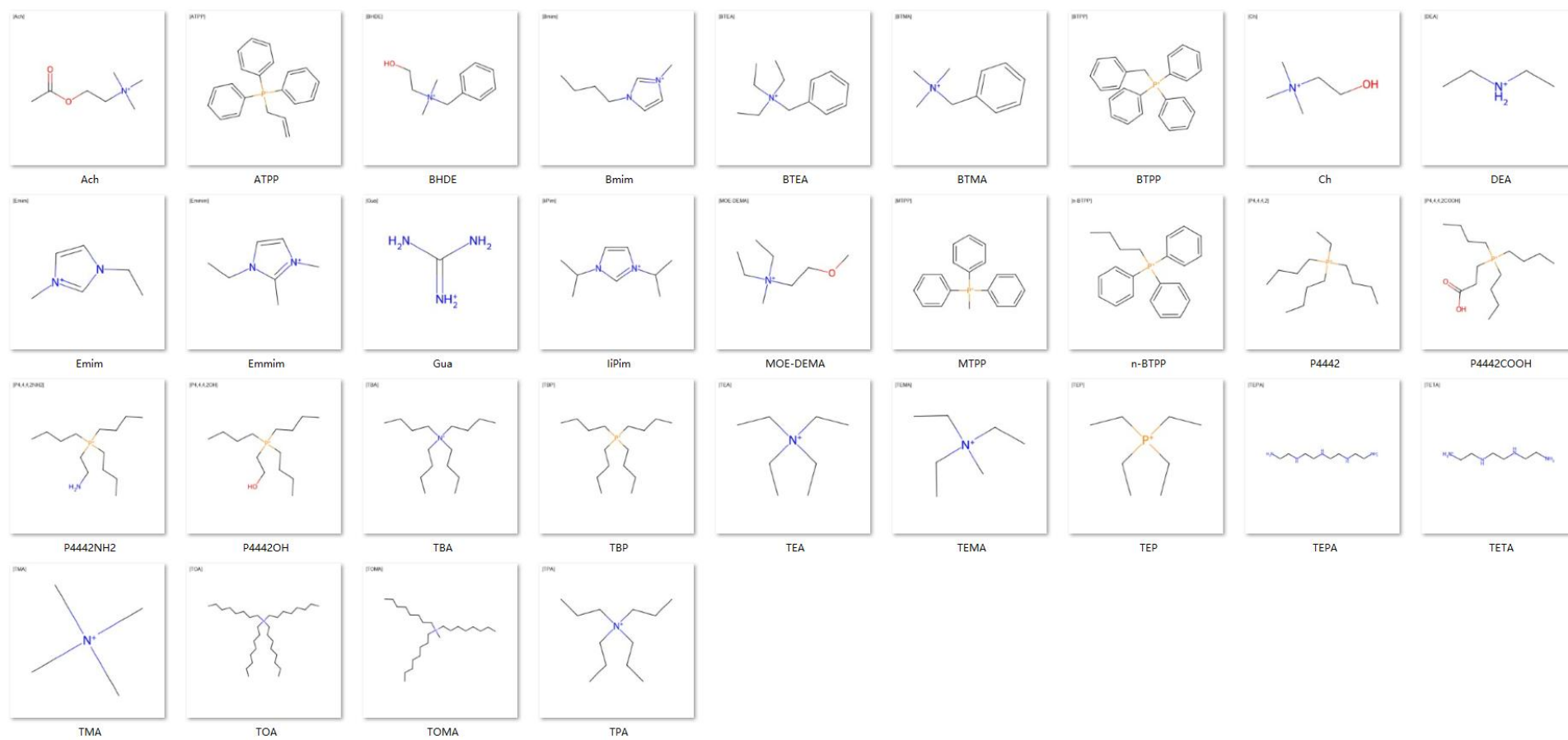


Figure S1. Typical structures of cations.

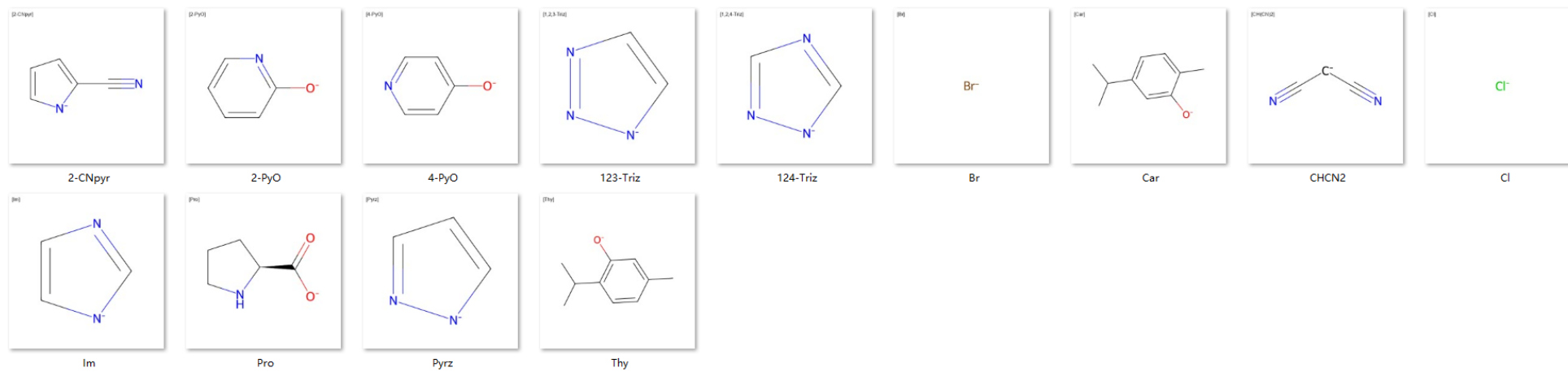


Figure S2. Typical structures of anions.

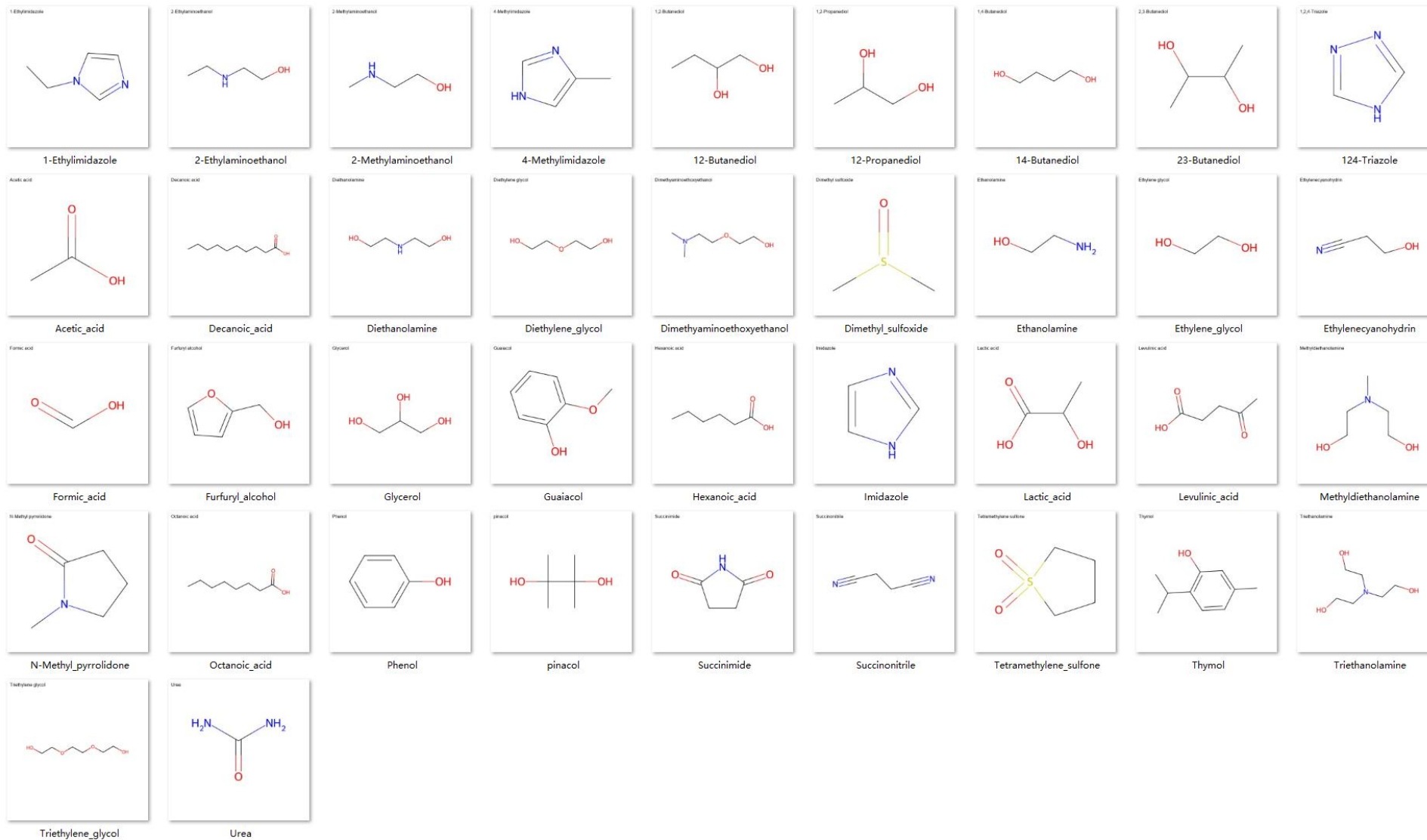


Figure S3. Typical structures of HBDs.

Models

RBF kernel

Support Vector Machine (SVM) is a supervised ML algorithm primarily used for classification, which finds an optimal hyperplane to maximize the margin between different classes and can handle non-linear data through kernel functions. Support Vector Regression (SVR) is a kind of SVM used in regression.

RBF kernel (hyperparameters: C, γ) is often the default and most popular choice for SVR, as described by the following equation:

$$K(x, x_i) = \exp(-\gamma \cdot \|x - x_i\|^2)$$

The regularization parameter C is a universal hyperparameter, which controls the overall tolerance for errors, and γ defines the local influence of data points, which monitors the amplitude of the kernel function.⁴¹ These parameters profoundly impact the model performance. Besides, the coefficients W and b can be obtained through minimizing the following equation:

$$\min_{W, b, \xi, \xi^*} \frac{1}{2} \|W\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

ξ_i and ξ_i^* are slack variables for each point, representing positive error and negative error, respectively. That is, slack variables allow regression errors to exist up to the value of ξ_i and ξ_i^* . The relationship among them is:

$$\begin{cases} y_i - \langle W, x_i \rangle - b \leq \varepsilon + \xi_i \\ \langle W, x_i \rangle + b - y_i \leq \varepsilon + \xi_i^* \\ \xi_i \geq 0, \xi_i^* \geq 0, i = 1, \dots, N \end{cases}$$

Least Squares Support Vector Machine (LSSVM) Model

Least Squares Support Vector Machine (LSSVM) for regression (LSSVR) is building directly upon SVR by replacing the inequality constraints and the ε -insensitive loss with equality constraints and a least squares cost function. Its optimization problem is:

$$\min_{W,b,e} \frac{1}{2} \|W\|^2 + \frac{\gamma}{2} \sum_{i=1}^N e_i^2$$
$$y_i = \langle W, x_i \rangle + b + e_i$$

where e_i represents the direct error for each sample, and the regularization parameter γ plays a role analogous to C in SVR, controlling the trade-off between model smoothness and fitting error. Thus, a faster and more straightforward training is obtained, making LSSVR efficient for regression tasks like predicting CO₂ absorption capacity of DESs.

Graph Neural Networks (GNNs) Model

Graph Neural Networks (GNNs) offer a paradigm shift by directly operating on molecular graphs, where atoms are represented as nodes and chemical bonds as edges. In graph theory, a graph G is defined as:

$$G = (V, E)$$

where V is a set of nodes and E is a set of edges. Each node can have a feature vector (e.g. atom type, charge, hybridization), and each edge can have features (e.g. bond type, length). Nodes and edges are computed by RDKit. The core operation of GNNs is message passing, which allows each node to iteratively gather and combine information from its neighboring nodes to refine its own feature representation.

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