Supporting Information

Title Hybrid Computational Approaches for Accurate Crystalline Density Prediction of *Cyclo*-Pentazolate Salts

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Table S1. Experimental data on crystalline densities (ρ_{expt}, g/cm^3) of pentazolate salts and the corresponding references

No	Formula	ρ_{expt}	Ref	*R* index	Measurement temperature (K)	CCDC identifier
1	$C_8H_{10}N_6$	1.430	S1	0.0360	128	1117381
2	$C_6H_5N_5$	1.417	S30	0.0313	173	183414
3	$H_{30}N_{15}O_{15}Fe$	1.428	S4	0.0420	193	2207237
4	$H_{30}N_{15}O_{15}Al$	1.384	S4	0.0599	150	2207238
5	$H_{22}N_{21}O_2Co$	1.664	S6	0.0239	193	2218042
6	$H_{15}N_{16}O_2Co$	1.733	S6	0.0842	194	2245589
7	$H_6N_5O_3Na$	1.471	S9	0.0381	170	1527747
8	$H_{10}N_{10}O_5Mn$	1.608	S9	0.0370	205	1527748
9	$H_{10}N_{10}O_5Fe$	1.599	S9	0.0349	205	1527749
10	$H_{10}N_{10}O_5Co$	1.696	S9	0.0408	170	1527750
11	$H_{20}N_{10}O_{10}Mg$	1.437	S9	0.0377	205	1527751
12	$C_2H_6N_6O_3$	1.666	S12	0.0377	205	1884821
13	$C_7H_9N_7O_3$	1.547	S12	0.0660	150	1885291
14	$C_2H_{12}N_{12}O$	1.462	S12	0.0609	100	1901039
15	N_8Cu	2.623	S15	0.0488	173	1816844
16	N_5Ag	3.015	S15	0.1063	173	1816845
17	$H_6N_6O_6Ba$	2.592	S15	0.0197	100	1816846
18	$H_6N_{31}O_6Ba_3Na$	2.338	S15	0.0320	100	1816847
19	$C_5H_{10}N_{20}$	1.660	S18	0.0402	173	1589904
20	$C_2H_7N_9O$	1.596	S18	0.0436	173	1589905
21	$C_2H_7N_9O_2$	1.681	S18	0.0858	173	1589906
22	$H_8N_6O_3$	1.491	S19	0.0452	173	1881964
23	$C_2H_6N_{10}$	1.618	S19	0.0488	150	1883082
24	CH_8N_{10}	1.465	S19	0.0388	173	1883605
25	$C_3H_7N_{13}$	1.645	S19	0.0572	173	1884809
26	$C_2H_8N_{10}$	1.524	S19	0.0432	150	1885298
27	CH_7N_9	1.476	S19	0.0674	150	1885299
28	N_5K	2.002	S19	0.0246	150	1885286
29	$H_{16}N_{10}O_8Zn$	1.669	S23	0.0302	205	1544795
30	$H_{38}N_{25}OCl_3Co_2$	1.634	S13	0.0421	296	2192804
31	$C_2H_4N_{14}Na_2$	1.728	S26	0.0485	173	1575478
32	CH_6N_8	1.515	S2	0.0281	153.15	1838393
33	$C_4H_{12}N_6$	1.245	S2	0.0490	153.15	1838395
34	H_5N_7	1.620	S2	0.0283	153.15	1880431
35	H_4N_6O	1.636	S2	0.0304	153.15	1880432
36	H_4N_6	1.520	S2	0.0407	153.15	1880433
37	$C_4H_{15}N_{15}O_3$	1.520	S3	0.0587	173	1874758
38	$C_{10}H_{26}N_{25}O_4Cl$	1.617	S3	0.0570	173	1589207
39	$H_{16}N_{10}O_8Co$	1.694	S5	0.0226	172.99	1553603
40	$H_{25}N_{34}O_3Cl$	1.340	S7	0.0580	123.01	1790635
41	$H_6N_5O_3Li$	1.369	S8	0.0517	100	2083862
42	N_5Li	1.279	S8	0.0401	140.15	2097922
43	$C_3H_8N_8O_2$	1.525	S10	0.0617	296	2015719
44	$C_2H_7N_7O$	1.393	S10	0.0394	296	2015718
45	$H_{10}N_{16}O_{10}Pb_4$	3.913	S11	0.0452	296	2104205

No	Formula	ρ_{expt}	Ref	*R* index	Measurement temperature (K)	CCDC identifier
46	HN_5OPb	4.537	S11	0.0302	293	2104203
47	$H_{22}N_{21}O_2Co$	1.647	S13	0.0336	296	2192795
48	$C_7H_{10}N_{18}O_2$	1.722	S14	0.0560	173	2015527
49	$C_4H_7N_{13}O$	1.673	S14	0.0387	170	2015456
50	$C_3H_7N_{11}O$	1.635	S14	0.0474	100	2015523
51	$C_4H_{16}N_{18}$	1.480	S16	0.0751	293.15	1977128
52	$C_6H_{22}N_{24}$	1.483	S16	0.0940	293	1977133
53	$C_3H_6N_{12}$	1.706	S17	0.0249	210	1973516
54	$C_6H_{13}N_{21}$	1.664	S17	0.0457	193	1973517
55	$C_3H_8N_{10}O$	1.486	S17	0.0611	173.15	1978993
56	$C_4H_9N_{15}$	1.630	S17	0.0403	193	1987674
57	$C_3H_7N_{13}$	1.649	S17	0.0568	193	1973518
58	$C_4H_{14}N_{16}O_2$	1.608	S20	0.0498	296	2194173
59	$C_4H_7N_5O_4Na_2$	1.709	S21	0.0415	100	2208014
60	$CH_8N_{10}O_3Na_2$	1.614	S22	0.0551	100	1894600
61	$H_{18}N_{19}Co$	1.716	S13	0.0776	170	2192794
62	$H_6N_{15}O_9ClPb_4$	4.417	S11	0.0275	296	2104206
63	$C_4H_{16}N_{25}O_5S_2Na_5$	1.654	S31	0.0407	296	2008732
64	$H_{10}N_{12}O_2$	1.510	S24	0.0309	150	1977776
65	CH_6N_{12}	1.638	S25	0.0303	173	2159866
66	$C_5H_{13}N_{17}O_2$	1.639	S27	0.0344	273.15	2027160
67	$H_{28}N_{37}Cl$	1.341	S28	0.0381	150.02	1887874
68	$H_3N_{11}Ag_2$	3.200	S29	0.0310	123.15	1880691
69	$H_{16}N_{10}O_8Co$	1.694	S5	0.0226	172.99	1553603

Table S2. Experimental data on the asymmetric cell parameters of salts **1-69**

No	Space group	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
1	$P2_1/m$	4.077	10.925	10.042		98.370	
2	$P2_1/c$	6.576	13.819	7.599		92.120	
3	$P2_1/n$	16.8316	14.7115	20.1791		93.400	
4	$P2_1/n$	16.7321	14.5671	20.0005		92.771	
5	$C2/c$	9.3725	12.5676	14.0566		100.960	
6	$P2_1/n$	13.1316	7.2567	13.2826		90.481	
7	*Cmcm*	6.905	13.874	6.930			
8	*Fmmm*	12.342	17.368	6.537			
9	*Fmmm*	12.330	17.444	6.570			
10	*Fmmm*	12.144	17.114	6.465			
11	$P\bar{1}$	7.1765	7.1963	9.2589	90.768	107.122	117.675
12	$P2_1/c$	8.0506	8.6457	9.4293		100.072	
13	$P\bar{1}$	7.350	7.518	10.912	83.875	77.392	60.740
14	$P2/n$	8.320	6.152	9.817		95.190	
15	$Ima2$	8.944	7.3884	6.731			
16	*Fddd*	11.904	15.240	17.282			
17	*Pnma*	9.134	7.520	12.069			
18	$P6_3/m$	15.168		7.532			
19	$C2/c$	9.728	10.219	14.345		100.519	

No	Space group	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
20	$P2_1/c$	7.537	13.286	7.215		94.130	
21	$P2_1/c$	12.138	10.025	14.091		119.324	
22	$P2_1/c$	3.685	14.638	11.575		90.320	
23	$P\overline{1}$	5.298	7.156	10.106	100.047	104.076	104.089
24	$P\overline{1}$	6.2136	7.7039	8.5102	71.562	87.896	70.411
25	$P2_1/c$	8.083	7.141	16.094		101.864	
26	$P2_1/c$	3.6171	20.792	10.069		97.773	
27	$P2_1/n$	8.429	6.861	11.434		98.964	
28	$Pnma$	7.835	6.304	7.332			
29	$Fmmm$	12.293	17.319	6.536			
30	$C2/m$	26.963	7.0239	13.9913		105.353	
31	$P3_221$	9.687		9.585			
32	$\overline{I}42d$	12.679		7.0988			
33	$P2_1/m$	5.786	8.571	7.867		99.590	
34	$P2_1/c$	6.4517	12.2378	5.4024		97.747	
35	$P2_1/c$	3.7489	14.7612	7.6841		96.265	
36	$Pcca$	9.4905	3.9137	10.3616			
37	$P\overline{1}$	6.7814	6.8399	16.536	93.162	98.922	111.079
38	$P\overline{1}$	6.6686	13.957	14.225	110.976	95.123	99.042
39	$Fmmm$	12.1536	17.1485	6.4578			
40	$Fd\overline{3}m$	17.9681					
41	$P2_1/n$	8.6927	7.1231	10.337		96.477	
42	$Pm\overline{3}n$	16.8669					
43	$C2/c$	18.195	7.8672	10.760		119.993	
44	$P\overline{1}$	7.0953	7.274	7.4921	83.202	87.971	64.315
45	$R3$	8.9224		22.5833			
46	$P2_1$	7.6556	13.6507	8.5962		106.440	
47	$C2/c$	9.413	12.5823	14.1132		100.629	
48	$C2/m$	11.846	16.9336	7.5427		105.880	
49	$P2_1/c$	10.6099	9.0936	10.4443		94.097	
50	$P2_1/c$	4.9507	11.8376	14.9389		98.347	
51	$P2/c$	10.9417	11.1628	12.1956		107.610	
52	$Pbcn$	28.094	11.2556	12.1937			
53	$Fdd2$	20.9224	23.0614	6.7835			
54	$P2_1/n$	7.4376	11.9787	17.1287		97.116	
55	$P2_1/c$	6.335	12.001	12.101		103.377	
56	$P2_1/n$	8.3224	10.6171	12.9121		107.377	
57	$P2_1/c$	8.0832	7.1465	16.0269		101.553	
58	$P\overline{1}$	6.6303	7.8338	7.9449	117.137	93.126	111.674
59	$P\overline{1}$	6.845	7.2316	10.2686	71.886	71.147	82.079
60	$P3_221$	9.6556		18.7426			
61	$C2/m$	23.944	8.1821	13.7433		99.330	
62	$Pca2_1$	10.1088	13.552	13.4401			
63	$C222_1$	9.3283	30.151	9.6156			
64	$P2_1/c$	3.83966	13.19458	9.19097		96.7349	
65	$Iba2$	10.410	20.174	7.189			
66	$P\overline{1}$	6.76735	9.480	11.9242	67.465	81.548	81.726

No	Space group	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
67	$Fd\overline{3}m$	17.9311					
68	$P2_1/c$	9.1248	9.1238	9.8307		108.963	
69	*Fmmm*	12.1536	17.1485	6.4578			

Table S3. The calculated quantitative characteristics of the crystals packing of *cyclo*-pentazolate salts with organic cations

Salt	KPI	AHBL (Å)	VS (%)	AD (atoms/Å^3)
12	0.731	2.88195	85.71	0.1052
13	0.722	3.08518	90.82	0.1013
14	0.696	3.03393	96.36	0.1079
19	0.704	3.08694	99.20	0.0999
20	0.710	3.01812	95.21	0.1055
21	0.740	2.93238	91.43	0.1070
22	0.687	2.83518	85.13	0.1089
23	0.721	3.03346	99.22	0.1031
24	0.672	3.02750	99.30	0.1047
25	0.699	2.94121	99.21	0.1012
26	0.702	3.09697	99.27	0.1066
27	0.681	3.08241	99.30	0.1041
32	0.702	3.05893	99.28	0.1052
33	0.700	3.50420	99.41	0.1144
34	0.749	3.07758	99.23	0.1136
35	0.712	2.95357	92.27	0.1041
36	0.698	2.97430	99.28	0.1039
43	0.702	2.97921	90.55	0.1109
44	0.651	3.09738	95.13	0.0983
48	0.726	2.96669	95.21	0.1017
49	0.713	2.98030	96.30	0.0995
50	0.714	2.95388	95.85	0.1016
51	0.689	3.01278	99.29	0.1071
52	0.697	2.96377	99.29	0.1079
53	0.731	3.09053	99.17	0.1027
54	0.713	3.01516	99.20	0.1057
55	0.677	2.99356	95.99	0.0983
56	0.712	2.98287	99.21	0.1029
57	0.699	2.94314	99.20	0.1014
58	0.733	2.99188	94.81	0.1095
64	0.691	2.91228	93.58	0.1038
65	0.706	3.01800	99.21	0.1007
66	0.716	3.01144	94.96	0.1064

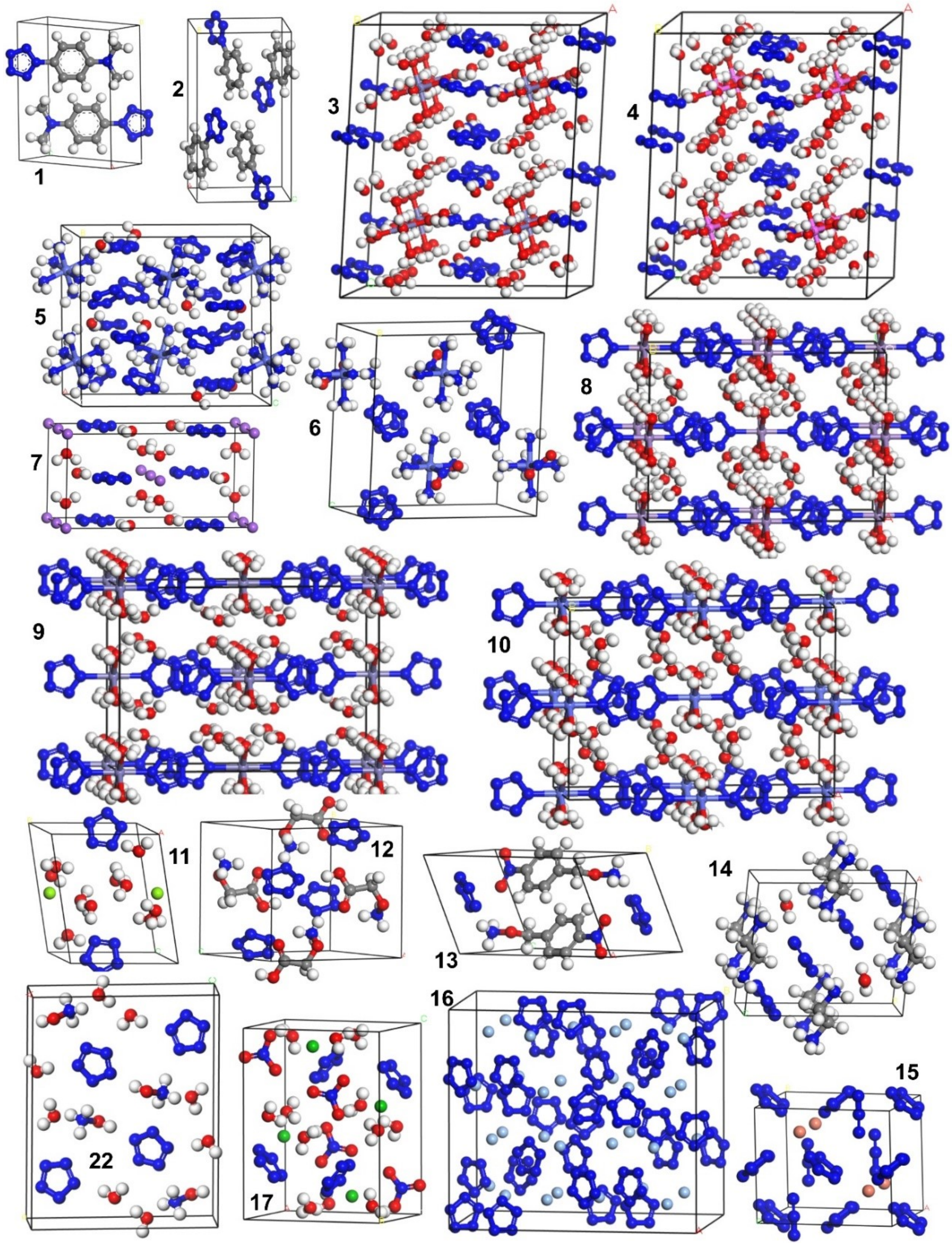


Figure S1. Crystal structures of the pentazolate salts studied in this work

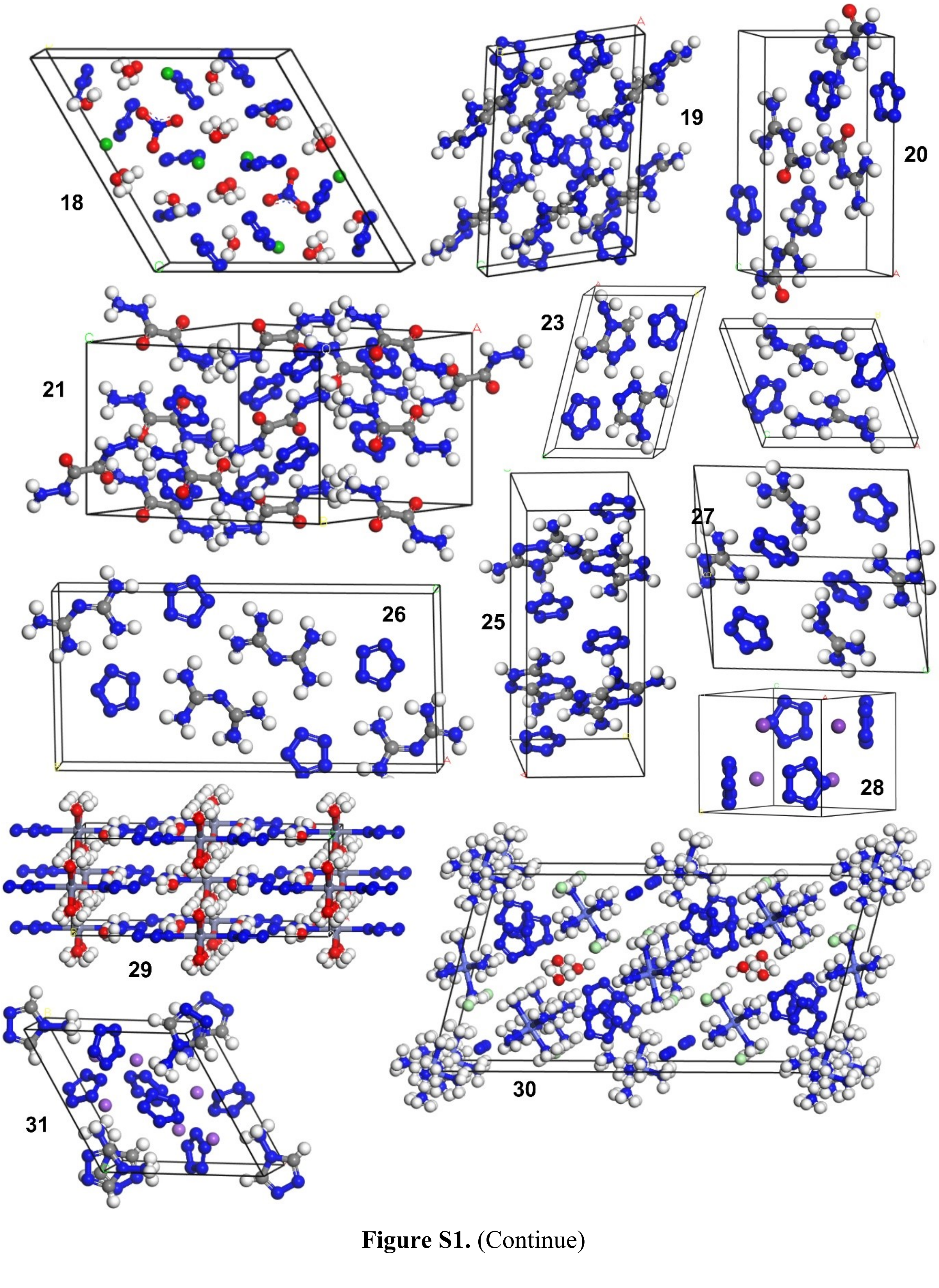
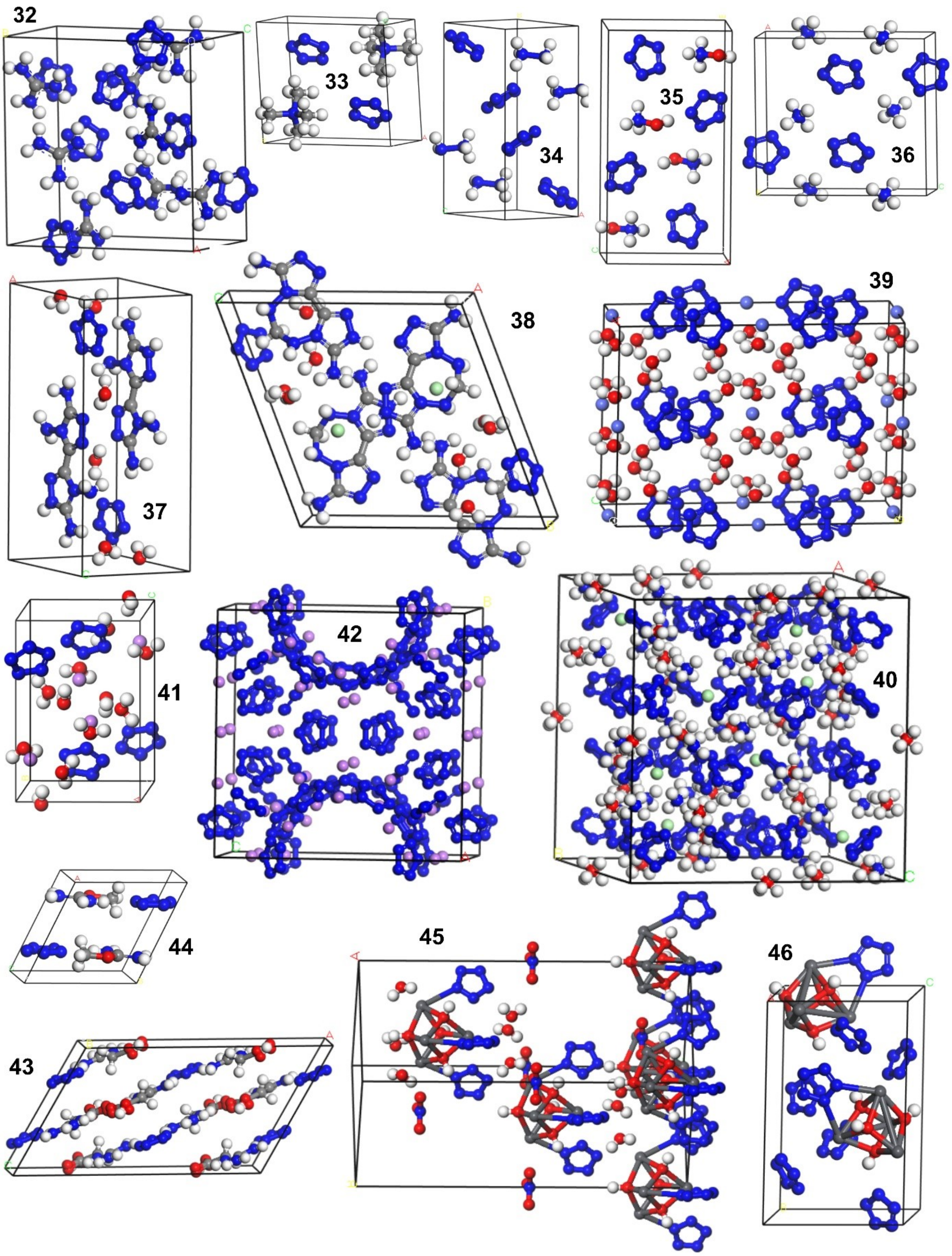


Figure S1. (Continue)



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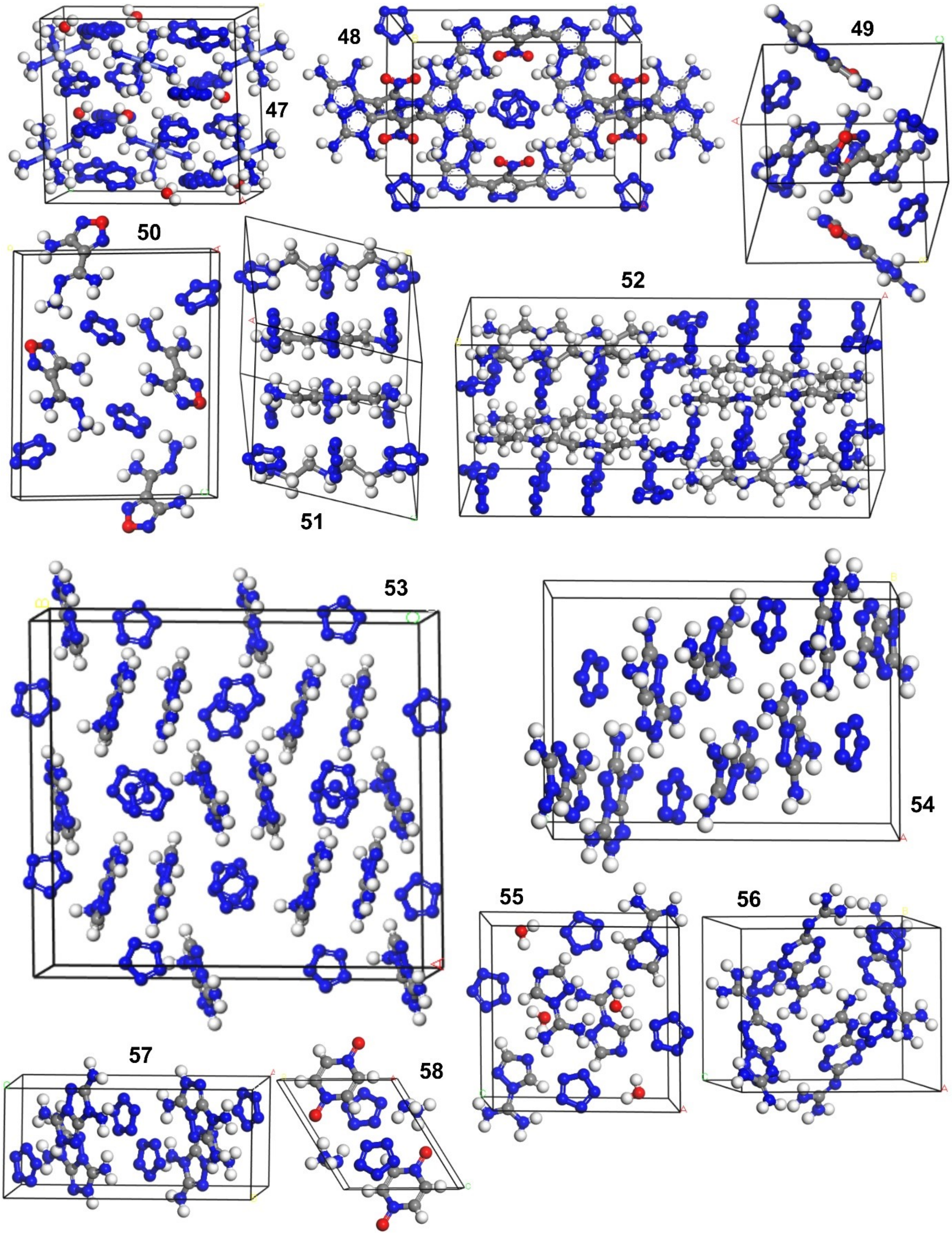

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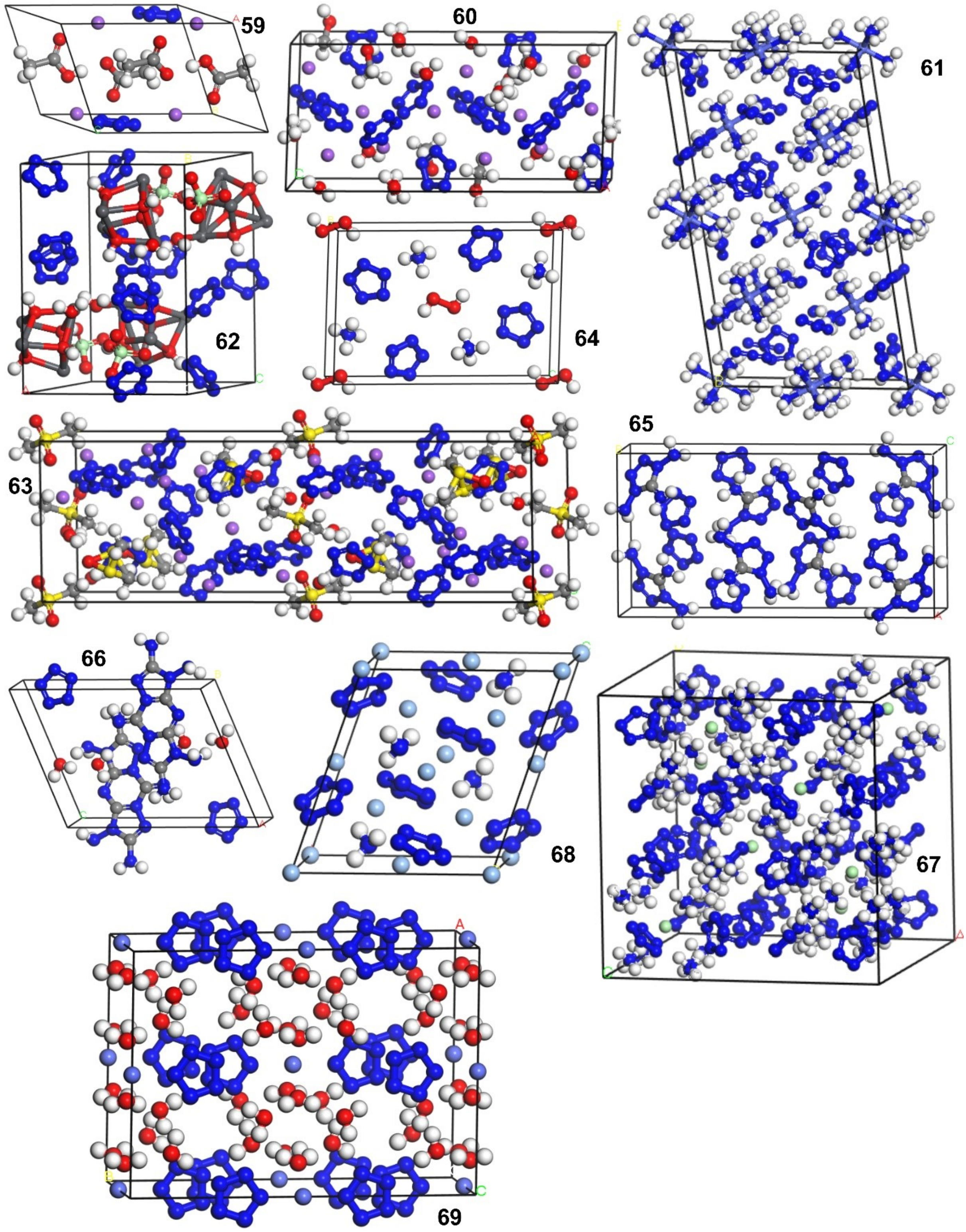

Figure S1. (Continue)

Table S4. The calculated descriptors used in Models A, B and C

No	ρ_{calcA}	R_{SA_V}	$\overline{\text{HOF}}$	ρ_{calcB}	ωH	ωC	ωN
1	1.338	0.958	22.280	0.842	0.505	0.053	0.442
2	1.406	1.044	33.913	0.914	0.490	0.034	0.476
3	1.388	1.478	46.680	0.818	0	0.056	0.392
4	1.226	1.478	50.727	0.774	0	0.060	0.414
5	1.496	1.357	99.720	0.789	0	0.055	0.722
6	1.535	1.343	87.194	0.813	0	0.046	0.679
7	1.477	1.338	4.982	0.650	0	0.041	0.476
8	1.721	1.392	90.312	0.861	0	0.035	0.491
9	1.732	1.398	81.150	0.873	0	0.035	0.490
10	1.759	1.399	71.824	0.885	0	0.035	0.485
11	1.359	1.499	3.347	0.797	0	0.059	0.407
12	1.525	1.195	21.451	0.951	0.148	0.037	0.518
13	1.522	1.060	32.550	0.898	0.351	0.038	0.410
14	1.352	1.256	61.768	0.841	0.109	0.055	0.763
15	2.849	1.371	296.008	1.278	0	0	0.638
16	3.137	1.319	183.944	1.712	0	0	0.394
17	2.438	1.165	37.852	0.854	0	0.019	0.260
18	2.643	1.093	113.928	0.839	0	0.006	0.447
19	1.589	1.052	73.260	0.952	0.171	0.029	0.800
20	1.469	1.160	30.831	0.915	0.139	0.041	0.728
21	1.564	1.137	34.261	0.924	0.127	0.037	0.667
22	1.376	1.405	16.475	0.834	0	0.058	0.600
23	1.488	1.163	61.449	0.922	0.141	0.036	0.823
24	1.378	1.179	50.652	0.885	0.075	0.050	0.875
25	1.555	1.108	59.140	0.969	0.160	0.031	0.809
26	1.358	1.156	39.044	0.884	0.139	0.047	0.814
27	1.453	1.208	51.068	0.883	0.083	0.049	0.869
28	2.272	1.033	115.508	0.520	0	0	0.642
29	1.585	1.497	30.354	0.959	0	0.046	0.401
30	1.511	1.387	126.831	0.755	0	0.061	0.557
31	1.840	1.167	87.435	0.680	0.089	0.015	0.726
32	1.384	1.240	51.627	0.878	0.092	0.047	0.861
33	0.981	1.114	31.731	0.748	0.333	0.084	0.583
34	1.496	1.313	74.791	0.870	0	0.049	0.951
35	1.604	1.299	69.432	0.895	0	0.039	0.807
36	1.364	1.343	77.951	0.865	0	0.046	0.954
37	1.433	1.176	18.570	0.896	0.149	0.047	0.654
38	1.424	1.139	25.026	0.929	0.201	0.044	0.588
39	1.579	1.446	32.626	0.849	0	0.047	0.408
40	1.421	1.366	78.799	0.873	0	0.043	0.814
41	1.385	1.441	2.036	0.698	0	0.046	0.535
42	1.445	1.299	126.006	0.697	0	0	0.910
43	1.347	1.131	23.694	0.911	0.191	0.043	0.596
44	1.371	1.203	36.268	0.875	0.165	0.049	0.676
45	3.611	1.380	177.953	1.877	0	0.008	0.183
46	4.437	1.331	259.891	2.002	0	0.003	0.238
47	1.509	1.357	99.720	0.789	0	0.055	0.722

No	ρ_{calcA}	R_{SA_V}	$\overline{\text{HOF}}$	ρ_{calcB}	ωH	ωC	ωN
48	1.589	0.976	44.431	0.993	0.222	0.027	0.667
49	1.603	1.060	52.687	0.969	0.190	0.028	0.719
50	1.549	1.119	51.367	0.953	0.169	0.033	0.723
51	1.318	1.167	84.454	0.852	0.152	0.051	0.797
52	1.358	1.142	88.983	0.848	0.167	0.052	0.781
53	1.550	1.112	66.151	0.952	0.171	0.029	0.800
54	1.575	1.088	49.273	0.966	0.190	0.035	0.775
55	1.355	1.197	38.691	0.889	0.180	0.040	0.700
56	1.518	1.076	42.736	0.950	0.180	0.034	0.786
57	1.506	1.106	59.140	0.966	0.160	0.031	0.809
58	1.450	1.235	53.665	0.886	0.151	0.044	0.704
59	1.652	1.216	23.218	0.642	0.204	0.030	0.298
60	1.523	1.266	38.001	0.640	0.047	0.032	0.551
61	1.499	1.347	133.400	0.774	0	0.053	0.775
62	4.143	1.344	217.049	1.982	0	0.005	0.172
63	1.690	1.190	52.216	0.674	0.071	0.024	0.520
64	1.526	1.367	59.690	0.868	0	0.048	0.800
65	1.521	1.140	70.051	0.939	0.065	0.033	0.903
66	1.495	1.122	31.234	0.940	0.175	0.038	0.694
67	1.411	1.361	76.883	0.857	0	0.049	0.891
68	3.495	1.336	136.844	1.549	0	0.008	0.413
69	1.595	1.446	88.893	0.849	0.047	0	0.408

Table S4. Continue

No	ωO	$\overline{\text{MW}}$	$\overline{\text{N}}$	$\overline{e}$	H/(N+O)	ρ_{calcC}
1	0	7.925	0.250	4.167	1.667	0.818
2	0	9.196	0.313	4.750	1.000	0.878
3	0.448	8.790	0.246	4.607	1.000	1.011
4	0.473	8.317	0.246	4.393	1.000	0.940
5	0.079	8.853	0.457	4.609	0.957	0.989
6	0.097	9.711	0.471	5.000	0.833	1.041
7	0.326	9.805	0.333	5.067	0.750	0.983
8	0.281	10.965	0.385	5.577	0.667	1.107
9	0.280	11.000	0.385	5.615	0.667	1.117
10	0.277	11.118	0.385	5.654	0.667	1.133
11	0.464	8.403	0.244	4.439	1.000	0.933
12	0.296	9.536	0.353	4.941	0.667	0.994
13	0.201	9.200	0.269	4.769	0.900	0.922
14	0.073	8.155	0.444	4.296	0.923	0.911
15	0	19.511	0.889	9.444	0.000	1.448
16	0	29.650	0.833	13.667	0.000	1.893
17	0.297	17.022	0.316	8.000	0.500	1.373
18	0.099	20.664	0.660	9.574	0.162	1.411
19	0	10.008	0.571	5.143	0.500	0.984
20	0.092	9.112	0.474	4.737	0.700	0.957
21	0.169	9.457	0.450	4.900	0.636	0.984
22	0.343	8.241	0.353	4.353	0.889	0.962

No	***ωO***	$\overline{\mathrm{MW}}$	$\overline{\mathrm{N}}$	$\overline{e}$	**H/(N+O)**	ρ_{calcC}
23	0	9.452	0.556	4.889	0.600	0.966
24	0	8.428	0.526	4.421	0.800	0.929
25	0	9.790	0.565	5.043	0.538	0.977
26	0	8.608	0.500	4.500	0.800	0.924
27	0	8.537	0.529	4.471	0.778	0.933
28	0	18.189	0.833	9.000	0.000	1.149
29	0.366	9.988	0.286	5.143	0.889	1.062
30	0.025	9.111	0.362	4.725	1.462	0.989
31	0	12.279	0.636	6.182	0.286	1.019
32	0	8.674	0.533	4.533	0.750	0.938
33	0	6.554	0.273	3.545	2.000	0.770
34	0	8.591	0.583	4.500	0.714	0.955
35	0.154	9.461	0.545	4.909	0.571	1.016
36	0	8.807	0.600	4.600	0.667	0.967
37	0.149	8.683	0.405	4.541	0.833	0.937
38	0.107	9.029	0.379	4.697	0.897	0.936
39	0.373	9.803	0.286	5.057	0.889	1.073
40	0.082	9.284	0.540	4.825	0.676	0.995
41	0.366	8.735	0.333	4.533	0.750	0.896
42	0	12.829	0.833	6.333	0.000	0.944
43	0.170	8.959	0.381	4.667	0.800	0.944
44	0.110	8.537	0.412	4.471	0.875	0.923
45	0.131	30.575	0.400	13.250	0.385	2.178
46	0.054	36.780	0.625	15.750	0.167	2.308
47	0.079	8.853	0.457	4.609	0.957	0.989
48	0.085	10.224	0.486	5.243	0.500	0.988
49	0.063	10.127	0.520	5.200	0.500	0.990
50	0.075	9.689	0.500	5.000	0.583	0.976
51	0	8.323	0.474	4.368	0.889	0.906
52	0	8.277	0.462	4.346	0.917	0.900
53	0	10.008	0.571	5.143	0.500	0.984
54	0	9.483	0.525	4.900	0.619	0.956
55	0.080	9.098	0.455	4.727	0.727	0.946
56	0	9.543	0.536	4.929	0.600	0.961
57	0	9.790	0.565	5.043	0.538	0.977
58	0.101	8.841	0.444	4.611	0.778	0.941
59	0.272	10.687	0.227	5.455	0.778	0.950
60	0.189	10.588	0.417	5.417	0.615	0.983
61	0	9.032	0.500	4.684	0.947	0.995
62	0.118	34.983	0.429	15.086	0.250	2.252
63	0.119	11.814	0.439	6.000	0.533	1.007
64	0.152	8.757	0.500	4.583	0.714	0.977
65	0	9.797	0.632	5.053	0.500	1.001
66	0.093	9.278	0.459	4.811	0.684	0.957
67	0	8.817	0.561	4.606	0.757	0.963
68	0	23.302	0.688	10.875	0.273	1.734
69	0.373	9.803	0.286	5.057	0.889	1.073

Table S5. Molecular properties calculated using PM7 method

No	HOF (kJ/mol)	*S* (Å^2)	*V* (Å^3)	No	HOF (kJ/mol)	*S* (Å^2)	*V* (Å^3)
1	534.7	216.3	225.8	**36**	779.5	136.7	101.8
2	542.6	168.1	161.0	**37**	687.1	421.9	358.7
3	2847.5	968.5	655.4	**38**	1651.7	730.8	641.7
4	3094.4	968.5	655.4	**39**	1141.9	584.5	404.2
5	4587.1	700.4	516.1	**40**	4964.3	914.8	669.7
6	2964.6	545.4	406.1	**41**	30.5	270.7	187.8
7	74.7	302.6	226.2	**42**	756.0	143.4	110.4
8	2348.1	460.9	331.2	**43**	497.6	233.7	206.6
9	2109.9	457.8	327.5	**44**	616.5	199.4	165.8
10	1867.4	457.2	326.8	**45**	7118.1	899.3	651.5
11	137.2	648.3	432.4	**46**	2079.1	195.6	147.0
12	364.7	203.6	170.4	**47**	4587.1	700.4	516.1
13	846.3	282.3	266.3	**48**	1643.9	371.7	381.0
14	1667.7	328.6	261.7	**49**	1317.2	277.0	261.4
15	2664.1	188.4	137.4	**50**	1130.1	250.3	223.6
16	1103.7	137.1	103.9	**51**	3209.3	433.5	371.4
17	719.2	440.9	378.5	**52**	4627.1	580.0	507.8
18	5354.6	1264.2	1157.0	**53**	1389.2	245.4	220.8
19	2564.1	387.0	367.9	**54**	1970.9	427.3	392.8
20	585.8	219.5	189.2	**55**	851.2	269.4	225.1
21	685.2	232.9	204.8	**56**	1196.6	302.7	281.3
22	280.1	235.9	167.9	**57**	1360.2	257.6	233.0
23	1106.1	214.6	184.5	**58**	1932.0	443.4	359.0
24	962.4	213.2	180.9	**59**	510.8	445.6	366.5
25	1360.2	257.7	232.5	**60**	912.0	502.2	396.8
26	780.9	225.1	194.7	**61**	5069.2	597.4	443.5
27	868.1	198.5	164.3	**62**	7596.7	830.3	617.9
28	693.0	216.6	209.8	**63**	2976.3	1189.5	999.6
29	1062.4	545.5	364.4	**64**	1432.6	330.8	242.1
30	8751.3	1154.8	832.3	**65**	1331.0	226.0	198.3
31	1923.6	463.5	397.2	**66**	1155.7	409.6	365.1
32	774.4	183.9	148.3	**67**	5074.3	923.6	678.7
33	698.1	214.8	192.9	**68**	2189.5	321.6	240.7
34	897.5	155.6	118.5	**69**	3111.3	584.5	404.2
35	763.8	151.0	116.3				

Table S6. The calculated crystal densities by the proposed models (g/cm^3) and the corresponding mean absolute percentage error (MAPE, %) of the Train46 set

No	Model A	MAPE	Model B	MAPE	Model C	MAPE
1	1.424	0	1.428	0	1.370	4
2	1.478	4	1.383	2	1.563	10
3	1.463	2	1.480	4	1.532	7
4	1.317	5	1.395	1	1.400	1
5	1.588	5	1.586	5	1.606	3
6	1.589	8	1.655	5	1.690	2
7	1.540	5	1.584	8	1.512	3

No	Model A	MAPE	Model B	MAPE	Model C	MAPE
8	1.748	9	1.662	3	1.740	8
9	1.760	10	1.662	4	1.746	9
10	1.783	5	1.672	1	1.784	5
11	1.440	0	1.442	0	1.388	3
12	1.588	5	1.624	3	1.557	7
13	1.585	2	1.574	2	1.545	0
14	1.491	2	1.456	0	1.478	1
15	2.493	5	2.636	0	2.400	9
16	2.988	1	3.042	1	3.273	9
17	2.500	4	2.566	1	2.328	10
18	2.481	6	2.424	4	2.500	7
19	1.622	2	1.720	4	1.622	2
20	1.553	3	1.562	2	1.550	3
21	1.626	3	1.646	2	1.563	7
22	1.485	0	1.440	3	1.454	2
23	1.557	4	1.568	3	1.582	2
24	1.517	4	1.571	7	1.503	3
25	1.601	3	1.627	1	1.607	2
26	1.481	3	1.526	0	1.523	0
27	1.580	7	1.531	4	1.512	2
28	2.012	1	1.941	3	1.814	9
29	1.641	2	1.605	4	1.644	2
30	1.582	3	1.646	1	1.613	1
31	1.763	2	1.615	7	1.688	2
32	1.507	1	1.484	2	1.523	1
33	1.156	7	1.228	1	1.256	1
34	1.626	0	1.531	6	1.505	7
35	1.666	2	1.582	3	1.550	5
36	1.489	2	1.502	1	1.519	0
37	1.530	1	1.543	2	1.513	0
38	1.506	7	1.600	1	1.552	4
39	1.636	3	1.610	5	1.663	2
40	1.505	12	1.528	14	1.565	17
41	1.470	7	1.339	2	1.361	1
42	1.291	1	1.305	2	1.494	17
43	1.437	6	1.589	4	1.534	1
44	1.480	6	1.482	6	1.507	8
45	3.874	1	3.935	1	4.018	3
46	4.570	1	4.494	1	4.374	4

Table S7. The calculated crystal densities by the proposed models (g/cm^3) and the corresponding MAPE (%) of the Test23 set

No	Model A	MAPE	Model B	MAPE	Model C	MAPE
47	1.600	3	1.586	4	1.606	2
48	1.622	6	1.769	3	1.632	5
49	1.635	2	1.677	0	1.625	3

No	Model A	MAPE	Model B	MAPE	Model C	MAPE
50	1.603	2	1.616	1	1.593	3
51	1.456	2	1.542	4	1.502	2
52	1.493	1	1.556	5	1.499	1
53	1.586	7	1.620	5	1.622	5
54	1.635	2	1.607	3	1.591	4
55	1.446	3	1.478	1	1.554	5
56	1.580	3	1.618	1	1.594	2
57	1.556	6	1.631	1	1.607	3
58	1.545	4	1.473	8	1.531	5
59	1.714	0	1.669	2	1.552	9
60	1.563	3	1.579	2	1.570	3
61	1.586	8	1.666	3	1.643	4
62	4.486	2	4.475	1	4.161	6
63	1.703	3	1.733	5	1.644	1
64	1.629	8	1.467	3	1.505	0
65	1.567	4	1.703	4	1.592	3
66	1.569	4	1.589	3	1.565	5
67	1.527	14	1.508	12	1.541	15
68	3.313	4	2.747	14	3.022	6
69	1.650	3	1.565	8	1.662	2

Table S8. The calculated densities (g/cm^3) for the Train46 set salts obtained as mean values of models AB, BC, AC and ABC along with the corresponding MAPE (%) values

No	AB	MAPE	BC	MAPE	AC	MAPE	ABC	MAPE
1	1.426	0	1.399	2	1.397	2	1.407	2
2	1.430	1	1.473	4	1.520	7	1.475	4
3	1.472	3	1.506	5	1.498	5	1.492	4
4	1.356	2	1.397	1	1.359	2	1.371	1
5	1.587	5	1.596	4	1.597	4	1.593	4
6	1.622	6	1.672	3	1.640	5	1.645	5
7	1.562	6	1.548	5	1.526	4	1.545	5
8	1.705	6	1.701	6	1.744	8	1.717	7
9	1.711	7	1.704	7	1.753	10	1.723	8
10	1.727	2	1.728	2	1.783	5	1.746	3
11	1.441	0	1.415	2	1.414	2	1.423	1
12	1.606	4	1.591	5	1.572	6	1.590	5
13	1.579	2	1.560	1	1.565	1	1.568	1
14	1.473	1	1.467	0	1.485	2	1.475	1
15	2.564	2	2.518	4	2.446	7	2.509	4
16	3.015	0	3.157	5	3.130	4	3.101	3
17	2.533	2	2.447	6	2.414	7	2.465	5
18	2.453	5	2.462	5	2.491	7	2.468	6
19	1.671	1	1.671	1	1.622	2	1.655	0
20	1.558	2	1.556	3	1.551	3	1.555	3
21	1.636	3	1.605	5	1.595	5	1.612	4
22	1.462	2	1.447	3	1.470	1	1.460	2

No	AB	MAPE	BC	MAPE	AC	MAPE	ABC	MAPE
23	1.563	3	1.575	3	1.570	3	1.569	3
24	1.544	5	1.537	5	1.510	3	1.531	4
25	1.614	2	1.617	2	1.604	2	1.612	2
26	1.504	1	1.525	0	1.502	1	1.510	1
27	1.555	5	1.522	3	1.546	5	1.541	4
28	1.976	1	1.877	6	1.913	4	1.922	4
29	1.623	3	1.624	3	1.642	2	1.630	2
30	1.614	1	1.629	0	1.598	2	1.614	1
31	1.689	2	1.651	4	1.725	0	1.689	2
32	1.496	1	1.504	1	1.515	0	1.505	1
33	1.192	4	1.242	0	1.206	3	1.213	3
34	1.578	3	1.518	6	1.566	3	1.554	4
35	1.624	1	1.566	4	1.608	2	1.599	2
36	1.496	2	1.511	1	1.504	1	1.504	1
37	1.537	1	1.528	1	1.522	0	1.529	1
38	1.553	4	1.576	3	1.529	5	1.553	4
39	1.623	4	1.636	3	1.649	3	1.636	3
40	1.517	13	1.547	15	1.535	15	1.533	14
41	1.404	3	1.350	1	1.415	3	1.390	2
42	1.298	2	1.399	9	1.393	9	1.363	7
43	1.513	1	1.562	2	1.486	3	1.520	0
44	1.481	6	1.495	7	1.494	7	1.490	7
45	3.904	0	3.976	2	3.946	1	3.942	1
46	4.532	0	4.434	2	4.472	1	4.479	1

Table S9. The calculated densities (g/cm^3) for the Test23 set salts obtained as mean values of models AB, BC, AC and ABC along with the corresponding MAPE (%) values

No	AB	MAPE	BC	MAPE	AC	MAPE	ABC	MAPE
47	1.593	3	1.596	3	1.603	3	1.598	3
48	1.696	2	1.701	1	1.627	6	1.674	3
49	1.656	1	1.651	1	1.630	3	1.645	2
50	1.610	2	1.605	2	1.598	2	1.604	2
51	1.499	1	1.522	3	1.479	0	1.500	1
52	1.524	3	1.528	3	1.496	1	1.516	2
53	1.603	6	1.621	5	1.604	6	1.609	6
54	1.621	3	1.599	4	1.613	3	1.611	3
55	1.462	2	1.516	2	1.500	1	1.493	0
56	1.599	2	1.606	1	1.587	3	1.597	2
57	1.593	3	1.619	2	1.581	4	1.598	3
58	1.509	6	1.502	7	1.538	4	1.516	6
59	1.692	1	1.611	6	1.633	4	1.645	4
60	1.571	3	1.574	2	1.566	3	1.571	3
61	1.626	5	1.654	4	1.614	6	1.631	5
62	4.480	1	4.318	2	4.324	2	4.374	1
63	1.718	4	1.689	2	1.673	1	1.693	2
64	1.548	2	1.486	2	1.567	4	1.533	2

No	AB	MAPE	BC	MAPE	AC	MAPE	ABC	MAPE
65	1.635	0	1.648	1	1.580	4	1.621	1
66	1.579	4	1.577	4	1.567	4	1.574	4
67	1.517	13	1.524	14	1.534	14	1.525	14
68	3.030	5	2.884	10	3.168	1	3.027	5
69	1.608	5	1.614	5	1.656	2	1.626	4

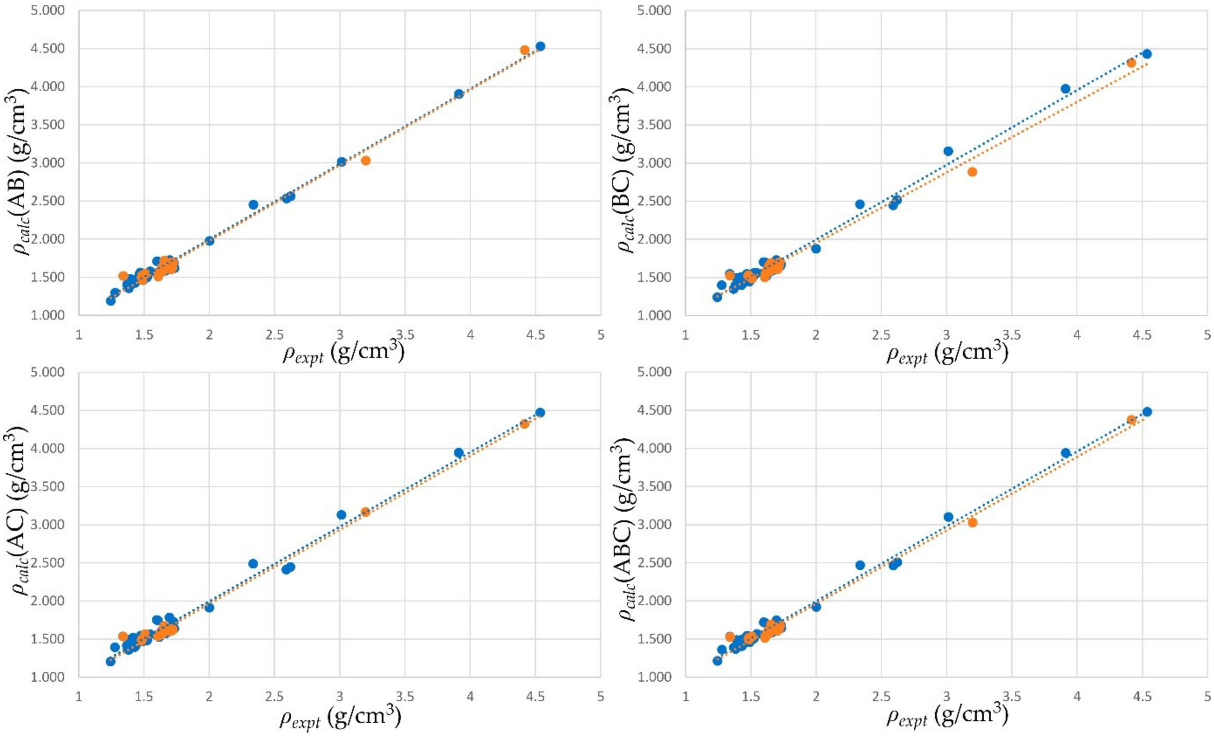

Figure S2. Correlations of the calculated (d_c) and measured (d_m) densities for the training set (blue markers) and test set (red markers) salts obtained as mean values

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