Significance of crystal habit sphericity in determination of impact sensitivity of bistetrazole-based energetic salts

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SUPPORTING INFORMATION

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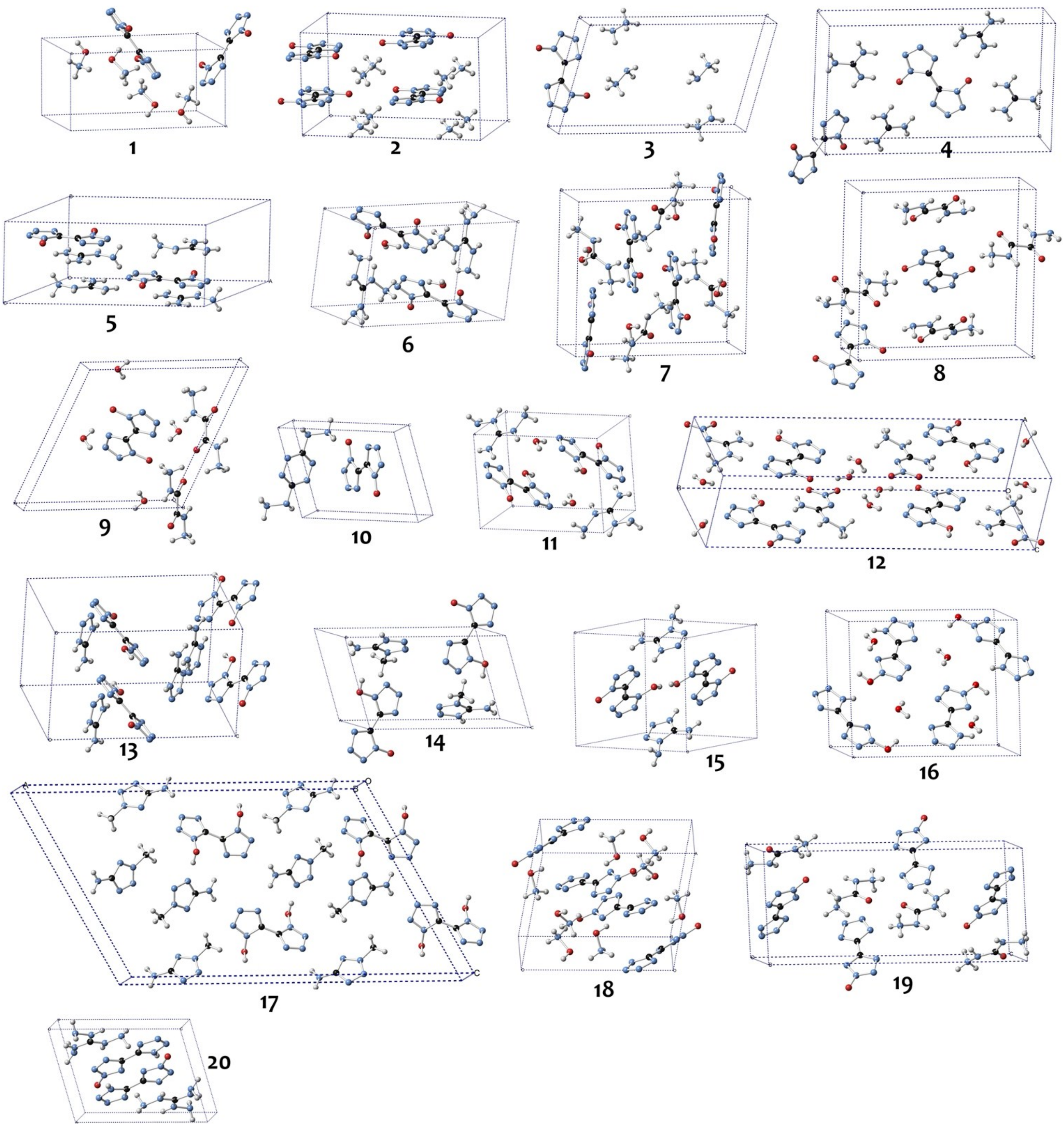

Fig. S1. Crystal packing of the studied energetic salts.

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

Salt	Space group	*a* (Å)	*b* (Å)	*c* (Å)	*α* (º)	*β* (º)	*γ* (º)	Ref
1	$P2_1/c$	5.527 (5.426)	11.523 (11.660)	6.480 (6.501)		96.10 (95.26)		[24]
2	$I222$	7.001 (7.527)	8.850 (7.531)	12.684 (13.291)				[39]
3	$P\overline{1}$	3.601 (3.660)	8.696 (8.670)	14.810 (14.711)	101.60 (101.10)	94.80 (94.95)	97.35 (97.74)	[39]
4	$P2_1/c$	3.567 (3.605)	17.211 (17.123)	9.532 (9.548)		98.52 (97.73)		[39]
5	$C2/m$	15.007 (14.724)	6.047 (6.182)	8.517 (8.702)		121.72 (123.28)		[39]
6	$P\overline{1}$	7.050 (7.117)	8.087 (8.090)	10.629 (10.544)	100.15 (100.36)	101.60 (102.07)	105.31 (105.13)	[39]
7	$P2_1/c$	7.027 (6.994)	12.764 (12.7121)	11.636 (11.5676)		94.40 (93.51)		[39]
8	$P2_1/c$	4.554 (4.554)	12.302 (12.424)	12.964 (12.943)		93.64 (93.77)		[39]
9	$P2_1/c$	11.439 (11.712)	4.781 (4.760)	11.320 (11.367)		113.66 (115.65)		[39]
10	$P\overline{1}$	4.824 (4.845)	6.794 (6.786)	9.465 (9.392)	75.69 (75.12)	76.37 (76.63)	89.00 (88.73)	[39]
11	$P\overline{1}$	7.424 (7.405)	7.875 (7.926)	9.550 (9.475)	93.931 (93.64)	90.18 (90.44)	106.50 (106.27)	[39]
12	$P2_1/n$	6.224 (6.275)	26.243 (26.188)	7.465 (7.408)		93.94 (93.55)		[39]
13	$C2/c$	7.446 (7.425)	9.197 (9.175)	13.760 (13.687)		99.12 (98.79)		[39]
14	$P\overline{1}$	6.282 (6.291)	7.409 (7.396)	11.858 (11.878)	106.79 (107.43)	99.98 (99.93)	98.77 (98.49)	[39]
15	$P\overline{1}$	7.519 (7.449)	8.576 (8.402)	8.497 (8.651)	93.03 (91.72)	114.52 (114.59)	92.70 (92.70)	[39]
16	$C2/c$	27.212 (27.041)	3.737 (3.763)	16.766 (16.874)		117.49 (117.62)		[39]
17	$P2_1/c$	4.911 (4.900)	13.067 (13.081)	9.964 (9.893)		102.27 (102.07)		[40]
18	$P2_1/n$	9.137 (9.046)	8.485 (8.459)	11.046 (11.096)		99.39 (99.37)		[40]
19	$P2_1/n$	8.347 (8.438)	5.543 (5.440)	19.805 (19.786)		92.86 (93.38)		[40]
20	$P\overline{1}$	7.293 (7.322)	7.426 (7.363)	9.850 (9.819)	84.59 (85.38)	75.04 (74.16)	84.81 (84.56)	[40]

Table S2. The asymmetric cell volumes, relative errors of their estimation, experimental friction sensitivity, energies of the frontier crystal orbitals and oxygen balance.

Salt	V_{exper} (Å^3)	V_{calcd} (Å^3)	δ (%)	FS (N)	E_{HOCO} (eV)	E_{LUCO} (eV)	OB (%)
1	410.36	409.57	0.85	120[a]	-6.200	-2.602	-27.1
2	785.53	753.41	0.61	360[b]	-5.848	-2.742	-47.0
3	447.78	450.88	-0.10	252[b]	-5.387	-2.573	-47.8
4	579.06	584.03	-1.42	360[b]	-5.653	-2.22	-66.6
5	658.15	662.2	0.94	324[b]	-5.703	-2.404	-65.4
6	555.7	555.15	0.75	120[b]	-5.935	-2.769	-49.3
7	1041.07	1026.53	-0.50	240[b]	-6.088	-2.767	-40.3
8	723.84	730.72	-0.26	360[b]	-6.145	-3.171	-51.2
9	566.99	571.26	-0.11	288[b]	-6.062	-3.159	-41.8
10	291.58	290.12	-1.05	80[b]	-5.699	-4.269	-51.2
11	533.99	532.58	-0.13	168[b]	-6.317	-3.025	-49.1
12	1216.32	1215.02	-1.18	192[b]	-6.212	-3.214	-27.1
13	931.19	921.47	0.49	72[b]	-6.118	-2.916	-40.8
14	508.25	507.59	-0.72	240[b]	-6.192	-3.010	-56.5
15	496.85	491.06	-0.98	160[b]	-6.054	-2.859	-41.5
16	1513.94	1521.38	-0.95	360[b]	-6.098	-2.678	-117.9
17	624.57	620.1	-1.14	30[c]	-6.658	-2.988	-37.2
18	845.98	837.74	0.85	160[c]	-6.086	-2.384	-36.3
19	915.25	906.65	0.61	240[c]	-5.995	-2.293	-52.4
20	511.92	506.13	-0.10	240[c]	-6.088	-2.954	-62.0

[a] Ref. 24, [b] Ref. 39, [c] Ref. 40.

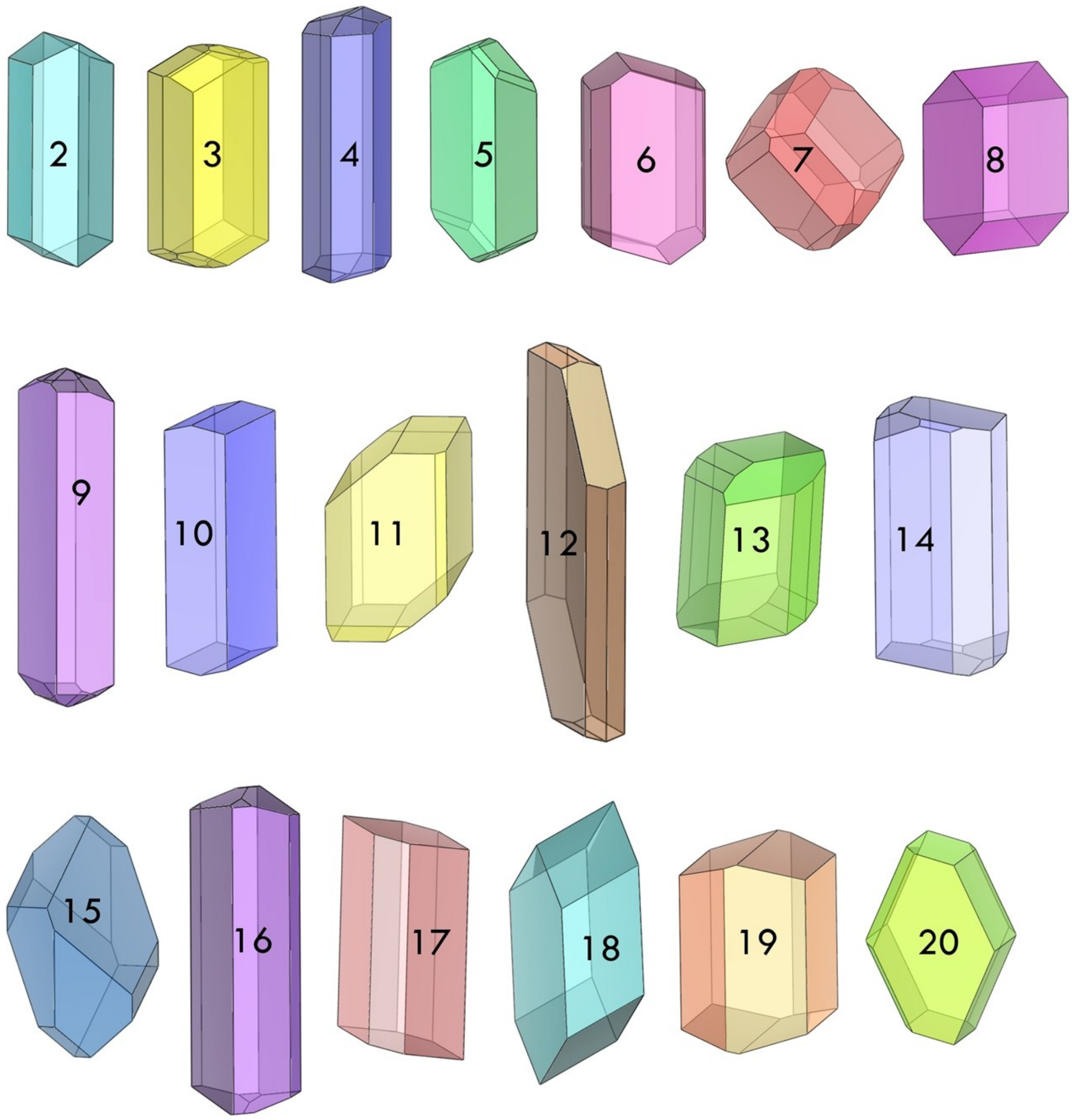

Fig. S2. The predicted crystal habits of salts **2-20**.

Table S3. The selected crystal habit properties for salts 2-20.

Salt 2	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 2)	2	-21.18	1.00	37.19
	(0 1 1)	4	-33.70	1.59	38.37
	(1 0 1)	4	-49.92	2.36	24.44
Salt 3	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-17.84	1.00	47.30
	(0 1 0)	2	-30.13	1.69	16.26
	(0 1 -1)	2	-28.79	1.61	16.12
	(1 0 0)	2	-60.64	3.40	2.41
	(1 0 -1)	2	-61.01	3.42	0.25
	(1 -1 -1)	2	-57.60	3.23	5.66
	(1 -1 1)	2	-57.88	3.24	0.54
	(1 -1 -2)	2	-57.34	3.21	0.14
	(1 1 -1)	2	-59.68	3.35	0.23
	(1 -1 2)	2	-54.16	3.04	4.70
	(1 1 -2)	2	-56.21	3.15	0.86
	(1 1 -3)	2	-52.87	2.96	3.65
	(1 2 -2)	2	-53.69	3.01	1.89
Salt 4	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 2 0)	2	-35.43	1.00	33.33
	(0 1 1)	4	-39.96	1.13	51.57
	(1 0 0)	2	-122.61	3.46	0.82
	(1 1 0)	4	-120.59	3.40	7.94
	(1 1 1)	4	-111.06	3.13	6.34
Salt 5	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-44.81	2.96	18.71
	(2 0 -1)	2	-15.13	1.00	65.14
	(1 1 0)	4	-75.79	5.01	11.52
	(1 1 -1)	4	-75.79	5.01	2.42
	(1 1 1)	4	-75.79	5.01	2.21
Salt 6	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-13.77	1.00	45.57
	(0 1 0)	2	-22.65	1.64	17.82
	(0 1 -1)	2	-24.43	1.77	9.87
	(1 0 0)	2	-32.53	2.36	15.56
	(1 -1 0)	2	-35.68	2.59	8.19
	(0 1 1)	2	-22.76	1.65	2.48
	(1 0 1)	2	-30.75	2.23	0.52
Salt 7	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 1 1)	4	-38.45	1.43	36.07
	(1 0 0)	2	-26.97	1.00	26.05
	(0 2 0)	2	-49.35	1.83	3.94
	(1 1 0)	4	-39.02	1.45	4.71
	(0 0 2)	2	-45.90	1.70	4.58
	(1 1 -1)	4	-34.85	1.29	22.15
	(1 1 1)	4	-42.58	1.58	2.37
	(1 0 2)	2	-50.21	1.86	0.14
Salt 8	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 1 1)	4	-28.68	1.85	35.76
	(0 0 2)	2	-15.52	1.00	41.30
	(1 0 0)	2	-36.34	2.34	22.93

Table S3. Continued.

Salt 9	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(1 0 0)	2	-11.81	1.00	55.41
	(0 0 2)	2	-18.48	1.56	34.44
	(1 1 0)	4	-71.48	6.05	2.43
	(0 1 1)	4	-71.48	6.05	3.87
	(1 1 -1)	4	-71.48	6.05	3.86
Salt 10	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-6.59	1.00	54.50
	(0 1 1)	2	-11.19	1.70	33.04
	(1 0 1)	2	-30.13	4.57	6.98
	(1 0 0)	2	-31.06	4.71	5.48
Salt 11	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 1 0)	2	-20.20	1.00	32.85
	(0 0 1)	2	-20.53	1.02	30.15
	(1 0 1)	2	-23.63	1.17	19.37
	(0 1 -1)	2	-27.57	1.36	3.24
	(1 0 0)	2	-31.60	1.56	10.16
	(1 -1 0)	2	-36.46	1.80	4.24
Salt 12	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 2 0)	2	-7.06	1.00	74.70
	(0 1 1)	4	-61.83	8.76	5.64
	(0 2 1)	4	-34.96	4.95	12.93
	(1 1 0)	2	-44.82	6.35	6.73
Salt 13	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	*Rhkl*	S_{rel} (%)
	(0 0 2)	2	-33.00	1.00	38.63
	(1 1 2)	4	-48.88	1.48	9.93
	(1 1 1)	4	-50.95	1.54	11.28
	(1 1 0)	4	-53.03	1.61	34.10
	(0 2 0)	2	-68.91	2.09	6.06
Salt 14	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-21.55	1.00	38.45
	(0 1 -2)	2	-24.11	1.12	16.47
	(0 1 -1)	2	-27.49	1.28	24.15
	(1 0 0)	2	-48.24	2.24	15.97
	(1 0 -1)	2	-54.12	2.51	3.19
	(1 -1 1)	2	-54.48	2.53	0.47
	(1 -1 0)	2	-60.83	2.82	1.31
Salt 15	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-21.21	1.00	31.67
	(1 -1 -1)	2	-22.78	1.07	22.83
	(0 1 0)	2	-27.64	1.30	21.59
	(0 1 1)	2	-28.23	1.33	4.58
	(1 0 0)	2	-30.43	1.43	14.89
	(1 0 -1)	2	-35.92	1.69	4.44
Salt 16	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(2 0 0)	2	-76.58	1.00	42.55
	(2 0 -2)	2	-87.87	1.15	33.68
	(0 0 2)	2	-104.82	1.37	10.52
	(1 1 1)	4	-296.08	3.87	12.23
	(1 1 -1)	4	-316.97	4.14	1.02

Table S3. Continued.

Salt 17	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 1 1)	4	-41.43	1.00	64.15
	(0 2 0)	2	-49.94	1.21	15.07
	(1 0 0)	2	-82.07	1.98	20.78
Salt 18	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(1 0 -1)	2	-13.64	1.00	56.36
	(0 0 2)	2	-33.47	2.45	13.86
	(0 1 1)	4	-36.04	2.64	29.78
Salt 19	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 2)	2	-62.10	1.00	30.42
	(1 0 -1)	2	-76.24	1.23	22.57
	(1 0 1)	2	-81.97	1.32	15.63
	(0 1 1)	4	-89.62	1.44	31.38
Salt 20	(*hkl*)	Multiplicity	E_{att} (kJ mol^{-1})	R_{hkl}	S_{rel} (%)
	(0 0 1)	2	-19.02	1.00	38.24
	(1 1 0)	2	-23.54	1.24	19.99
	(1 0 0)	2	-25.14	1.32	20.90
	(1 1 1)	2	-30.27	1.59	3.62
	(1 0 1)	2	-31.87	1.68	4.93
	(0 1 0)	2	-36.38	1.91	12.33

Table S4. Decomposition schemes for the studied energetic salts according to the H_2O–CO_2 arbitrary.

Salt	The H_2O–CO_2 arbitrary equation
1	$C_2H_8N_{10}O_4 = 2C + 4H_2O + 5N_2$
2	$C_2H_8N_{10}O_2 = C + CH_4 + 2H_2O + 5N_2$
3	$2C_2H_{10}N_{12}O_2 = C + 3CH_4 + 4H_2O + 12N_2$
4	$C_4H_{12}N_{14}O_2 = 2C + 2CH_4 + 2H_2O + 7N_2$
5	$2C_4H_{14}N_{16}O_2 = 3C + 5CH_4 + 4H_2O + 16N_2$
6	$2C_3H_{12}N_{14}O_3 = 3C + 3CH_4 + 6H_2O + 14N_2$
7	$2C_3H_{10}N_{12}O_4 = 5C + CH_4 + 8H_2O + 12N_2$
8	$2C_6H_{14}N_{16}O_6 = 11C + CH_4 + 12H_2O + 16N_2$
9	$C_4H_{12}N_{12}O_6 = 4C + 6H_2O + 6N_2$
10	$C_4H_8N_{16}O_2 = 3C + CH_4 + 2H_2O + 8N_2$
11	$4C_3H_{11}N_{13}O_3 = 7C + 5CH_4 + 12H_2O + 26N_2$
12	$4C_3H_{11}N_{13}O_6 = 11C + CO_2 + 22H_2O + 26N_2$
13	$4C_3H_5N_{13}O_2 = 11C + CH_4 + 8H_2O + 26N_2$
14	$4C_4H_7N_{13}O_2 = 13C + 3CH_4 + 8H_2O + 26N_2$
15	$2C_3H_6N_{14}O_2 = 5C + CH_4 + 4H_2O + 14N_2$
16	$C_6H_{12}N_{18}O_2 = 4C + 2CH_4 + 2H_2O + 9N_2$
17	$C_2H_4N_8O_2 = 2C + 2H_2O + 4N_2$
18	$2C_2H_8N_{10}O_3 = 3C + CH_4 + 6H_2O + 10N_2$
19	$C_3H_8N_{12}O_2 = 2C + CH_4 + 2H_2O + 6N_2$
20	$C_3H_{10}N_{14}O = C + 2CH_4 + H_2O + 7N_2$

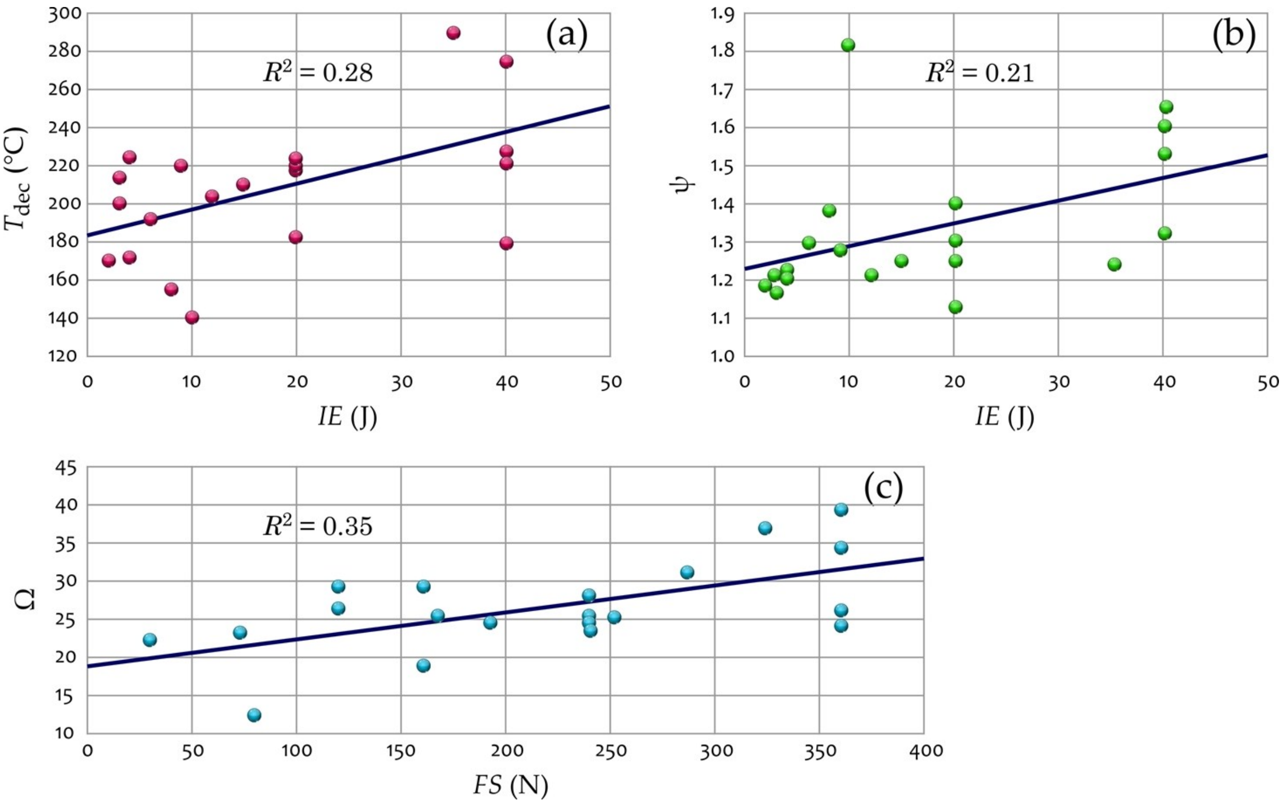

Fig. S3. Separate correlation of decomposition temperature (a), crystal habit sphericity (b) with impact sensitivity and function Ω with friction sensitivity (c).