RADICAL PAIR FORMATION DUE TO COMPRESSION-INDUCED ELECTRON TRANSFER IN CRYSTALS OF ENERGETIC SALTS

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Phys. Chem. Chem. Phys.

SUPPORTING INFORMATION

LIST OF SUPPLEMENTARY FIGURES AND TABLES:

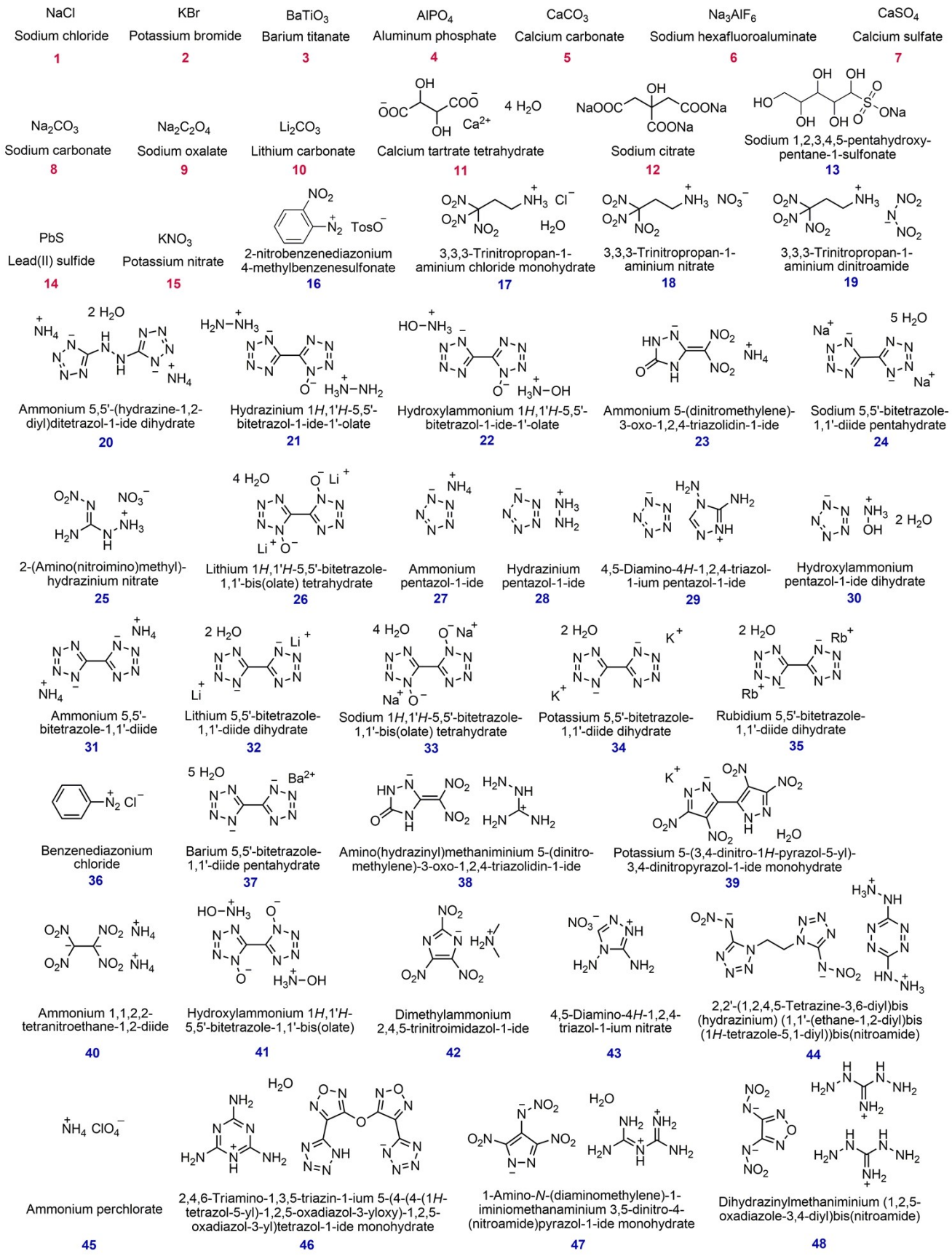


Fig. S1. Chemical formulas and full names of the salts studied.

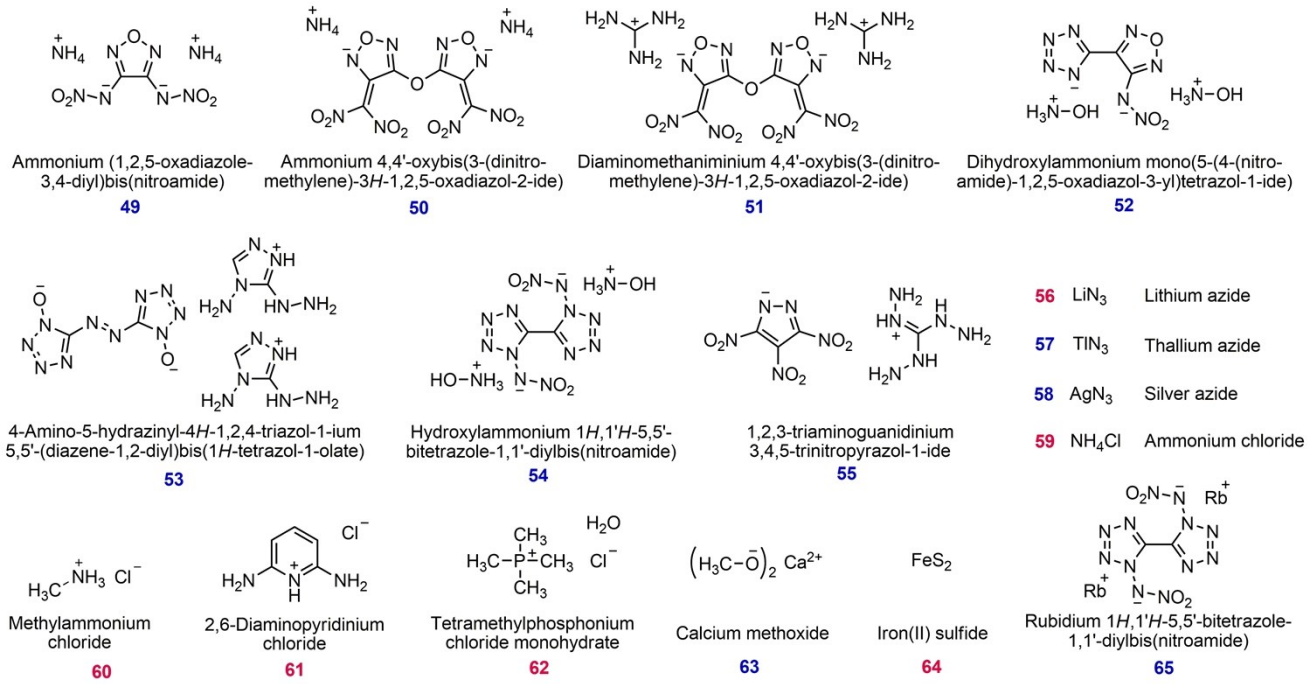


Fig. S1. Continue.

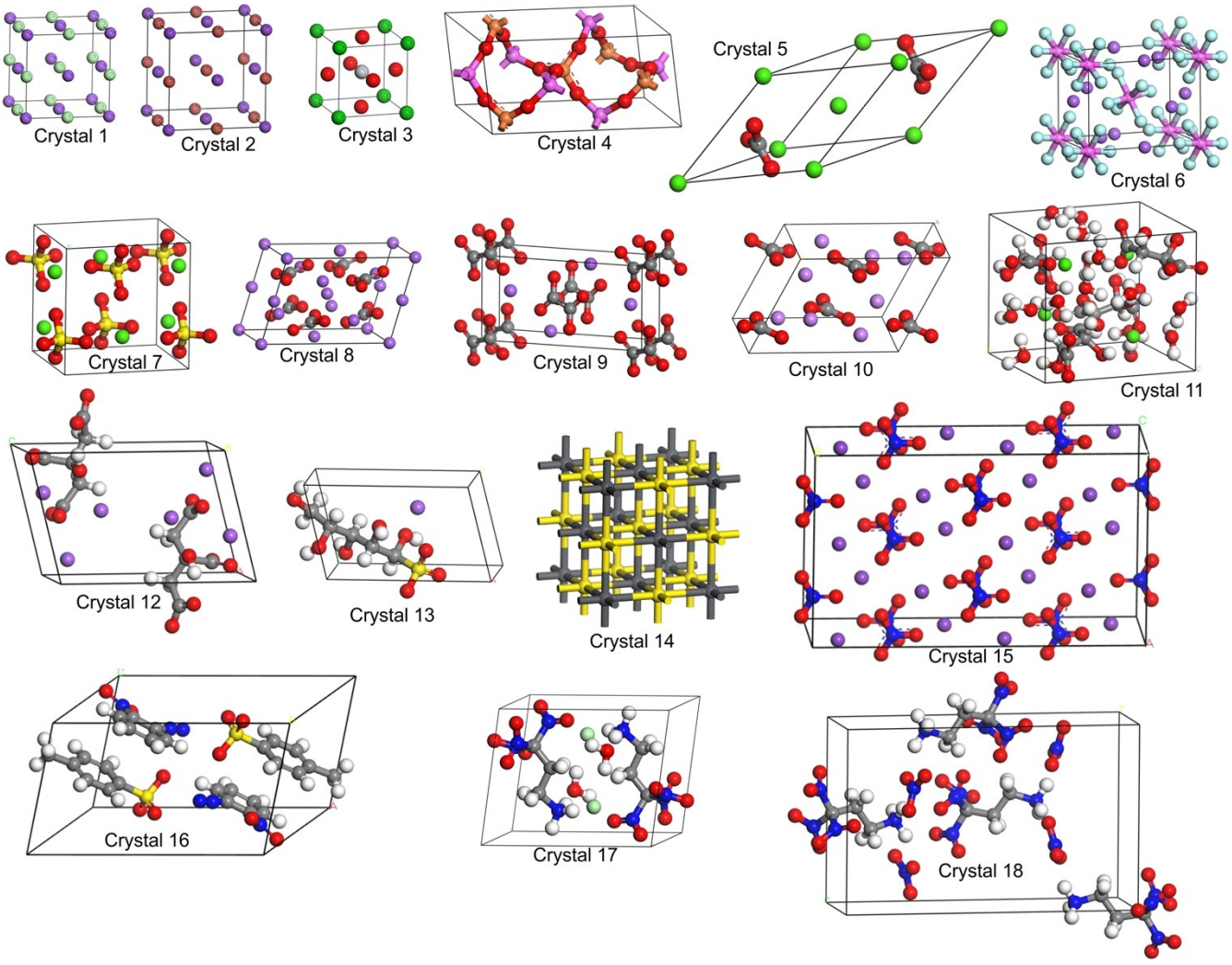


Fig. S2. Crystal structures of the salts studied.

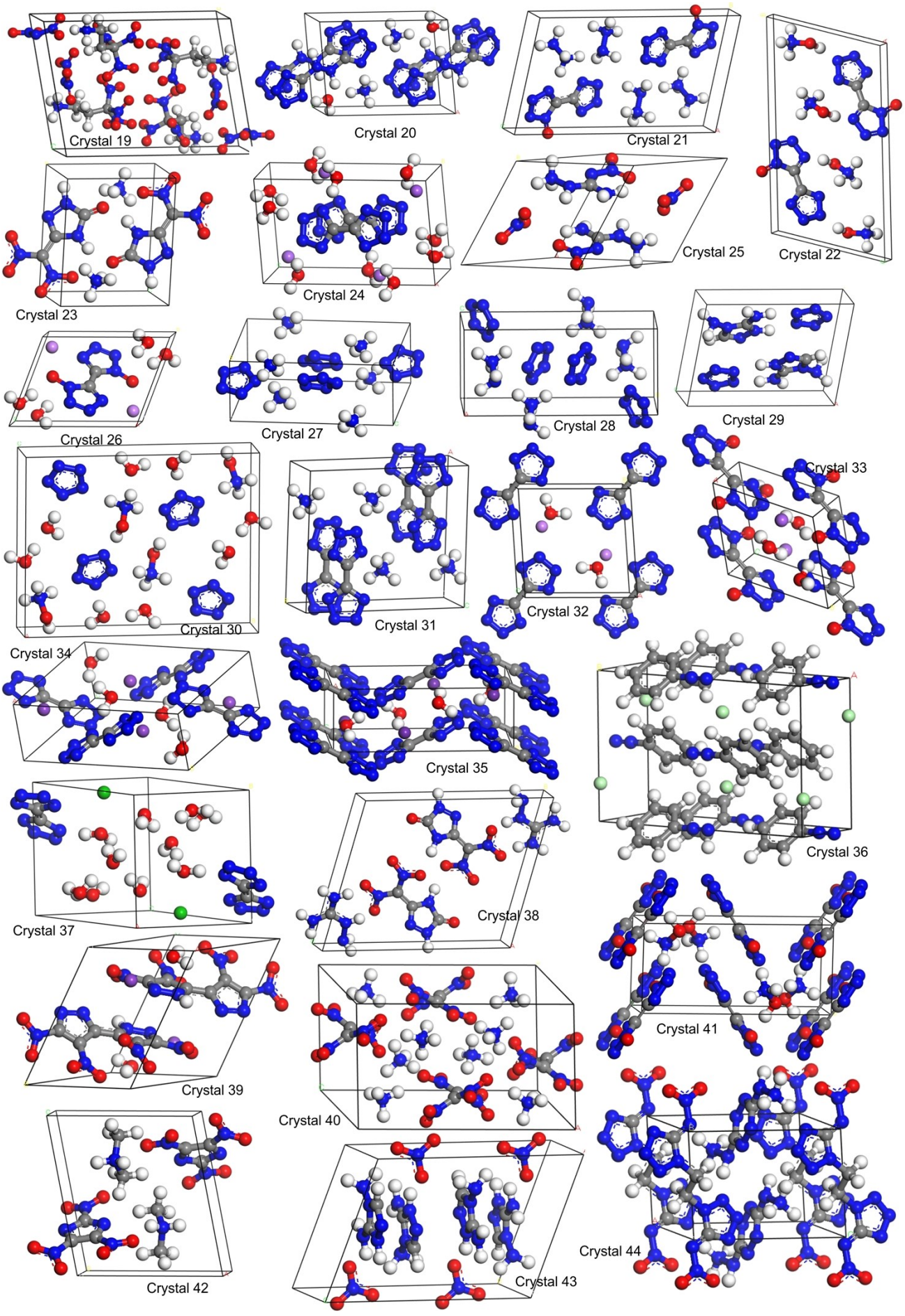


Fig. S2. Continue.

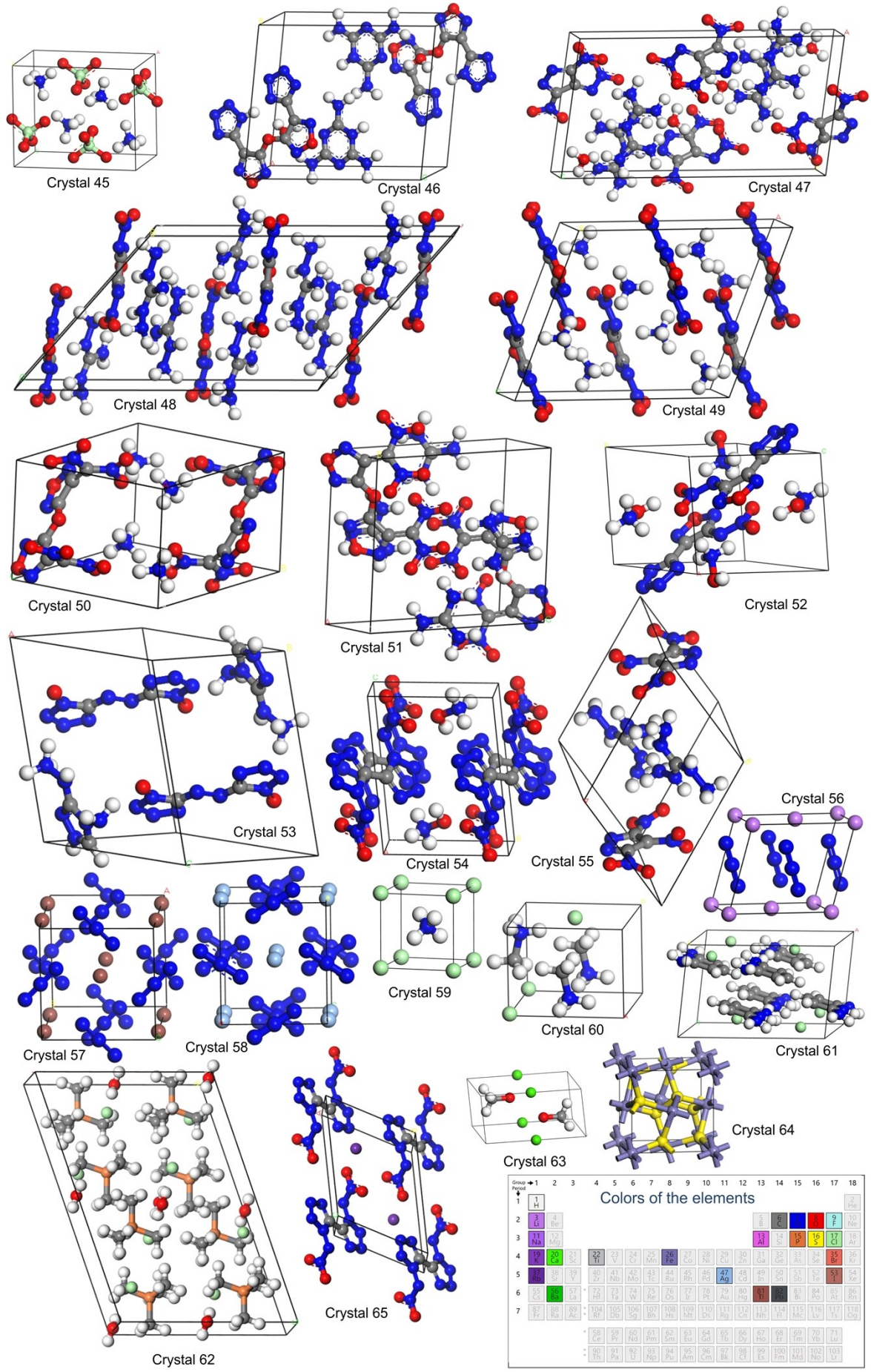


Fig. S2. Continue.

Table S1. The calculated and experimental (in parentheses) asymmetric cell parameters of the salts studied.

Crystal	Space group	*a*	*b*	*c*	*α*	*β*	*γ*
1	$Fm\bar{3}m$	5.672 (5.640)					
2	$Fm\bar{3}m$	6.597 (6.597)					
3	$Pm\bar{3}m$	3.954 (4.010)					
4	$P3_12_1$	5.053 (4.942)		11.092 (10.945)			
5	$R\bar{3}c$	6.351 (6.375)			46.5 (46.1)		
6	$P2_1/n$	5.276 (5.402)	5.546 (5.596)	7.534 (7.756)		90.9 (90.3)	
7	*Amma*	7.016 (6.991)	7.012 (6.996)	6.326 (6.238)			
8	$C2/m$	8.804 (8.825)	5.288 (5.194)	5.921 (5.953)		104.8 (101.8)	
9	$P2_1/a$	10.299 (10.350)	5.334 (5.260)	3.442 (3.460)		91.4 (92.9)	
10	$C/2c$	8.369 (8.359)	4.972 (4.973)	6.111 (6.198)		114.5 (114.8)	
11	$P2_12_12_1$	9.488 (9.631)	10.455 (10.573)	9.109 (9.215)			
12	$P2_1$	7.337 (7.347)	5.366 (5.435)	10.747 (11.034)		103.9 (103.9)	
13	$P1$	4.840 (4.856)	5.911 (5.850)	8.880 (8.795)	76.0 (76.5)	81.6 (81.5)	71.5 (71.4)
14	$Fm\bar{3}m$	5.863 (5.930)					
15	$Cmc2_1$	10.892 (10.904)	18.429 (18.455)	6.362 (6.421)			
16	$P\bar{1}$	7.489 (7.509)	7.572 (7.546)	13.611 (13.672)	78.6 (78.6)	76.7 (75.7)	75.3 (75.6)
17	$P\bar{1}$	6.770 (6.743)	7.826 (7.805)	10.154 (10.066)	89.8 (90.4)	99.2 (98.8)	113.9 (114.1)
18	$P2_12_12_1$	5.698 (5.662)	10.293 (10.283)	16.382 (16.258)			
19	$P\bar{1}$	6.766 (6.709)	11.381 (11.255)	15.394 (15.214)	75.1 (75.5)	79.4 (79.3)	75.5 (75.7)
20	$P\bar{1}$	4.018 (3.824)	7.093 (6.967)	9.670 (9.920)	82.4 (80.5)	90.6 (88.7)	86.1 (79.5)
21	$P\bar{1}$	3.614 (3.655)	8.441 (8.436)	14.289 (14.338)	102.8 (103.6)	96.4 (96.6)	93.2 (93.3)
22	$P\bar{1}$	3.628 (3.606)	8.020 (8.019)	14.833 (14.798)	105.5 (105.1)	91.8 (91.7)	96.5 (96.0)
23	$P\bar{1}$	6.764 (6.785)	7.092 (7.137)	8.070 (7.965)	84.3 (85.1)	75.0 (74.0)	84.6 (84.9)
24	$P\bar{1}$	7.199 (7.209)	7.429 (7.462)	10.679 (10.775)	82.2 (81.3)	76.6 (76.5)	68.5 (67.6)
25	$P\bar{1}$	7.288 (7.175)	7.181 (7.202)	7.909 (7.856)	65.8 (66.1)	63.1 (65.3)	66.1 (68.5)
26	$P\bar{1}$	5.280 (5.345)	6.343 (6.363)	8.228 (8.300)	105.4 (105.9)	97.6 (98.2)	112.3 (111.5)
27	*Pcca*	9.488 (9.399)	3.956 (3.954)	10.353 (10.362)			

Table S1. Continue.

Crystal	Space group	*a*	*b*	*c*	*α*	*β*	*γ*
28	$P2_1/c$	6.554	12.076	5.369		97.9	
		(6.453)	(12.247)	(5.407)		(97.8)	
29	$P\bar{1}$	5.315	7.128	10.174	100.6	103.9	103.7
		(5.298)	(7.156)	(10.106)	(100.0)	(104.1)	(104.1)
30	$P2_1/c$	3.630	14.796	11.443		90.8	
		(3.685)	(14.638)	(11.575)		(90.3)	
31	*Pban*	9.123	10.691	3.669			
		(9.130)	(10.763)	(3.666)			
32	$P\bar{1}$	3.353	7.368	7.490	83.2	86.5	80.4
		(3.368)	(7.362)	(7.501)	(82.9)	(87.1)	(80.8)
33	$P\bar{1}$	5.587	6.471	8.354	99.5	97.0	111.7
		(5.681)	(6.451)	(8.355)	(100.3)	(97.3)	(111.8)
34	$P2_1/c$	3.836	11.347	9.750		93.6	
		(3.851)	(11.316)	(9.735)		(93.0)	
35	$P2_1/c$	4.051	11.355	9.990		94.6	
		(4.088)	(11.328)	(9.948)		(93.5)	
36	$C222_1$	15.050	4.860	9.011			
		(15.152)	(4.928)	(9.044)			
37	$P\bar{1}$	7.417	7.876	9.272	89.3	74.0	88.7
		(7.440)	(8.162)	(9.259)	(88.6)	(73.7)	(88.9)
38	$P\bar{1}$	3.630	10.997	13.276	107.4	94.6	98.6
		(3.648)	(10.984)	(13.201)	(107.2)	(95.4)	(99.1)
39	$P\bar{1}$	7.336	8.853	10.809	105.1	94.9	108.7
		(7.354)	(9.047)	(10.724)	(105.6)	(94.5)	(108.9)
40	$P2_1/n$	9.322	7.865	13.152		107.8	
		(9.255)	(7.800)	(13.135)		(107.9)	
41	$P2_1/c$	5.527	11.523	6.480		96.10	
		(5.426)	(11.660)	(6.501)		(95.26)	
42	$P2_1$	8.516	6.163	9.507		100.9	
		(8.484)	(6.144)	(9.439)		(100.6)	
43	$P2_1/c$	8.764	6.132	12.401		110.0	
		(8.527)	(6.265)	(12.760)		(112.0)	
44	$P\bar{1}$	6.796	7.639	8.737	96.6	101.7	115.5
		(6.771)	(7.562)	(8.712)	(96.5)	(101.9)	(115.0)
45	*Pnma*	8.859	6.043	7.241			
		(9.130)	(5.790)	(7.470)			
46	$P\bar{1}$	6.535	10.776	12.326	84.8	76.4	84.2
		(6.691)	(10.822)	(12.259)	(85.2)	(76.7)	(84.7)
47	$P2_1/n$	9.758	7.062	18.405		97.9	
		(9.688)	(7.154)	(18.317)		(98.0)	
48	$C2/c$	18.570	8.268	12.572		131.4	
		(18.761)	(8.292)	(12.498)		(131.3)	
49	$C2/c$	12.136	7.489	10.175		111.2	
		(12.031)	(7.401)	(9.981)		(109.4)	
50	$P\bar{1}$	7.724	9.367	10.495	93.8	104.4	99.8
		(7.691)	(9.290)	(10.564)	(94.5)	(104.2)	(100.4)
51	$P\bar{1}$	8.747	10.374	10.661	79.0	86.0	72.2
		(8.882)	(10.251)	(10.718)	(78.1)	(83.7)	(71.3)
52	$P\bar{1}$	7.118	8.205	9.176	83.7	71.2	73.0
		(7.130)	(8.131)	(9.057)	(83.4)	(71.7)	(72.5)
53	$P\bar{1}$	8.262	8.374	10.743	89.3	109.5	117.5
		(7.972)	(8.192)	(10.269)	(90.4)	(110.2)	(115.5)
54	$P\bar{1}$	5.176	6.649	8.476	96.9	90.2	97.9
		(5.242)	(6.769)	(8.400)	(96.4)	(89.2)	(97.5)
55	$P\bar{1}$	5.065	10.742	11.565	65.3	77.7	85.8
		(5.113)	(10.676)	(11.579)	(66.3)	(78.5)	(84.9)

Table S1. Continue.

Crystal	Space group	*a*	*b*	*c*	*α*	*β*	*γ*
56	$C2/m$	5.602 (5.627)	3.282 (3.319)	4.854 (4.979)		104.1 (107.4)	
57	$I4/mcm$	6.131 (6.208)		7.591 (7.355)			
58	*Ibam*	6.186 (5.617)	5.366 (5.915)	6.364 (6.006)			
59	$P\bar{4}3m$	3.806 (3.860)					
60	$Pmn2_1$	5.971 (6.040)	4.813 (5.050)	6.202 (6.040)			
61	$C2/m$	10.805 (10.763)	9.046 (9.076)	6.811 (6.635)		96.7 (95.4)	
62	$C2/c$	11.818 (11.762)	8.667 (8.628)	17.591 (17.604)		108.6 (107.5)	
63	$P\bar{3}m1$	3.688 (3.642)		8.019 (8.311)			
64	$Pa\bar{3}$	5.317 (5.428)					
65	$P\bar{1}$	5.356 (5.303)	7.077 (7.063)	8.621 (8.568)	66.5 (66.8)	86.3 (86.7)	71.1 (70.0)

Table S2. The relative errors $\delta = (V_{theor} - V_{exper})/V_{exper}$ of the asymmetric cell volumes estimation.

Salt	V_{theor} (Å^3)	V_{exper} (Å^3)	δ (%)	Salt	V_{theor} (Å^3)	V_{exper} (Å^3)	δ (%)
1	182.48	179.41	1.71	**34**	423.55	423.65	-0.02
2	287.10	287.10	0.00	**35**	458.05	459.82	-0.38
3	61.82	64.48	-4.13	**36**	659.09	675.31	-2.40
4	283.21	267.31	5.95	**37**	520.51	539.45	-3.51
5	123.07	122.72	0.29	**38**	495.64	493.36	0.46
6	220.42	234.46	-5.99	**39**	630.95	639.35	-1.31
7	311.22	305.09	2.01	**40**	918.12	902.31	1.75
8	266.51	267.10	-0.22	**41**	410.36	409.57	0.19
9	189.03	188.12	0.48	**42**	489.97	483.62	1.31
10	231.39	233.89	-1.07	**43**	626.26	632.03	-0.91
11	903.59	938.35	-3.70	**44**	390.27	385.38	1.27
12	410.73	427.70	-3.97	**45**	387.65	394.88	-1.83
13	233.10	229.52	1.56	**46**	837.34	858.38	-2.45
14	201.54	208.53	-3.35	**47**	1256.27	1257.16	-0.07
15	1277.04	1292.12	-1.17	**48**	1447.96	1460.71	-0.87
16	718.54	719.40	-0.12	**49**	862.20	838.27	2.85
17	484.41	476.49	1.66	**50**	720.04	713.73	0.88
18	960.80	946.58	1.50	**51**	904.08	903.47	0.07
19	1099.94	1068.31	2.96	**52**	485.07	475.31	2.05
20	272.48	256.29	6.32	**53**	612.48	558.43	9.68
21	420.96	425.21	-1.00	**54**	286.79	293.67	-2.34
22	412.37	410.15	0.54	**55**	558.44	567.10	-1.53
23	371.13	368.54	0.70	**56**	86.56	88.73	-2.45
24	516.10	519.82	-0.72	**57**	285.34	283.46	0.66
25	324.17	327.54	-1.03	**58**	211.25	199.55	5.86
26	237.27	243.11	-2.40	**59**	55.13	57.51	-4.14
27	388.59	385.09	0.91	**60**	178.24	184.23	-3.25
28	420.90	423.36	-0.58	**61**	661.18	645.27	2.47
29	351.47	349.18	0.66	**62**	1707.69	1703.83	0.23
30	614.54	624.37	-1.57	**63**	109.07	110.24	-1.06
31	357.85	360.24	-0.66	**64**	150.31	159.93	-6.02
32	181.00	182.10	-0.60	**65**	282.72	276.06	2.41
33	271.21	273.38	-0.79				

Table S3. The Mulliken (M) and Hirshfeld (H) partial charges (e^-) at different pressures along with the frontier molecular orbitals energies (eV).

Salt	0 GPa		20 GPa		50 GPa		100 GPa		Anion		Cation	
	M	H	M	H	M	H	M	H	E_{HOMO}	E_{LUMO}	E_{HOMO}	E_{LUMO}
1	0.621	0.210	0.595	0.170	0.565	0.170	0.525	0.180	-0.769	5.89	-39.53	-6.98
2	0.713	0.250	0.707	0.190	0.687	0.170	0.673	0.170	-0.860	4.81	-26.73	-6.00
3	0.714	0.200	0.681	0.194	0.663	0.200	0.651	0.205	3.820	4.79	-32.66	-11.98
4	0.610	0.193	0.600	0.173	0.640	0.160	0.720	0.149	9.031	11.42	-108.48	-32.58
5	0.731	0.195	0.684	0.166	0.651	0.146	0.609	0.130	5.791	9.00	-45.15	-14.24
6	0.793	0.288	0.822	0.262	0.852	0.259	0.877	0.260	5.912	10.34	-39.53	-6.98
7	0.890	0.181	0.920	0.139	0.960	0.120	1.000	0.106	3.606	8.33	-45.15	-14.24
8	0.950	0.270	0.970	0.262	0.987	0.257	1.010	0.263	5.791	9.00	-39.53	-6.98
9	0.750	0.283	0.705	0.240	0.710	0.238	0.740	0.243	3.685	8.11	-39.53	-6.98
10	1.062	0.190	1.218	0.150	1.373	0.128	1.510	0.113	5.791	9.00	-64.01	-6.93
11	0.750	0.220	0.705	0.120	0.710	0.107	0.740	0.100	1.523	6.38	-45.15	-14.24
12	1.062	0.290	1.217	0.260	1.373	0.257	1.397	0.270	4.891	8.89	-39.53	-6.98
13	1.230	0.260	1.721	0.250	1.979	0.249	2.310	0.241	-3.467	2.43	-39.53	-6.98
14	0.600	0.270	0.530	0.220	0.440	0.190	0.310	0.170	5.643	9.25	-28.28	-16.70
15	0.912	0.312	0.960	0.232	1.008	0.210	1.058	0.192	-1.204	4.42	-26.73	-6.00
16	0.861	0.600	0.686	0.510	0.510	0.419	0.286	0.296	-2.326	2.28	-13.18	-8.75
17	0.700	0.280	0.570	0.130	0.460	0.070	0.350	0.010	-0.769	5.89	-13.08	-7.86
18	0.792	0.383	0.733	0.188	0.690	0.100	0.600	0.000	-1.204	4.42	-13.08	-7.86
19	0.830	0.364	0.784	0.136	0.744	0.027	0.719	-0.085	-2.905	1.93	-13.08	-7.86
20	0.665	0.275	0.641	0.151	0.615	0.095	0.565	0.045	1.521	6.59	-22.46	-6.36
21	0.742	0.299	0.672	0.145	0.643	0.057	0.678	0.022	1.879	7.17	-14.16	-6.01
22	0.650	0.232	0.590	0.112	0.567	0.042	0.545	-0.005	1.879	7.17	-15.97	-6.38
23	0.773	0.343	0.725	0.163	0.690	0.080	0.688	0.010	-2.483	1.12	-22.46	-6.36
24	0.830	0.185	0.890	0.045	0.945	-0.005	1.005	-0.035	1.362	7.31	-39.53	-6.98
25	0.750	0.308	0.646	0.107	0.614	0.032	0.652	0.012	-1.204	4.42	-12.25	-6.46
26	0.820	0.125	0.830	0.021	0.835	-0.040	0.880	-0.085	1.645	7.08	-64.01	-6.93
27	0.730	0.310	0.660	0.115	0.635	0.040	0.725	0.005	-3.095	5.07	-22.46	-6.36
28	0.794	0.334	0.750	0.140	0.782	0.080	0.780	0.040	-3.095	5.07	-14.16	-6.01
29	0.800	0.343	0.737	0.136	0.743	0.043	0.763	0.003	-3.095	5.07	-12.02	-4.99
30	1.852	0.187	1.579	0.020	1.367	-0.023	1.100	-0.034	-3.095	5.07	-15.97	-6.38
31	0.675	0.270	0.620	0.115	0.655	0.070	0.645	0.015	1.362	7.31	-22.46	-6.36
32	0.836	0.134	0.820	0.024	0.816	-0.030	0.850	-0.070	1.362	7.31	-64.01	-6.93
33	0.794	0.165	0.817	0.045	0.862	-0.005	0.932	-0.035	1.645	7.08	-39.53	-6.98
34	0.910	0.216	0.996	0.116	1.056	0.056	1.120	0.024	1.362	7.31	-26.73	-6.00
35	0.940	0.234	1.010	0.124	1.090	0.066	1.160	0.016	1.362	7.31	-22.91	-5.50
36	0.819	0.420	0.689	0.221	0.560	0.130	0.411	0.041	-0.769	5.89	-12.59	-8.18
37	0.665	0.162	0.610	0.043	0.612	-0.006	0.591	-0.050	1.362	7.31	-32.66	-11.98
38	0.757	0.304	0.734	0.141	0.731	0.051	0.824	-0.001	-2.483	1.12	-12.77	-4.66
39	0.730	0.270	0.660	0.066	0.666	0.030	0.676	0.014	-4.350	-0.75	-26.73	-6.00
40	0.804	0.337	0.745	0.134	0.730	0.047	0.725	-0.032	0.970	4.98	-22.46	-6.36
41	0.730	0.265	0.695	0.130	0.650	0.075	0.635	0.025	1.645	7.08	-15.97	-6.38
42	0.860	0.310	0.791	0.014	0.744	-0.114	0.740	-0.210	-4.044	0.05	-16.45	-5.41
43	0.795	0.342	0.770	0.170	0.765	0.075	0.740	-0.008	-1.204	4.42	-12.02	-4.99
44	0.686	0.210	0.684	0.107	0.660	0.065	0.696	0.037	-0.716	4.20	-15.89	-13.76
45	0.810	0.355	0.703	0.120	0.657	-0.005	0.613	-0.085	-3.002	4.29	-22.46	-6.36
46	0.714	0.210	0.638	-0.042	0.604	-0.124	0.578	-0.204	-4.370	-0.01	-11.60	-5.23
47	0.743	0.283	0.681	0.091	0.614	0.003	0.768	0.000	1.052	4.29	-17.46	-10.76
48	0.780	0.294	0.747	0.070	0.727	-0.020	0.706	-0.114	1.168	5.52	-12.40	-4.33
49	0.790	0.334	0.720	0.166	0.720	0.108	0.682	0.018	1.168	5.52	-22.46	-6.36
50	0.803	0.361	0.759	0.134	0.755	0.041	0.755	-0.035	-1.244	3.24	-22.46	-6.36
51	0.807	0.319	0.737	0.062	0.784	-0.018	0.826	-0.080	-1.244	3.24	-13.39	-5.21
52	0.707	0.280	0.645	0.125	0.638	0.047	0.632	0.033	0.388	5.10	-15.97	-6.38
53	0.695	0.285	0.628	0.120	0.615	0.095	0.710	0.078	1.166	4.38	-11.67	-4.79
54	0.730	0.270	0.660	0.066	0.666	0.030	0.676	0.014	-0.502	4.35	-15.97	-6.38
55	0.845	0.325	1.414	0.304	1.395	0.180	1.340	0.035	-4.168	0.12	-12.09	-3.97

Table S3. Continue.

Salt	0 GPa		20 GPa		50 GPa		100 GPa		Anion		Cation	
	M	H	M	H	M	H	M	H	E_{HOMO}	E_{LUMO}	E_{HOMO}	E_{LUMO}
56	1.030	0.130	1.080	0.098	1.130	0.090	1.183	0.080	-0.04	6.12	-64.01	-6.93
57	0.700	0.320	0.730	0.230	0.820	0.220	1.120	0.303	-0.04	6.12	-17.08	-7.83
58	0.623	0.268	0.600	0.250	0.630	0.248	0.683	0.273	-0.04	6.12	-17.15	-10.66
59	0.700	0.257	0.568	0.078	0.468	-0.010	0.372	-0.080	-0.77	5.89	-22.46	-6.36
60	0.710	0.269	0.441	-0.079	0.511	-0.020	0.439	-0.079	-0.77	5.89	-17.12	-5.90
61	0.710	0.258	0.559	0.061	0.449	-0.041	0.331	-0.120	-0.77	5.89	-10.31	-5.66
62	0.711	0.269	0.570	0.020	0.469	-0.080	0.351	-0.160	-0.77	5.89	-14.73	-4.25
63	1.390	0.205	1.320	0.175	1.270	0.155	1.190	0.145	1.08	4.73	-45.15	-14.24
64	-0.020	0.060	-0.133	0.040	-0.287	0.020	-0.420	0.020	5.25	7.49	-28.09	-21.24
65	1.060	0.279	1.250	0.170	1.440	0.141	1.588	0.129	-0.50	4.35	-22.91	-5.50

Table S4. Decomposition equations applied for the calculations of the stored energy content (E_c).

Salt	Decomposition equation
1	$2NaCl = Na_2 + Cl_2$
2	$2KBr = K_2 + Br_2$
3	$BaTiO_3 = BaO + TiO_2$
4	$2AlPO_4 = Al_2O_3 + P_2O_5$
5	$CaCO_3 = CaO + CO_2$
6	$Na_3AlF_6 = 3NaF + AlF_3$
7	$CaSO_4 = CaO + SO_3$
8	$Na_2CO_3 = Na_2O + CO_2$
9	$Na_2C_2O_4 = Na_2O + CO_2 + CO$
10	$Li_2CO_3 = Li_2O + CO_2$
11	$C_4H_2O_6Ca + 4H_2O = CaO + 4CO + 5H_2O$
12	$2C_6H_5O_7Na_3 = 3Na_2O + 5H_2O + 6CO + 6C$
13	$8C_5H_{11}O_8SNa + 8H_2O = 8NaOH \cdot H_2O + 40H_2O + 8CO_2 + 32C + S_8$
14	$8PbS = 8Pb + S_8$
15	$4KNO_3 = 2N_2 + 2K_2O + 5O_2$
16	$16C_{13}H_{11}N_3O_5S = 24N_2 + 80H_2O + 8H_2S + S_8 + 208C$
17	$C_3H_7ClN_4O_6 + H_2O = 2N_2 + HCl + 4H_2O + 3CO$
18	$2C_3H_7N_5O_9 = 5N_2 + 7H_2O + CO + 5CO_2$
19	$4C_3H_7N_7O_{10} = 14N_2 + 14H_2O + 12CO_2 + O_2$
20	$C_2H_{14}N_{12}O_2 = N_2 + CH_4 + H_2 + H_2O$
21	$C_2H_{10}N_{12}O = 6N_2 + H_2O + 2CH_4$
22	$2C_2H_8N_{10}O_3 = 10N_2 + 6H_2O + CH_4 + 3C$
23	$C_3H_6N_6O_5 = 3N_2 + 3H_2O + 2CO + C$
24	$2C_2H_{10}N_8O_5Na_2 = 8N_2 + 4NaOH \cdot H_2O + 2H_2O + CH_4 + 3C$
25	$CH_6N_6O_5 = 3N_2 + 3H_2O + CO_2$
26	$C_2Li_2H_8N_8O_6 = 4N_2 + 2LiOH \cdot H_2O + CO + C + H_2O$
27	$H_4N_6 = 2H_2 + 3N_2$
28	$2H_5N_7 = 5H_2 + 7N_2$
29	$2C_2H_6N_{10} = 3CH_4 + C + 10N_2$
30	$H_4N_6O + 2H_2O = 3H_2O + H_2 + 3N_2$
31	$C_2H_8N_{10} = 2CH_4 + 5N_2$
32	$2C_2Li_2H_8N_8O_4 = 4H_3LiO_2 + CH_4 + 3C + 8N_2$
33	$C_2H_8N_8Na_2O_6 = 2H_3NaO_2 + H_2O + 4N_2 + CO + C$
34	$2C_2H_4K_2N_8O_2 = 4KOH + 8N_2 + CH_4 + 3C$
35	$2C_2H_4N_8O_2Rb_2 = 4RbOH + 8N_2 + CH_4 + 3C$
36	$C_6H_5ClN_2 = N_2 + HCl + CH_4 + 5C$
37	$2BaC_2H_{10}N_8O_5 + 10H_2O = 2BaO_{10}H_{18} + 8N_2 + CH_4 + 3C$
38	$2C_4H_9N_9O_5 = 9N_2 + 9H_2O + CO + 7C$
39	$C_6H_3KN_8O_9 = KOH + 4N_2 + H_2O + CO_2 + 5CO$
40	$C_2H_8N_6O_8 = 3N_2 + 4H_2O + 2CO_2$
41	$C_2H_8N_{10}O_4 = 5N_2 + 4H_2O + 2C$
42	$C_5H_8N_6O_6 = 3N_2 + 4H_2O + 2CO + 3C$

Table S4. Continue.

Salt	Decomposition equation
43	$C_2H_6N_6O_3 = 3N_2 + 3H_2O + 2C$
44	$C_2H_{14}N_{12}O_2 = 6N_2 + 2H_2O + 2CH_4 + H_2$
45	$2ClH_4NO_4 = N_2 + 4H_2O + Cl_2 + O_2$
46	$2C_9H_{10}N_{18}O_4 = 18N_2 + 8H_2O + CH_4 + 17C$
47	$2C_5H_{11}N_{11}O_7 = 11N_2 + 11H_2O + 3CO + 7C$
48	$2C_4H_{16}N_{16}O_5 = 16N_2 + 10H_2O + 3CH_4 + 5C$
49	$C_2H_8N_8O_5 = 4N_2 + 4H_2O + CO + C$
50	$C_6H_8N_{10}O_{11} = 5N_2 + 4H_2O + 5CO + CO_2$
51	$C_8H_{12}N_{14}O_{11} = 7N_2 + 6H_2O + 5CO + 3C$
52	$C_3H_8N_{10}O_5 = 5N_2 + 4H_2O + CO + 2C$
53	$C_4H_8N_{16}O_2 = 8N_2 + 2H_2O + CH_4 + 3C$
54	$C_2H_8N_{14}O_6 = 7N_2 + 4H_2O + 2CO$
55	$2C_4H_9N_{11}O_6 = 11N_2 + 9H_2O + 3CO + 5C$
56	$2LiN_3 = 2Li + 3N_2$
57	$2TlN_3 = 2Tl + 3N_2$
58	$2AgN_3 = 2Ag + 3N_2$
59	$2NH_4Cl = N_2 + 2HCl + 3H_2$
60	$2CH_6NCl = N_2 + 2HCl + 2CH_4 + H_2$
61	$4C_5H_8N_3Cl = 6N_2 + 4HCl + 7CH_4 + 13C$
62	$4C_4H_{14}OPCl = 4H_2O + 4HCl + 11CH_4 + 5C + 4P$
63	$C_2H_6O_2Ca = CaO + H_2O + CH_4 + C$
64	$4FeS_2 = 4Fe + S_8$
65	$C_2N_{12}O_4Rb_2 = 6N_2 + Rb_2O + CO_2 + CO$

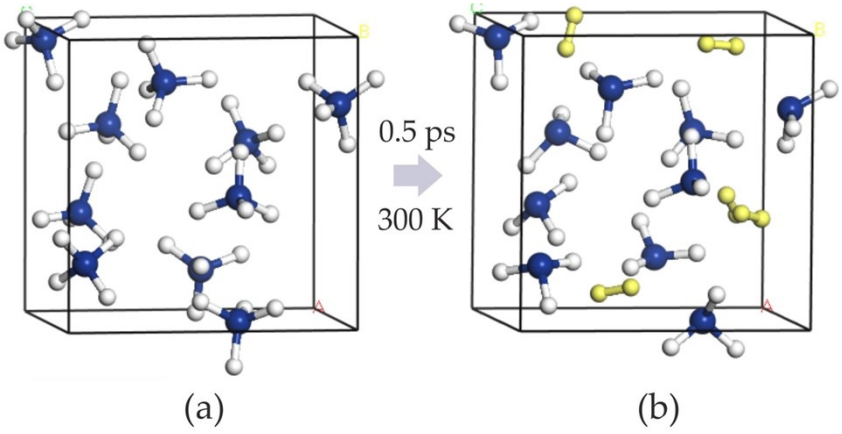
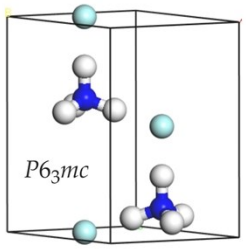
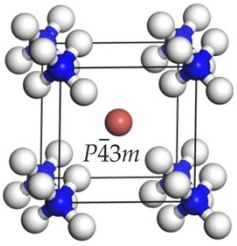


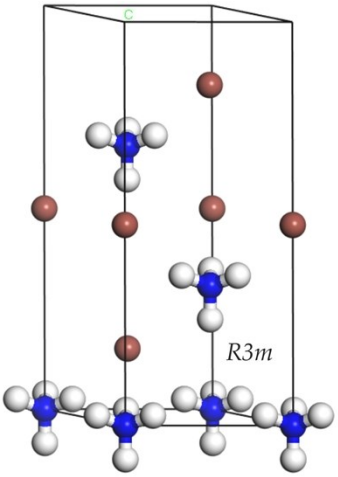
Fig. S3. NH_4• radicals before (a) and after (b) MD simulation at ambient conditions.



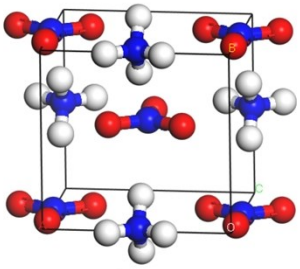
Crystal 66
Ammonium fluoride
a = 4.462 (4.439),
c = 7.113 (7.164)



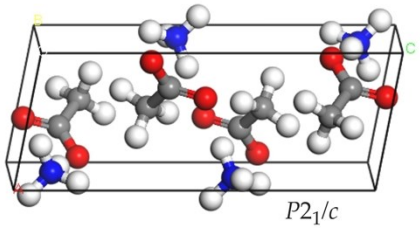
Crystal 67
Ammonium bromide
a = 4.055 (3.952)



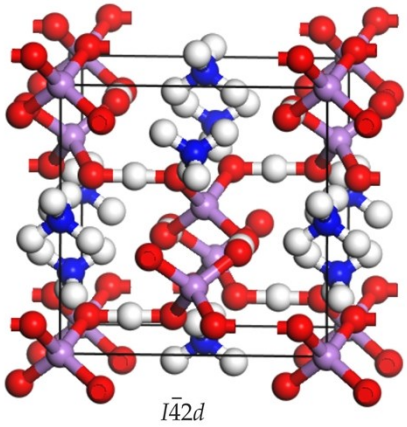
Crystal 68
Ammonium iodide
a = 5.091 (5.135),
c = 12.324 (12.577)



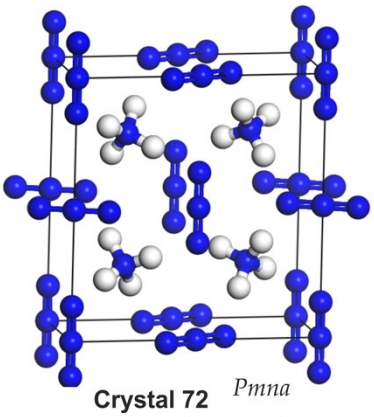
Crystal 69
Ammonium nitrate
a = 5.724 (5.651),
b = 5.455 (5.472)
c = 4.945 (4.883)



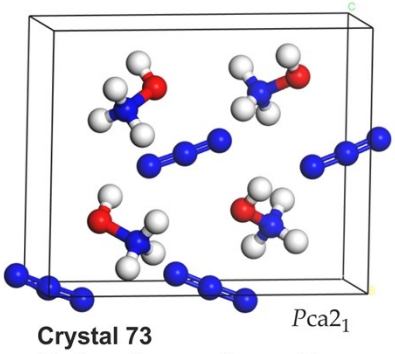
Crystal 70
Ammonium acetate
a = 4.723 (4.787), b = 7.599 (7.742)
c = 12.101 (7.164), β = 101.0 (100.8)



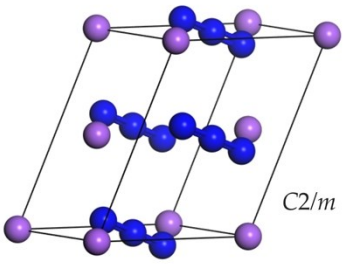
Crystal 71
Ammonium dihydrogenphosphate
a = 7.544 (7.700)
c = 7.627 (7.716)



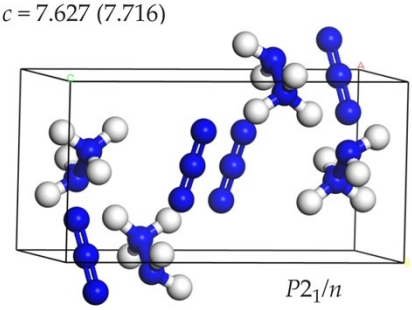
Crystal 72
Ammonium azide
a = 9.009 (8.933)
b = 3.722 (3.782)
c = 8.547 (8.652)



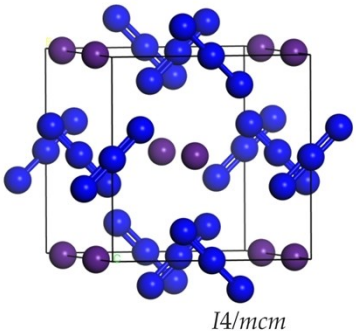
Crystal 73
Hydroxylammonium azide
a = 10.455, b = 3.711, c = 8.593



Crystal 74
α-Sodium azide
a = 6.371 (6.211), b = 3.648 (3.658),
c = 5.665 (5.323), β = 103.1 (108.4)



Crystal 75
Hydrazinium azide
a = 5.718 (5.641), b = 5.552 (5.521)
c = 10.958 (11.306), β = 93.9 (93.3)



Crystal 76
α-Cesium azide
a = 5.925 (6.541), c = 7.973 (8.091)

Cell parameters are given in angstroms and degrees

Fig. S4. Crystal structures along with the optimized and experimental (in parentheses) asymmetric cell parameters of salts **66**-**76**.

Table S5. Hirshfeld charges (e^-) of the cation in the NH_4X and XN_3 series at various pressures along with conceptual DFT parameters (eV) of the corresponding radicals (X•) obtained in terms of the adiabatic approximation.

Salt	X	0 GPa	20 GPa	50 GPa	100 GPa	I	A	η	χ	ω
66	F	0.260	0.172	0.110	0.080	17.78	3.51	14.27	10.65	3.97
67	Br	0.248	0.070	-0.033	-0.112	11.96	3.58	8.38	7.77	3.60
68	I	0.278	0.047	-0.057	-0.142	12.14	3.25	8.89	7.70	3.33
69	NO_3	0.370	0.176	0.070	-0.006	13.75	4.03	9.72	8.89	4.07
70	CH_3COO	0.306	0.220	0.174	0.116	11.41	3.15	8.26	7.28	3.21
71	H_2PO_4	0.330	0.140	0.014	-0.020	10.99	4.14	6.85	7.57	4.18
72	NH_4	0.280	0.133	0.053	-0.020	4.41	-1.27	5.68	1.57	0.22
73	NH_3OH	0.230	0.133	0.077	0.047	7.20	-3.76	10.96	1.72	0.13
74	Na	0.268	0.223	0.220	0.233	5.42	0.60	4.82	3.01	0.94
75	NH_3NH_2	0.310	0.173	0.090	0.047	7.20	-3.76	10.96	1.72	0.13
76	Cs	0.300	0.280	0.280	0.290	4.01	0.49	3.53	2.25	0.72

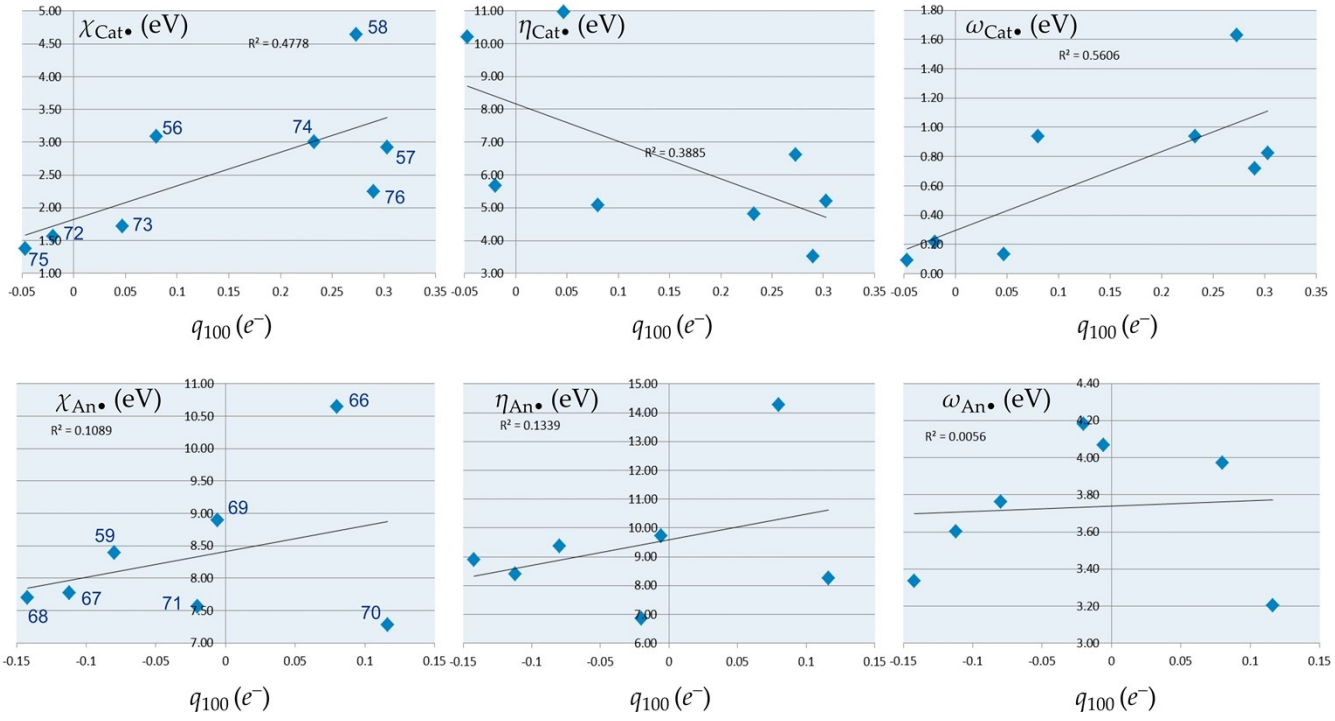


Fig. S5. Dependence of conceptual DFT parameters (χ, η and ω) on cationic charges at 100 GPa (q_{100}) for the NH_4X and XN_3 series salts.

Table S6. The frontier molecular orbital energies and conceptual DFT parameters (in eV) obtained in terms of the vertical approximation.

Salt	E_{HOMO}		E_{LUMO}		η		χ		ω	
	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•
1	-9.30	-3.51	-6.85	-1.77	-2.44	-1.74	8.08	2.64	-13.34	-2.01
2	-8.89	-2.90	-6.42	-1.60	-2.47	-1.30	7.66	2.25	-11.88	-1.95
3	-1.96	-8.28	0.04	-6.90	-2.00	-1.38	0.96	7.59	-0.23	-20.88
4	3.65	-25.37	5.78	-22.19	-2.13	-3.19	-4.71	23.78	-5.22	-88.76
5	-2.28	-9.87	1.11	-8.07	-3.39	-1.80	0.58	8.97	-0.05	-22.41
6	0.76	-3.51	3.61	-1.77	-2.85	-1.74	-2.19	2.64	-0.84	-2.01
7	-2.83	-9.87	-0.37	-8.07	-2.45	-1.80	1.60	8.97	-0.52	-22.41
8	-2.28	-3.51	1.11	-1.77	-3.39	-1.74	0.58	2.64	-0.05	-2.01
9	-2.46	-3.51	-0.37	-1.77	-2.09	-1.74	1.42	2.64	-0.48	-2.01
10	-2.28	-3.65	1.11	-1.51	-3.39	-2.14	0.58	2.58	-0.05	-1.55
11	-1.58	-9.87	0.96	-8.07	-2.55	-1.80	0.31	8.97	-0.02	-22.41
12	0.46	-3.51	1.38	-1.77	-0.92	-1.74	-0.92	2.64	-0.46	-2.01
13	-7.57	-3.51	-6.77	-1.77	-0.80	-1.74	7.17	2.64	-32.20	-2.01
14	0.33	-10.97	2.26	-9.54	-1.93	-1.43	-1.29	10.25	-0.43	-36.82
15	-10.50	-2.90	-6.97	-1.60	-3.53	-1.30	8.74	2.25	-10.80	-1.95
16	-7.67	-5.28	-6.26	-3.40	-1.41	-1.88	6.96	4.34	-17.15	-5.02
17	-9.30	-6.72	-6.85	-3.52	-2.44	-3.20	8.08	5.12	-13.34	-4.09
18	-10.50	-6.72	-6.97	-3.52	-3.53	-3.20	8.74	5.12	-10.80	-4.09
19	-9.71	-6.72	-6.04	-3.52	-3.67	-3.20	7.87	5.12	-8.45	-4.09
20	-3.03	-6.35	-0.93	-1.11	-2.10	-5.24	1.98	3.73	-0.93	-1.33
21	-3.49	-7.39	-1.37	-2.64	-2.12	-4.75	2.43	5.01	-1.39	-2.65
22	-3.49	-7.78	-1.37	-4.03	-2.12	-3.75	2.43	5.90	-1.39	-4.64
23	-7.57	-6.35	-5.35	-1.11	-2.22	-5.24	6.46	3.73	-9.38	-1.33
24	-3.21	-3.51	-1.44	-1.77	-1.77	-1.74	2.33	2.64	-1.53	-2.01
25	-10.50	-7.40	-6.97	-4.11	-3.53	-3.28	8.74	5.76	-10.80	-5.04
26	-2.81	-3.65	-1.31	-1.51	-1.50	-2.14	2.06	2.58	-1.41	-1.55
27	-7.99	-6.35	-5.43	-1.11	-2.56	-5.24	6.71	3.73	-8.80	-1.33
28	-7.99	-7.39	-5.43	-2.64	-2.56	-4.75	6.71	5.01	-8.80	-2.65
29	-7.99	-3.99	-5.43	-1.38	-2.56	-2.62	6.71	2.68	-8.80	-1.38
30	-7.99	-7.78	-5.43	-4.03	-2.56	-3.75	6.71	5.90	-8.80	-4.64
31	-3.21	-6.35	-1.44	-1.11	-1.77	-5.24	2.33	3.73	-1.53	-1.33
32	-3.21	-3.65	-1.44	-1.51	-1.77	-2.14	2.33	2.58	-1.53	-1.55
33	-2.81	-3.51	-1.31	-1.77	-1.50	-1.74	2.06	2.64	-1.41	-2.01
34	-3.21	-2.90	-1.44	-1.60	-1.77	-1.30	2.33	2.25	-1.53	-1.95
35	-3.21	-2.80	-1.44	-1.60	-1.77	-1.20	2.33	2.20	-1.53	-2.01
36	-9.30	-5.66	-6.85	-2.18	-2.44	-3.48	8.08	3.92	-13.34	-2.21
37	-3.21	-8.28	-1.44	-6.90	-1.77	-1.38	2.33	7.59	-1.53	-20.88
38	-7.57	-3.96	-5.35	-0.91	-2.22	-3.05	6.46	2.44	-9.38	-0.97
39	-8.68	-2.90	-6.89	-1.60	-1.79	-1.30	7.78	2.25	-16.97	-1.95
40	-3.00	-6.35	-1.21	-1.11	-1.79	-5.24	2.11	3.73	-1.24	-1.33
41	-2.81	-7.78	-1.31	-4.03	-1.50	-3.75	2.06	5.90	-1.41	-4.64
42	-9.23	-2.07	-7.07	-0.69	-2.15	-1.38	8.15	1.38	-15.43	-0.69
43	-10.50	-3.99	-6.97	-1.38	-3.53	-2.62	8.74	2.68	-10.80	-1.38
44	-3.16	-9.87	-2.50	-7.20	-0.66	-2.67	2.83	8.54	-6.08	-13.65
45	-10.18	-6.35	-7.25	-1.11	-2.93	-5.24	8.71	3.73	-12.95	-1.33
46	-7.21	-2.81	-4.24	-0.56	-2.97	-2.25	5.73	1.68	-5.52	-0.63
47	-3.40	-8.37	-1.37	-5.37	-2.03	-2.99	2.39	6.87	-1.40	-7.89
48	-3.06	-3.20	-0.89	-0.70	-2.17	-2.50	1.97	1.95	-0.90	-0.76
49	-3.06	-6.35	-0.89	-1.11	-2.17	-5.24	1.97	3.73	-0.90	-1.33
50	-3.87	-6.35	-3.34	-1.11	-0.52	-5.24	3.61	3.73	-12.40	-1.33
51	-3.87	-3.59	-3.34	-0.64	-0.52	-2.95	3.61	2.12	-12.40	-0.76
52	-3.64	-7.78	-1.84	-4.03	-1.81	-3.75	2.74	5.90	-2.08	-4.64
53	-3.53	-4.25	-1.59	-1.60	-1.94	-2.65	2.56	2.92	-1.69	-1.62
54	-3.96	-7.78	-3.00	-4.03	-0.96	-3.75	3.48	5.90	-6.34	-4.64
55	-9.88	-3.43	-7.45	-0.87	-2.42	-2.55	8.66	2.15	-15.48	-0.90
56	-8.49	-3.65	-5.50	-1.51	-2.99	-2.14	6.99	2.58	-8.17	-1.55
57	-8.49	-3.25	-5.50	-2.03	-2.99	-1.22	6.99	2.64	-8.17	-2.86

Table S6. Continue.

Salt	E_{HOMO}		E_{LUMO}		η		χ		ω	
	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•
58	-8.49	-5.33	-5.50	-3.46	-2.99	-1.87	6.99	4.39	-8.17	-5.16
59	-9.30	-6.35	-6.85	-1.11	-2.44	-5.24	8.08	3.73	-13.34	-1.33
60	-9.30	-2.37	-6.85	-0.98	-2.44	-1.39	8.08	1.68	-13.34	-1.01
61	-9.30	-2.97	-6.85	-0.73	-2.44	-2.24	8.08	1.85	-13.34	-0.77
62	-9.30	-1.85	-6.85	-1.02	-2.44	-0.83	8.08	1.44	-13.34	-1.24
63	-7.52	-9.87	-4.10	-8.07	-3.42	-1.80	5.81	8.97	-4.93	-22.41
64	0.40	-13.48	1.95	-11.64	-1.55	-1.83	-1.17	12.56	-0.44	-43.03
65	-3.96	-2.80	-3.00	-1.60	-0.96	-1.20	3.48	2.20	-6.34	-2.01

Table S7. The frontier molecular orbital energies and conceptual DFT parameters (in eV) obtained in terms of the adiabatic approximation.

Salt	E_{HOMO}		E_{LUMO}		η		χ		ω	
	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•
1	13.07	5.41	3.71	0.60	9.36	4.81	8.39	3.00	3.76	0.94
2	11.96	4.50	3.58	0.52	8.38	3.98	7.77	2.51	3.60	0.79
3	3.58	10.14	-1.91	5.22	5.49	4.91	0.84	7.68	0.06	6.00
4	-1.39	28.96	-7.37	18.93	5.99	10.03	-4.38	23.95	1.60	28.59
5	5.12	12.09	-3.54	6.15	8.65	5.94	0.79	9.12	0.04	7.00
6	0.57	5.41	-4.64	0.60	5.21	4.81	-2.04	3.00	0.40	0.94
7	5.27	12.09	-1.52	6.15	6.80	5.94	1.88	9.12	0.26	7.00
8	5.12	5.41	-3.54	0.60	8.65	4.81	0.79	3.00	0.04	0.94
9	0.32	5.41	-2.41	0.60	2.73	4.81	-1.05	3.00	0.20	0.94
10	5.12	5.62	-3.54	0.55	8.65	5.07	0.79	3.08	0.04	0.94
11	1.25	12.09	-0.57	6.15	1.82	5.94	0.34	9.12	0.03	7.00
12	-2.12	5.41	-4.06	0.60	1.94	4.81	-3.09	3.00	2.46	0.94
13	6.93	5.41	5.28	0.60	1.66	4.81	6.11	3.00	11.26	0.94
14	2.20	13.83	-4.04	7.01	6.23	6.82	-0.92	10.42	0.07	7.96
15	13.75	4.50	4.03	0.52	9.72	3.98	8.89	2.51	4.07	0.79
16	8.31	7.01	4.33	1.79	3.98	5.22	6.32	4.40	5.02	1.86
17	13.07	7.05	3.71	4.26	9.36	2.80	8.39	5.66	3.76	5.72
18	13.75	7.05	4.03	4.26	9.72	2.80	8.89	5.66	4.07	5.72
19	11.68	7.05	4.66	4.26	7.03	2.80	8.17	5.66	4.75	5.72
20	4.58	4.40	-0.33	-1.27	4.91	5.68	2.12	1.57	0.46	0.22
21	5.09	6.45	-0.25	-3.71	5.34	10.16	2.42	1.37	0.55	0.09
22	5.09	7.20	-0.25	-3.76	5.34	10.96	2.42	1.72	0.55	0.13
23	9.22	4.40	3.89	-1.27	5.33	5.68	6.55	1.57	4.03	0.22
24	4.62	5.41	-0.08	0.60	4.70	4.81	2.27	3.00	0.55	0.94
25	13.75	6.54	4.03	3.75	9.72	2.79	8.89	5.14	4.07	4.74
26	5.25	5.62	-0.15	0.55	5.40	5.07	2.55	3.08	0.60	0.94
27	10.55	4.40	2.39	-1.27	8.16	5.68	6.47	1.57	2.56	0.22
28	10.55	6.45	2.39	-3.71	8.16	10.16	6.47	1.37	2.56	0.09
29	10.55	4.41	2.39	0.28	8.16	4.14	6.47	2.35	2.56	0.67
30	10.55	7.20	2.39	-3.76	8.16	10.96	6.47	1.72	2.56	0.13
31	4.62	4.40	-0.08	-1.27	4.70	5.68	2.27	1.57	0.55	0.22
32	4.62	5.62	-0.08	0.55	4.70	5.07	2.27	3.08	0.55	0.94
33	5.25	5.41	-0.15	0.60	5.40	4.81	2.55	3.00	0.60	0.94
34	4.62	4.50	-0.08	0.52	4.70	3.98	2.27	2.51	0.55	0.79
35	4.62	4.34	-0.08	0.49	4.70	3.85	2.27	2.41	0.55	0.76
36	13.07	6.78	3.71	1.10	9.36	5.68	8.39	3.94	3.76	1.37
37	4.62	10.14	-0.08	5.22	4.70	4.91	2.27	7.68	0.55	6.00
38	9.22	3.94	3.89	0.17	5.33	3.77	6.55	2.06	4.03	0.56
39	10.04	4.50	5.60	0.52	4.45	3.98	7.82	2.51	6.88	0.79
40	4.20	4.40	0.09	-1.27	4.11	5.68	2.14	1.57	0.56	0.22
41	5.25	7.20	-0.15	-3.76	5.40	10.96	2.55	1.72	0.60	0.13
42	10.80	3.75	5.59	-0.75	5.20	4.51	8.20	1.50	6.46	0.25
43	13.75	4.41	4.03	0.28	9.72	4.14	8.89	2.35	4.07	0.67
44	5.50	-2.24	1.84	7.80	3.66	-10.03	3.67	2.78	1.84	-0.38

Table S7. Continue.

Salt	E_{HOMO}		E_{LUMO}		η		χ		ω	
	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•	An•	Cat•
45	12.34	4.40	5.29	-1.27	7.05	5.68	8.82	1.57	5.52	0.22
46	8.18	4.00	5.54	0.31	2.64	3.69	6.86	2.16	8.92	0.63
47	4.70	9.22	0.17	4.54	4.53	4.68	2.44	6.88	0.66	5.06
48	4.76	3.72	0.26	-0.41	4.50	4.12	2.51	1.65	0.70	0.33
49	4.76	4.40	0.26	-1.27	4.50	5.68	2.51	1.57	0.70	0.22
50	5.92	4.40	2.31	-1.27	3.61	5.68	4.12	1.57	2.35	0.22
51	5.92	4.25	2.31	-0.44	3.61	4.70	4.12	1.90	2.35	0.39
52	5.38	7.20	0.71	-3.76	4.66	10.96	3.04	1.72	0.99	0.13
53	4.81	4.25	0.21	0.54	4.60	3.71	2.51	2.40	0.69	0.77
54	6.10	7.20	1.80	-3.76	4.30	10.96	3.95	1.72	1.81	0.13
55	11.55	3.71	5.89	-0.10	5.65	3.81	8.72	1.80	6.72	0.43
56	12.78	5.62	2.71	0.55	10.06	5.07	7.75	3.08	2.98	0.94
57	12.78	5.51	2.71	0.35	10.06	5.16	7.75	2.93	2.98	0.83
58	12.78	7.95	2.71	1.32	10.06	6.63	7.75	4.64	2.98	1.62
59	13.07	4.40	3.71	-1.27	9.36	5.68	8.39	1.57	3.76	0.22
60	13.07	4.14	3.71	-0.55	9.36	4.69	8.39	1.79	3.76	0.34
61	13.07	4.37	3.71	-0.67	9.36	5.04	8.39	1.85	3.76	0.34
62	13.07	3.05	3.71	-0.10	9.36	3.16	8.39	1.47	3.76	0.34
63	7.36	12.09	1.42	6.15	5.94	5.94	4.39	9.12	1.62	7.00
64	1.78	16.49	-3.67	7.44	5.45	9.05	-0.95	11.96	0.08	7.91
65	6.10	4.34	1.80	0.49	4.30	3.85	3.95	2.41	1.81	0.76

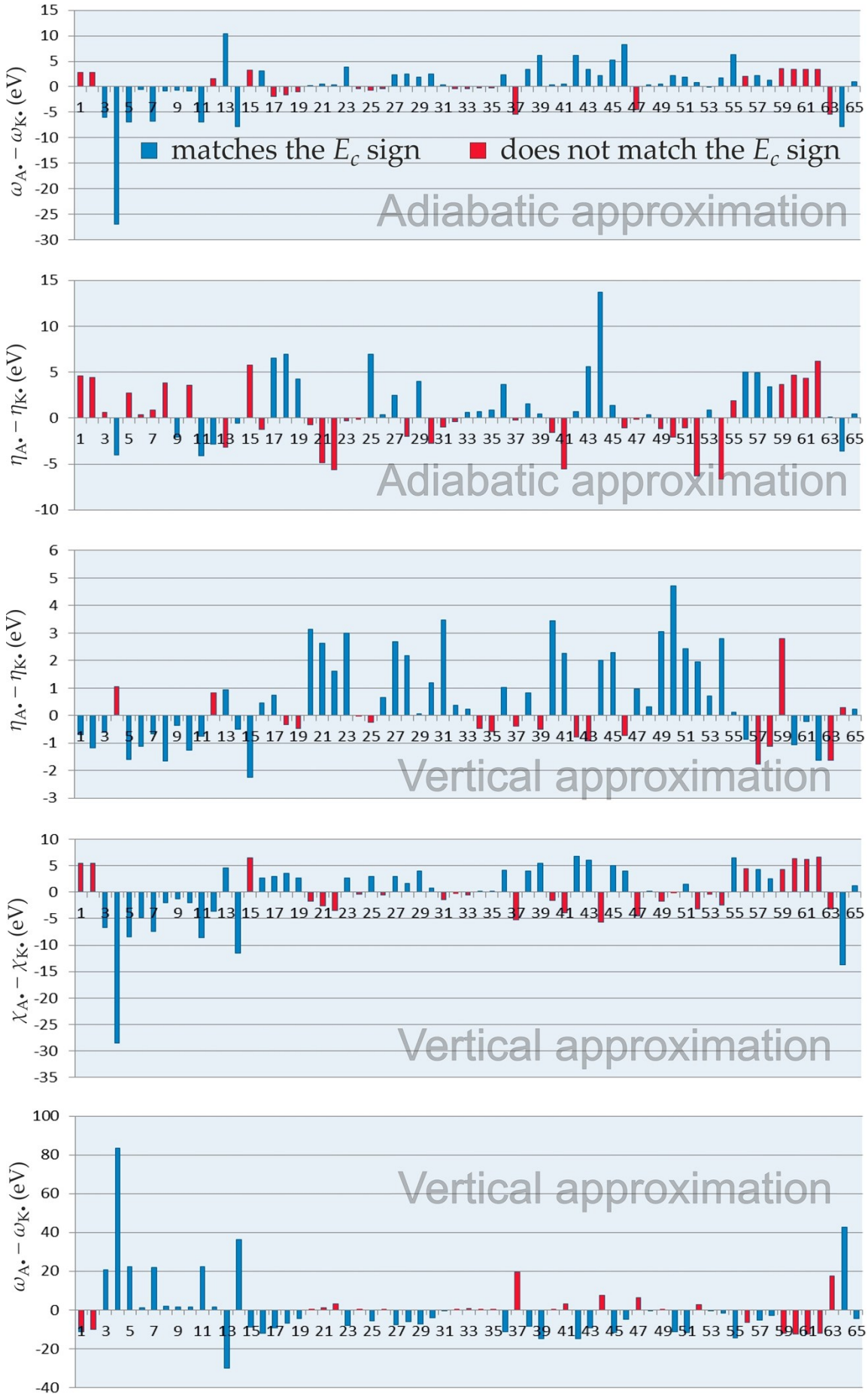


Fig. S6. Efficiency of various conceptual DFT parameters in distinguishing of compounds with the positive and negative energy content.