Supplementary Materials for

All-nitrogen cages and molecular crystals: Topological rules, stability, and pyrolysis paths

Konstantin P. Katin ^{1,2,*}, Valeriy B. Merinov ¹, Alexey I. Kochaev ³, Savas Kaya ⁴, and Mikhail M. Maslov ^{1,2}

¹Department of Condensed Matter Physics, National Research Nuclear University "MEPhI", Kashirskoe Sh. 31, Moscow, 115409, Russian Federation ²Laboratory of Computational Design of Nanostructures, Nanodevices, and Nanotechnologies, Research Institute for the Development of Scientific and Educational Potential of Youth, Aviatorov Str. 14/55, Moscow, 119620, Russia ³Ulyanovsk State University, 42 Leo Tolstoy str., Ulyanovsk, 432017, Russia ⁴Faculty of Science, Department of Chemistry, Cumhuriyet University, Sivas, Turkey

Correspondence to: Konstantin P. Katin¹ (E-mail: kpkatin@yandex.ru)



Figure S1. The chemical potential (a), hardness (b), softness (c), and electrophilicity index (d) versus the number of nitrogen atoms in the system obtained at the DFT/B3LYP/6-311G(d,p) level of theory. Letter designations correspond to designations in Figure 3 of the main text.

	X	Y	Z
	1.974281	-3.54882	1.566962
$\mathbf{N}_{\mathbf{c}}(\mathbf{a})$	2.759893	-2.81658	0.84954
1N4 (d)	3.309012	-2.0946	2.017838
	3.955617	-3.13679	1.661083
	0.654609	-0.28288	-0.09506
	-0.61949	-0.32061	-0.09657
N _c (b)	-0.03689	1.543085	0.076869
1 N 6 (D)	0.804816	-0.01767	1.456821
	-0.78872	-0.06447	1.455263
	-0.02581	1.122658	1.39963
	-1.90233	21.57072	-8.15687
	-3.02184	21.11975	-7.3215
	-4.16003	21.78409	-8.31595
$N_{c}(z)$	-3.03621	22.30851	-9.10151
1N8 (C)	-2.0188	20.42572	-9.06572
	-2.95327	19.86418	-8.08218
	-4.15819	20.50062	-9.02733
	-3.21904	21.13192	-9.96254

Table S1. Optimized cartesian coordinates of nitrogen nanosystems considered. Letter designations correspond to designations in Figure 3 of the main text.

	X	Y	Z
	0.855032	-0.41634	1.064775
	1.640693	-0.59239	0.023911
	0.910485	-1.79647	2.027199
N8 (d)	-0.01665	-2.58311	1.485876
N8 (d)	0.202055	-2.30192	-0.07199
	0.098833	-0.8439	-0.12384
	1.623719	-2.44565	-0.02426
	1.764121	-2.71742	1.301004
	0.494896	-0.15901	0.205152
	1.984502	0.091398	0.685034
	2.286184	1.4832	0.517819
	1.059617	2.125689	-0.12236
$\mathbf{N}_{\mathbf{r}}(\mathbf{z})$	-0.054	1.08834	-0.23829
IN10 (e)	0.138089	-0.06399	1.682604
	1.38712	0.146028	2.085835
	1.726402	1.966301	1.897637
	0.58059	2.395455	1.2195
	-0.55646	1.58353	1.16072
	-1.22131	-0.77077	1.941333
	0.193991	-0.6536	1.362254
	-1.80348	-1.8239	1.057681
	-0.71834	-1.87271	2.862668
N _{to} (f)	-1.19515	-2.9207	1.86735
1 10 (1)	0.193652	-2.48226	-0.02918
	-1.39271	-1.7759	-0.18169
	0.172935	-1.04646	0.01886
	0.620776	-1.83193	2.171414
	0.223396	-2.96238	1.283194
	1.165275	-0.05786	0.005737
	0.167689	0.627716	3.086965
	-0.69189	1.784047	1.510439
	-0.32228	-0.13053	0.15186
	1.120571	1.43442	0.05177
$N_{in}(\alpha)$	-0.36316	1.385733	0.179045
1 N 12 (g)	0.74733	-0.66934	2.216269
	-0.61609	-0.61236	1.466344
	-1.12092	0.542847	2.277769
	0.606106	1.750523	2.281101
	1.67961	1.536212	1.507121
	1.727769	-0.28014	1.424326

Table S1. Continued.

Table S1. Continued.

	Х	Y	Z
	-0.08242	-0.08234	-0.05374
	1.481021	-0.08273	-0.05372
	2.211014	1.181891	-0.05386
	1.43043	2.535872	-0.0551
	-0.03092	2.536309	-0.05491
$N_{\rm ec}(\mathbf{b})$	-0.81197	1.182555	-0.05349
1 N 12 (11)	-0.03142	-0.11127	1.455422
	1.430156	-0.11149	1.455518
	2.210932	1.241532	1.453981
	1.481282	2.50656	1.454029
	-0.08124	2.506814	1.454497
	-0.81145	1.24194	1.454308
	-11.7349	-0.14765	-1.27289
	-11.3583	-1.30886	-0.55228
	-12.4285	-1.0598	0.845271
	-11.686	-0.01538	1.452442
	-11.9767	1.224507	0.571666
N. ()	-11.0472	1.016373	-0.51426
IN12 (I)	-13.0878	0.063941	-1.18436
	-13.5516	-0.50672	0.301213
	-13.2708	0.971225	0.030176
	-9.89341	0.417078	0.069468
	-10.108	-1.09505	-0.04645
	-10.3367	-0.26116	1.360476
	1.470755	1.073213	2.470626
	2.064811	2.144793	1.814687
	1.692693	3.379792	2.681463
	0.80759	2.677656	0.72031
	-0.83649	0.85719	2.679764
	0.398043	0.482397	1.813549
N _L (3)	0.496013	3.732767	1.787996
1 N 14 (J)	1.16574	2.916301	3.903214
	1.139274	1.404699	3.841525
	-0.3725	1.381985	3.902141
	-0.70286	3.252592	2.456455
	-1 18576	2.055541	1.786856
	1.10570		
	-0.37938	2.92733	3.818075

Table S1. Continued.

	Х	Y	Ζ
	1.716658	0.052466	1.889343
	0.576944	0.56281	2.61156
	3.513166	1.654607	1.820469
	2.984269	0.605278	2.601474
	2.899063	1.627763	0.557347
	1.711678	0.633481	0.579954
	0.691686	1.791921	0.546465
NI (ma)	1.852312	2.833349	0.530135
IN16 (m)	2.50689	2.678149	3.84267
	0.9608	2.562042	3.848856
	1.039137	1.020028	3.891062
	2.598339	1.081813	3.879506
	1.81758	3.455321	1.804813
	2.940685	3.077889	2.569546
	0.06316	1.806353	1.838229
	0.534973	2.972449	2.544615
	1.697317	-0.64693	-1.01219
	1.886324	0.773209	-0.4702
	0.496141	-0.71597	-1.89614
	-0.08583	0.596681	-2.05253
	0.851111	1.633734	-1.03457
	-0.52973	-1.59513	-1.26743
	-1.69608	-0.71147	-0.99202
	-1.39592	0.597371	-1.51871
	-0.00374	-2.08968	0.013769
NL. (m)	-0.88563	-1.5306	1.098488
1N20 (II)	-1.9255	-0.63964	0.482624
	1.388583	-1.53581	0.161565
	1.393515	-0.72147	1.386002
	-0.01894	-0.71836	1.970083
	1.724557	0.685989	1.005665
	0.558307	1.533755	1.350307
	-0.51263	0.689424	1.933909
	-1.67014	0.781674	1.006392
	-1.33868	1.644171	-0.11793
	0.021951	2.044704	0.061894

Table S1. Continued.

	x	Y	Z
	1.150377	-2.02336	0.436005
	-0.00179	-2.39461	-0.33615
	2.017763	-1.20529	-0.41362
	-0.00149	-1.44082	-1.73357
	1.240457	-0.71922	-1.68838
	2.360677	-0.02541	0.390668
	2.044012	1.16152	-0.42325
	1.264168	0.750082	-1.65778
	1.494861	0.00049	1.654036
N24 (0)	0.741453	-1.26344	1.67438
	-0.7444	-1.2629	1.674275
	0.746356	1.272107	1.649901
	-0.747	1.272682	1.649888
	-1.49672	0.001663	1.653944
	1.188507	2.02895	0.421803
	-2.02045	-1.20361	-0.41378
	-1.15376	-2.02248	0.435838
	-2.36252	-0.02345	0.39069
	-2.04485	1.163369	-0.42309
	-1.18843	2.029973	0.421993
	0.000164	2.367307	-0.38956
	-1.24288	-0.71816	-1.68827
	-1.2655	0.751288	-1.65764
	-0.00033	1.506457	-1.64201