Electronic Supplementary Material (ESI) for New Journal of Chemistry.

A UNIFIED MODEL OF IMPACT SENSITIVITY OF METAL AZIDES

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New Journal of Chemistry

SUPPORTING INFORMATION

LIST OF SUPPLEMENTARY FIGURES AND TABLES:

Table S1. The experimental and calculated (GGA/NCP/PBE-Grimme) volumes of asymmetric cells (V, Å^3) and the corresponding relative errors (δ, %)

Azide	V_{exper}	V_{calcd}	δ
$Cu(N_3)_2$	376.3	364.95	-3.11
CuN_3	418.26	402.33	-3.96
$Pb(N_3)_2$	1218.51	1193.07	-2.13
$Hg_2(N_3)_2$	261.55	258.77	-1.07
$Hg(N_3)_2$	421.1	415.49	-1.35
$Ba(N_3)_2$	224.89	217.5	-3.40
$Sr(N_3)_2$	824.3	841.08	2.00
$Ca(N_3)_2$	743.13	759.16	2.11
AgN_3	199.55	210.06	5.00
TlN_3	283.46	285.34	0.66
CsN_3	346.17	329.75	-4.98
RbN_3	299.38	293.05	-2.16
KN_3	265.09	262.27	-1.08
NaN_3	114.76	115.17	0.36
LiN_3	88.73	86.57	-2.50

Table S2. The calculated asymmetric cell parameters for several metal azides and relative errors of the cell volumes estimation

Azide	a (Å)	b (Å)	c (Å)	β (°)	V_{cell} (Å^3)	δ (%)
LiN_3	5.651[a]	3.268	5.672	123.2	87.65	-1.23
	(5.626)[b]	(3.317)	(5.035)	(106.7)	(90.00)	(1.41)
	5.848[c]	*3.327*	*6.031*	*126.9*	*93.84*	*5.45*
NaN_3	6.346	3.652	5.614	112.7	120.03	4.39
	(6.218)	(3.660)	(5.413)	(107.9)	(117.23)	(2.11)
	6.489	*3.741*	*5.611*	*113.5*	*124.91*	*8.13*
KN_3	6.096		6.995		259.94	-1.98
	(6.154)		(7.063)		(267.49)	(0.90)
	6.191		*7.198*		*275.89*	*3.91*
CuN_3	8.108		5.870		385.89	-8.39
	(8.734)		(5.852)		(446.41)	(6.31)
	9.775		*5.842*		*558.21*	*25.07*
TlN_3	6.162		7.727		293.40	3.39
	(6.286)		(7.348)		(290.35)	(2.37)
	6.381		*7.434*		*302.69*	*6.35*
AgN_3	5.400	6.176	6.302		210.17	5.05
	(5.654)	(5.981)	(5.971)		(201.92)	(1.17)
	5.353	*6.980*	*6.567*		*245.37*	*18.67*

[a]Calculated in this work using GGA/USP/PBE-Grimme 540 eV approach.
[b]Calculated by Zhu *et al*. [46, 48] using GGA/USP/PW91 500 eV approach.
[c]Calculated in this work using GGA/USP/PW91 500 eV approach.

The PW91 functional is described in the following paper: J. P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244-13249.

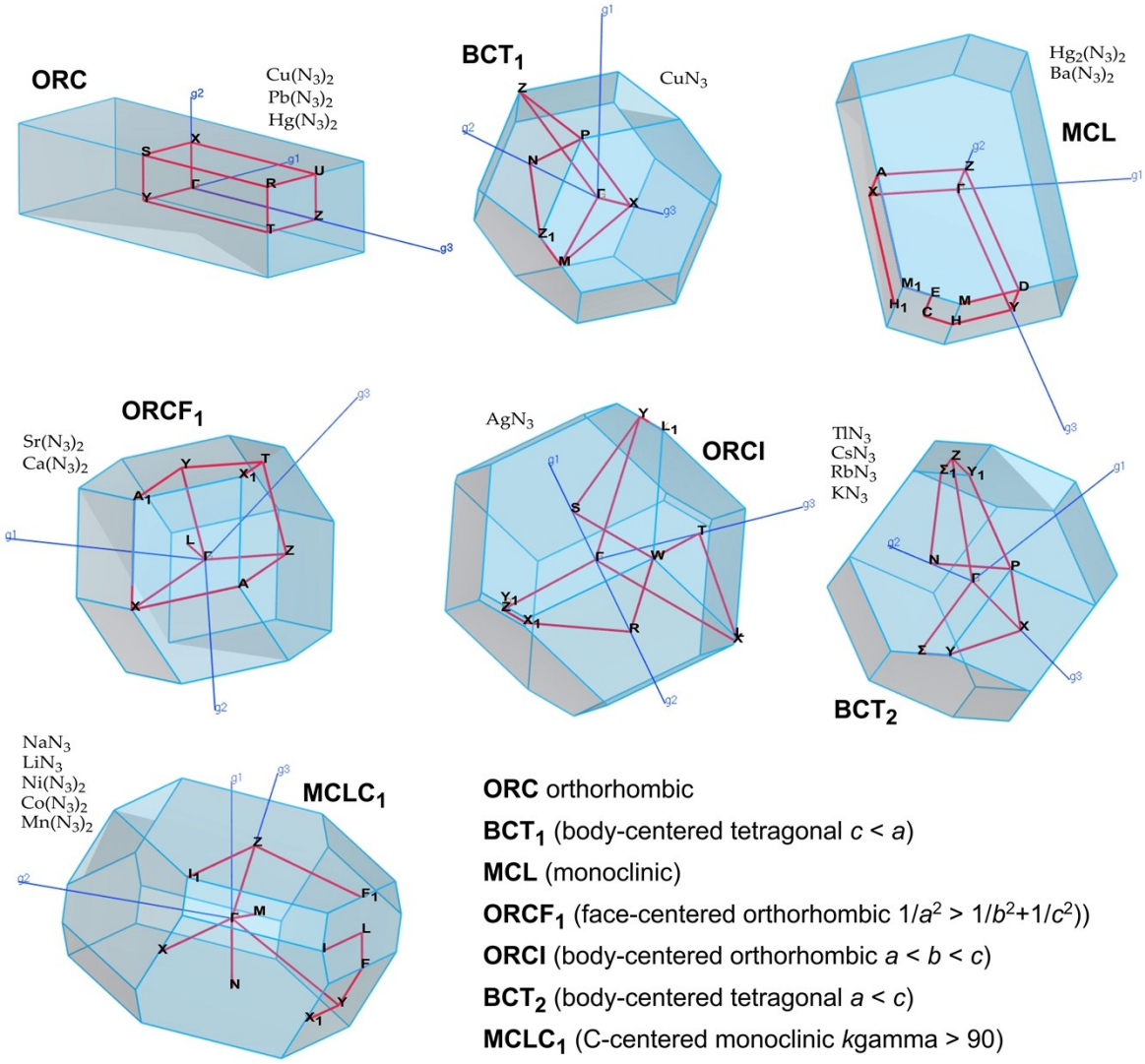


Fig. S1. The Brillouin zones for different Bravais lattices of the studied metal azides along with the corresponding high-symmetry points.

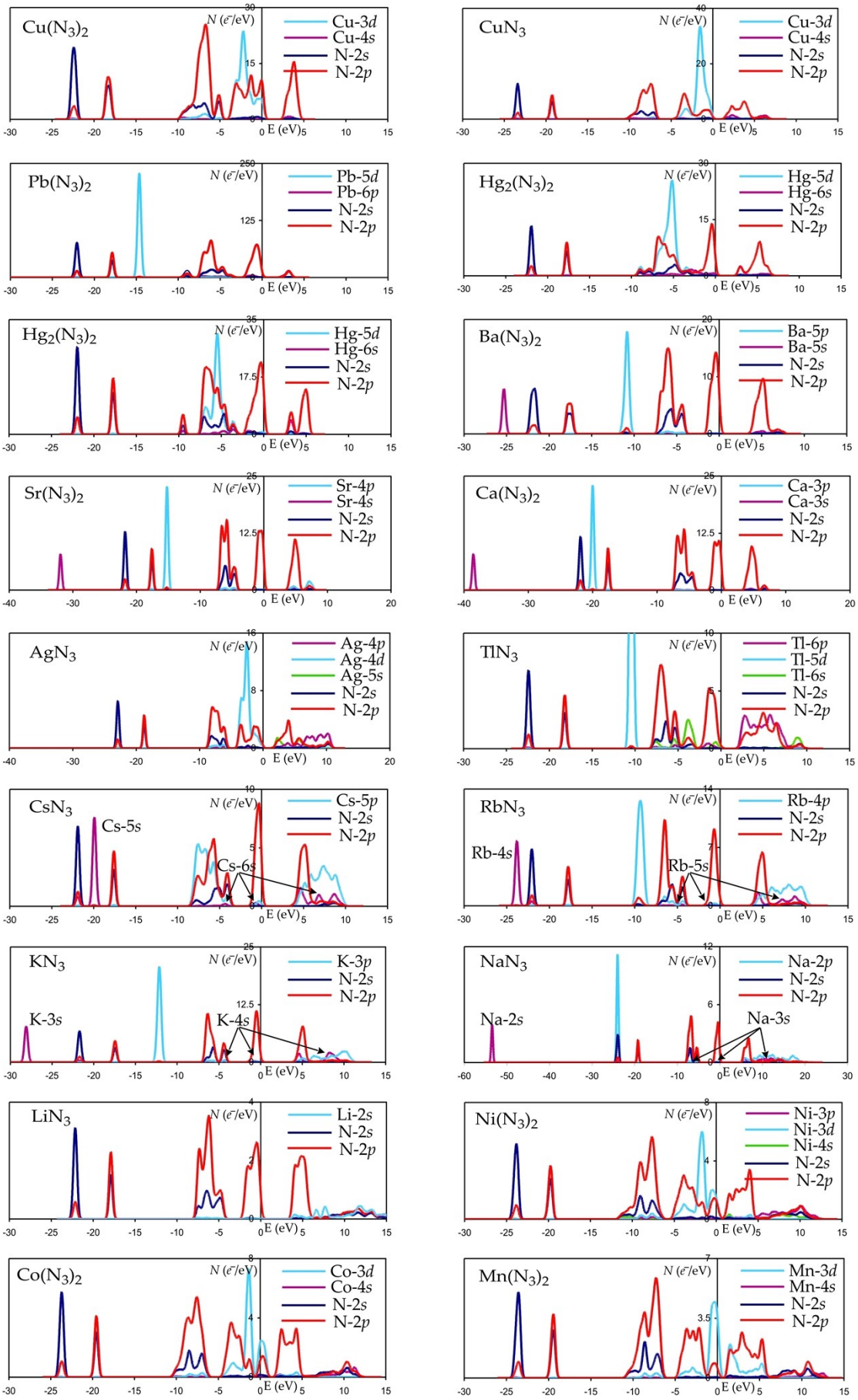


Fig. S2. Partial densities of states with contribution from each element.

Table S3. The calculated elastic stiffness constants C_{ij} (GPa) for the studied metal azides

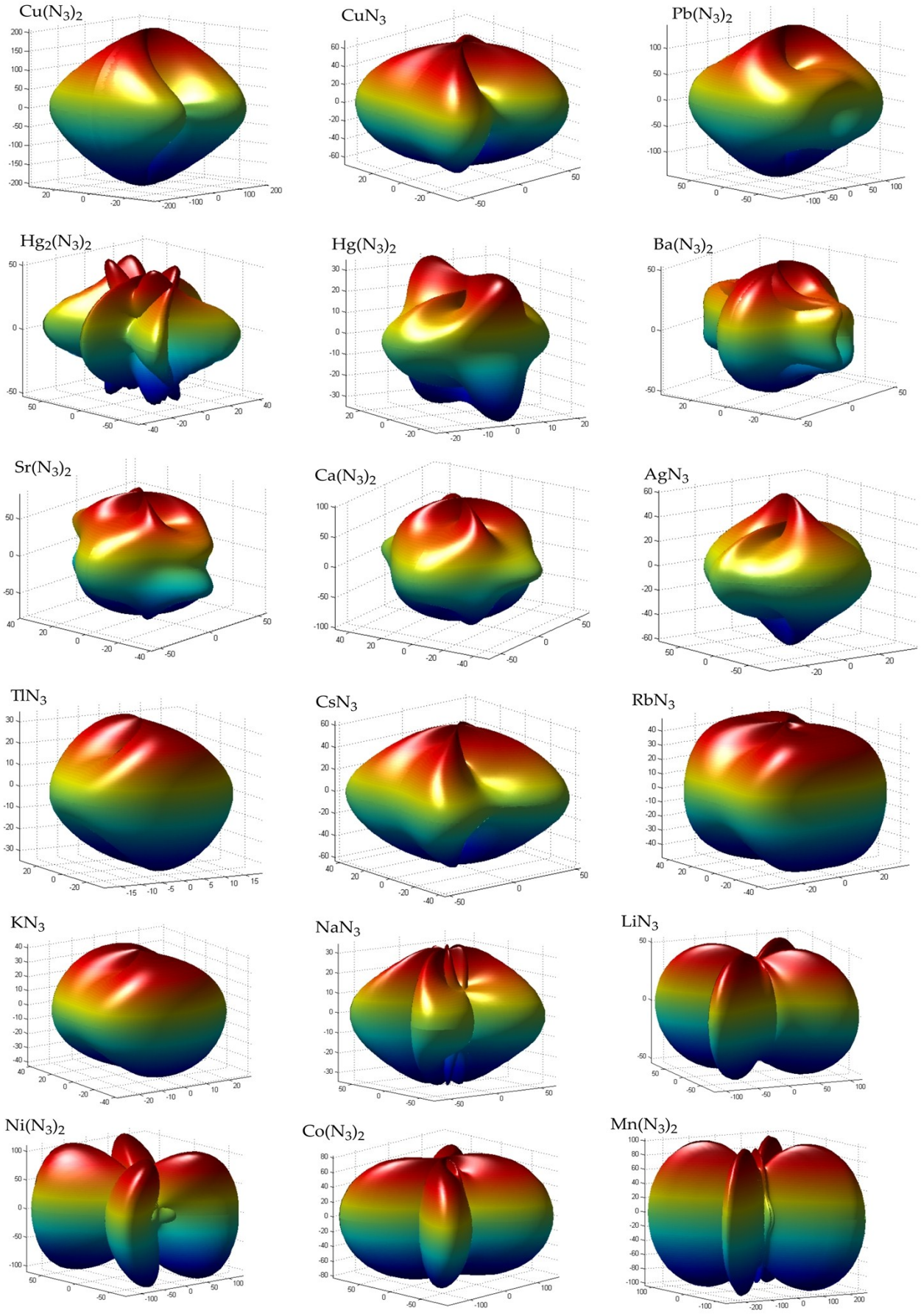
$Cu(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	23.1075	17.0806	-0.5764			
	2	17.0806	21.5254	-2.7043			
	3	-0.5764	-2.7043	209.1780			
	4				13.6358		
	5					21.9733	
	6						4.3037
CuN_3	C_{ij}	1	2	3	4	5	6
	1	54.26230	26.46580	81.59645			-1.61670
	2	26.46580	54.26230	81.59645			1.61670
	3	81.59645	81.59645	226.28990			
	4				20.39310		
	5					20.39310	
	6	-1.61670	1.61670				13.34675
$Pb(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	83.3687	14.3587	27.8305			
	2	14.3587	59.7650	1.2472			
	3	27.8305	1.2472	155.2280			
	4				33.1113		
	5					55.7299	
	6						72.4230
$Hg_2(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	78.19015	29.40680	12.78550		17.74075	
	2	29.40680	66.71835	19.97875		-8.69700	
	3	12.78550	19.97875	49.45555		-1.14940	
	4				11.76570		-4.91905
	5	17.74075	-8.69700	-1.14940		12.18560	0.00000
	6				-4.91905		23.91480
$Hg(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	30.93765	17.02395	10.49545			
	2	17.02395	39.60965	5.11557			
	3	10.49545	5.11557	26.54680			
	4				5.36875		
	5					8.78745	
	6						18.28205
$Ba(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	60.21615	34.60623	24.69983		-3.78483	
	2	34.60623	45.77765	29.17403		2.07892	
	3	24.69983	29.17403	71.21430		0.00177	
	4				18.28425		1.19493
	5	-3.78483	2.07892	0.00177		9.36520	
	6				1.19493		15.72795
$Sr(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	49.76815	33.08403	21.52977			
	2	33.08403	78.96260	47.46667			
	3	21.52977	47.46667	87.00985			
	4				35.16190		
	5					11.88285	
	6						22.02015

Table S3. Continue

$Ca(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	57.66655	25.78108	22.74610			
	2	25.78108	96.55870	53.00910			
	3	22.74610	53.00910	97.01055			
	4				42.92125		
	5					16.56600	
	6						17.36430
AgN_3	C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
	1	140.11750	32.58857	62.08125			
	2	32.58857	71.41730	23.31928			
	3	62.08125	23.31928	68.25925			
	4				9.63590		
	5					13.65710	
	6						22.44345
TlN_3	C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
	1	47.40900	19.14090	17.56585			
	2	19.14090	47.40900	17.56585			
	3	17.56585	17.56585	28.44065			
	4				9.00335		
	5					9.00335	
	6						17.40110
CsN_3	C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
	1	48.45230	17.67115	35.14475			
	2	17.67115	48.45230	35.14475			
	3	35.14475	35.14475	87.24115			
	4				26.75565		
	5					26.75565	
	6						8.73185
RbN_3	C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
	1	66.04495	33.55950	27.79575			
	2	33.55950	66.04495	27.79575			
	3	27.79575	27.79575	52.57890			
	4				20.67670		
	5					20.67670	
	6						25.63975
KN_3	C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
	1	55.19035	22.82375	17.22010			
	2	22.82375	55.19035	17.22010			
	3	17.22010	17.22010	37.51490			
	4				15.57970		
	5					15.57970	
	6						19.76855
NaN_3	C_{ij}	**1**	**2**	**3**	**4**	**5**	**6**
	1	60.78215	11.45225	24.36428		20.43180	
	2	11.45225	30.66110	15.91190		-0.70365	
	3	24.36428	15.91190	57.25825		20.49870	
	4				14.45780		-4.91028
	5	20.43180	-0.70365	20.49870		21.75110	
	6				-4.91028		10.36085

Table S3. Continue

LiN_3	C_{ij}	1	2	3	4	5	6
	1	62.30320	9.99705	15.07720		14.14512	
	2	9.99705	47.42085	10.06298		2.50440	
	3	15.07720	10.06298	82.47510		41.98515	
	4				17.39370		0.55283
	5	14.14512	2.50440	41.98515		38.52455	
	6				0.55283		20.40030
$Ni(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	57.68115	22.74192	54.07585		-26.38350	
	2	22.74192	70.92665	32.96775		-7.57758	
	3	54.07585	32.96775	152.56630		-60.53380	
	4				-14.60855		-9.53603
	5	-26.38350	-7.57758	-60.53380		53.61255	
	6				-9.53603		11.28270
$Co(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	54.06385	22.35940	34.31295		-19.13505	
	2	22.35940	92.32280	32.85895		-7.11115	
	3	34.31295	32.85895	146.79795		-48.60145	
	4				18.97485		-5.27448
	5	-19.13505	-7.11115	-48.60145		40.12690	
	6				-5.27448		18.15975
$Mn(N_3)_2$	C_{ij}	1	2	3	4	5	6
	1	68.78775	17.63945	63.11488		-19.88445	
	2	17.63945	101.09560	28.72285		-7.08015	
	3	63.11488	28.72285	224.67485		-87.93343	
	4				22.94985		-2.70165
	5	-19.88445	-7.08015	-87.93343		46.96705	
	6				-2.70165		17.81750



Equations are given from: J. F. Nye, Physical properties of crystals, Oxford University Press Inc., Oxford, 1985.

Fig. S3. Graphical presentation of the Young modulus of the metal azides studied in this work

Table S4. The calculated total energies of the cationic and corresponding neutral states of the metals as well as the HOMO and LUMO energies of the cations.

Cation	E_{HOMO} (eV)	E_{LUMO} (eV)	E (M^{n+}) (a. u.)	E (M^0) (a. u.)
Cu^{2+}	-30.37	-21.44	-1685.69	-1686.80
Cu^{+}	-15.39	-11.09	-1686.51	-1686.80
Pb^{2+}	-28.99	-16.96	-19666.20	-19666.90
Hg^{+}	-15.89	-13.43	-19187.00	-19187.34
Hg^{2+}	-30.00	-22.44	-19186.30	-19187.34
Ba^{2+}	-31.66	-12.08	-8271.36	-8271.90
Sr^{2+}	-38.16	-12.87	-3217.57	-3218.17
Ca^{2+}	-44.94	-13.78	-721.57	-722.22
Ag^{+}	-16.94	-10.47	-5522.48	-5522.76
Tl^{+}	-17.39	-7.66	-18956.00	-18956.15
Cs^{+}	-19.82	-4.87	-7429.60	-7429.72
Rb^{+}	-22.99	-5.32	-3030.15	-3030.29
K^{+}	-26.50	-5.45	-633.02	-633.16
Na^{+}	-39.35	-6.50	-170.39	-170.57
Li^{+}	-63.84	-6.42	-8.22	-8.41
Ni^{2+}	-30.31	-22.81	-1549.74	-1550.61
Co^{2+}	-24.67	-20.47	-1420.83	-1421.75
Mn^{2+}	-27.29	-19.07	-1185.13	-1185.98