Таблица 4.

Сродство к электрону и структурные параметры $R\text{-}N_2^+ + e = R\text{-}N_2\bullet$

№	Reaction	ΔE, kJ/mol	ΔG, kJ/mol	LUMO, Eh		Ring Deviation *, Å		Angle C-N-N		Dist. C-N *, Å		Dist. N-N *, Å	
				$R\text{-}N_2^+$	$R\text{-}N_2\bullet$	$R\text{-}N_2^+$	$R\text{-}N_2\bullet$	$R\text{-}N_2^+$	$R\text{-}N_2\bullet$	$R\text{-}N_2^+$	$R\text{-}N_2\bullet$	$R\text{-}N_2^+$	$R\text{-}N_2\bullet$
1	$CH_3\text{-}N_2^+(S) + e = CH_3\text{-}N_2\bullet(D)$	-710.76	-718.93	-0.326390	-0.073650			180	123	1.4558	1.5088	1.1029	1.1769
2	$CH_3\text{-}N_2^+(T) + e = CH_3\text{-}N_2\bullet(D)$	-1186.53	-1172.72	-0.541320	-0.073650			127	123	1.3932	1.5088	1.2321	1.1769
3	$C_2H_5\text{-}N_2^+(S) + e = C_2H_5\text{-}N_2\bullet(D)$	-685.45	-692.89	-0.309530	-0.070120			178	123	1.4893	1.5258	1.1032	1.1760
4	$C_2H_5\text{-}N_2^+(T) + e = C_2H_5\text{-}N_2\bullet(D)$	-1124.05	-1101.51	-0.500610	-0.070120			124	123	1.4161	1.5258	1.2098	1.1760
5	$1\text{-}CH_3\text{-}C_2H_4\text{-}N_2^+(S) + e = 1\text{-}CH_3\text{-}C_2H_4\text{-}N_2\bullet(D)$	-663.62	-669.66	-0.293210	-0.065620			178	124	1.5442	1.5522	1.1033	1.1737
6	$1\text{-}CH_3\text{-}C_2H_4\text{-}N_2^+(T) + e = 1\text{-}CH_3\text{-}C_2H_4\text{-}N_2\bullet(D)$	-1069.99	-1054.03	-0.443500	-0.065620			122	124	1.4319	1.5522	1.1949	1.1737
7	$1,1\text{-}(CH_3)_2\text{-}C_2H_3\text{-}N_2^+(S) + e = 1,1\text{-}(CH_3)_2\text{-}C_2H_3\text{-}N_2\bullet(D)$	-580.40	-549.08	-0.314080	-0.065670			**Break C-NN bond****					
8	$1,1\text{-}(CH_3)_2\text{-}C_2H_3\text{-}N_2^+(T) + e = 1,1\text{-}(CH_3)_2\text{-}C_2H_3\text{-}N_2\bullet(D)$	-1032.86	-1017.14	-0.415860	-0.065670			**Break C-NN bond****					
9	$Pyridine\text{-}2\text{-}N_2^+(S) + e = Pyridine\text{-}2\text{-}N_2\bullet(D)$	-676.81	-685.53	-0.312160	-0.089210	0.0003	0.0002	179	124	1.4249	1.4748	1.1090	1.1818
10	$Pyridine\text{-}2\text{-}N_2^+(T) + e = Pyridine\text{-}2\text{-}N_2\bullet(D)$	-930.49	-922.30	-0.411250	-0.089210	0.2280	0.0002	137	124	1.4089	1.4748	1.1708	1.1818
11	$Pyridine\text{-}3\text{-}N_2^+(S) + e = Pyridine\text{-}3\text{-}N_2\bullet(D)$	-684.21	-691.43	-0.314260	-0.091320	0.0007	0.0008	178	125	1.3788	1.4570	1.1145	1.1845
12	$Pyridine\text{-}3\text{-}N_2^+(T) + e = Pyridine\text{-}3\text{-}N_2\bullet(D)$	-919.85	-912.16	-0.412520	-0.091320	0.1537	0.0008	124	125	1.4357	1.4570	1.1854	1.1845
13	$Pyridine\text{-}4\text{-}N_2^+(S) + e = Pyridine\text{-}4\text{-}N_2\bullet(D)$	-703.64	-710.58	-0.324880	-0.099840	0.0000	0.0001	180	124	1.3961	1.4642	1.1108	1.1829
14	$Pyridine\text{-}4\text{-}N_2^+(T) + e = Pyridine\text{-}4\text{-}N_2\bullet(D)$	-902.35	-896.87	-0.385000	-0.099840	0.0002	0.0001	180	124	1.3407	1.4642	1.1406	1.1829
15	$Pyrazine\text{-}2\text{-}N_2^+(S) + e = Pyrazine\text{-}2\text{-}N_2\bullet(D)$	-709.56	-717.36	-0.328560	-0.107850	0.0004	0.0001	178	124	1.4177	1.4655	1.1098	1.1841
16	$Pyrazine\text{-}2\text{-}N_2^+(T) + e = Pyrazine\text{-}2\text{-}N_2\bullet(D)$	-927.00	-920.24	-0.402910	-0.107850	0.0193	0.0001	166	124	1.3487	1.4655	1.1446	1.1841
17	$Pyrimidine\text{-}2\text{-}N_2^+(S) + e = Pyrimidine\text{-}2\text{-}N_2\bullet(D)$	-696.50	-703.20	-0.322520	-0.086040	0.0003	0.0403	180	124	1.4750	1.4694	1.1050	1.1807

№	Reaction	ΔE, kJ/mol	ΔG, kJ/mol	LUMO, Eh		Ring Deviation *, Å		Angle C-N-N		Dist. C-N *, Å		Dist. N-N *, Å	
				R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•
18	Pyrimidine-2-N_2^+(T) + e = Pyrimidine-2-N_2•(D)	-924.22	-918.54	-0.402420	-0.086040	0.0003	0.0403	180	124	1.3310	1.4694	1.1450	1.1807
19	Pyrimidine-4-N_2^+(S) + e = Pyrimidine-4-N_2•(D)	-724.76	-730.82	-0.335000	-0.104740	0.0001	0.0310	178	124	1.4490	1.4705	1.1064	1.1823
20	Pyrimidine-4-N_2^+(T) + e = Pyrimidine-4-N_2•(D)	-914.68	-911.94	-0.396630	-0.104740	0.0005	0.0310	179	124	1.3436	1.4705	1.1393	1.1823
21	Pyrimidine-5-N_2^+(S) + e = Pyrimidine-5-N_2•(D)	-717.42	-723.67	-0.329610	-0.105390	0.0003	0.0003	180	124	1.3745	1.4525	1.1148	1.1851
22	Pyrimidine-5-N_2^+(T) + e = Pyrimidine-5-N_2•(D)	-925.49	-919.00	-0.394600	-0.105390	0.0002	0.0003	180	124	1.3322	1.4525	1.1442	1.1851
23	1,2,3-Triazine-4-N_2^+(S) + e = 1,2,3-Triazine-4-N_2•(D)	-767.47	-772.13	-0.354470	-0.123530	0.0005	0.0241	176	123	1.4319	1.4665	1.1073	1.1819
24	1,2,3-Triazine-4-N_2^+(T) + e = 1,2,3-Triazine-4-N_2•(D)	-885.50	-886.96	-0.384860	-0.123530	0.0002	0.0241	180	123	1.3371	1.4665	1.1375	1.1819
25	1,2,3-Triazine-5-N_2^+(S) + e = 1,2,3-Triazine-5-N_2•(D)	-754.94	-761.43	-0.360700	-0.127790	0.0002	0.0002	180	180	1.3883	1.3286	1.1125	1.1535
26	1,2,3-Triazine-5-N_2^+(T) + e = 1,2,3-Triazine-5-N_2•(D)	-864.95	-867.86	-0.382160	-0.127790	0.0004	0.0002	180	180	1.3371	1.3286	1.1352	1.1535
27	1,2,4-Triazine-3-N_2^+(S) + e = 1,2,4-Triazine-3-N_2•(D)	-740.00	-745.64	-0.342270	-0.113080	0.0006	0.0425	178	124	1.4584	1.4610	1.1051	1.1813
28	1,2,4-Triazine-3-N_2^+(T) + e = 1,2,4-Triazine-3-N_2•(D)	-877.11	-875.60	-0.387590	-0.113080	0.0009	0.0425	180	124	1.3332	1.4610	1.1403	1.1813
29	1,2,4-Triazine-5-N_2^+(S) + e = 1,2,4-Triazine-5-N_2•(D)	-769.09	-772.26	-0.355380	-0.126890	0.0010	0.0267	176	123	1.4461	1.4669	1.1075	1.1826
30	1,2,4-Triazine-5-N_2^+(T) + e = 1,2,4-Triazine-5-N_2•(D)	-863.84	-864.31	-0.382590	-0.126890	0.0001	0.0267	180	123	1.3449	1.4669	1.1353	1.1826
31	1,2,4-Triazine-6-N_2^+(S) + e = 1,2,4-Triazine-6-N_2•(D)	-753.96	-761.06	-0.348200	-0.118240	0.0003	0.0116	180	123	1.4036	1.4623	1.1102	1.1835
32	1,2,4-Triazine-6-N_2^+(T) + e = 1,2,4-Triazine-6-N_2•(D)	-882.45	-882.63	-0.387580	-0.118240	0.0005	0.0116	179	123	1.3318	1.4623	1.1396	1.1835
33	1,3,5-Triazine-2-N_2^+(S) + e = 1,3,5-Triazine-2-N_2•(D)	-749.56	-758.71	-0.342070	-0.100570	0.0005	0.0160	180	127	1.5140	1.4559	1.1031	1.1780
34	1,3,5-Triazine-2-N_2^+(T) + e = 1,3,5-Triazine-2-N_2•(D)	-958.88	-958.97	-0.417670	-0.100570	0.0006	0.0160	180	127	1.3517	1.4559	1.1343	1.1780
35	N-O-Pyridine-2-N_2^+(S) + e = N-O-Pyridine-2-N_2•(D)	-687.27	-693.31	-0.317800	-0.098210	0.0003	0.0004	179	126	1.3630	1.4233	1.1160	1.1942
36	N-O-Pyridine-2-N_2^+(T) + e = N-O-Pyridine-2-N_2•(D)	-834.85	-829.41	-0.374990	-0.098210	0.0018	0.0004	179	126	1.3324	1.4233	1.1449	1.1942
37	N-O-Pyridine-3-N_2^+(S) + e = N-O-Pyridine-3-N_2•(D)	-713.76	-720.51	-0.322550	-0.103700	0.0017	0.0004	180	125	1.3877	1.4613	1.1126	1.1832

№	Reaction	ΔE, kJ/mol	ΔG, kJ/mol	LUMO, Eh		Ring Deviation *, Å		Angle C-N-N		Dist. C-N *, Å		Dist. N-N *, Å	
				R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•
38	N-O-Pyridine-3-N_2^+(T) + e = N-O-Pyridine-3-N_2•(D)	-840.37	-836.16	-0.369880	-0.103700	0.0003	0.0004	178	125	1.3399	1.4613	1.1441	1.1832
39	N-O-Pyridine-4-N_2^+(S) + e = N-O-Pyridine-4-N_2•(D)	-644.24	-654.89	-0.311690	-0.096690	0.0001	0.0001	180	180	1.3635	1.3281	1.1193	1.1555
40	N-O-Pyridine-4-N_2^+(T) + e = N-O-Pyridine-4-N_2•(D)	-787.67	-786.96	-0.370370	-0.096690	0.0000	0.0001	180	180	1.3414	1.3281	1.1427	1.1555
41	Ph-N_2^+(S) + e = Ph-N_2•(D)	-654.34	-661.87	-0.300120	-0.080430	0.0000	0.0005	180	125	1.3832	1.4602	1.1138	1.1838
42	Ph-N_2^+(T) + e = Ph-N_2•(D)	-901.66	-890.54	-0.406100	-0.080430	0.0153	0.0005	126	125	1.4093	1.4602	1.1914	1.1838
43	4-NO_2-Ph-N_2^+(S) + e = 4-NO_2-Ph-N_2•(D)	-682.75	-690.66	-0.324090	-0.127070	0.0001	0.0005	180	180	1.3887	1.3409	1.1126	1.1507
44	4-NO_2-Ph-N_2^+(T) + e = 4-NO_2-Ph-N_2•(D)	-869.55	-868.76	-0.363560	-0.127070	0.0000	0.0005	180	180	1.3651	1.3409	1.1220	1.1507
45	4-CH_3O-Ph-N_2^+(S) + e = 4-CH_3O-Ph-N_2•(D)	-616.93	-624.53	-0.274560	-0.069170	0.0003	0.0003	180	125	1.3636	1.4506	1.1193	1.1856
46	4-CH_3O-Ph-N_2^+(T) + e = 4-CH_3O-Ph-N_2•(D)	-806.86	-801.47	-0.368430	-0.069170	0.0204	0.0003	123	125	1.4355	1.4506	1.1912	1.1856
47	Pyrrole-2-N_2^+(S) + e = Pyrrole-2-N_2•(D)	-655.52	-662.06	-0.291020	-0.069620	0.0015	0.0003	178	126	1.3369	1.4083	1.1243	1.1935
48	Pyrrole-2-N_2^+(T) + e = Pyrrole-2-N_2•(D)	-823.78	-818.79	-0.387900	-0.069620	0.0001	0.0003	122	126	1.3955	1.4083	1.2021	1.1935
49	Pyrrole-3-N_2^+(S) + e = Pyrrole-3-N_2•(D)	-622.69	-631.14	-0.282580	-0.057890	0.0006	0.0001	178	126	1.3494	1.4279	1.1179	1.1889
50	Pyrrole-3-N_2^+(T) + e = Pyrrole-3-N_2•(D)	-827.45	-821.49	-0.388090	-0.057890	0.0002	0.0001	122	126	1.4209	1.4279	1.1929	1.1889
51	Pyrazole-3-N_2^+(S) + e = Pyrazole-3-N_2•(D)	-671.37	-679.66	-0.308180	-0.072070	0.0003	0.0001	179	125	1.3684	1.4341	1.1129	1.1878
52	Pyrazole-3-N_2^+(T) + e = Pyrazole-3-N_2•(D)	-927.12	-920.92	-0.422460	-0.072070	0.0167	0.0001	124	125	1.3913	1.4341	1.1991	1.1878
53	Pyrazole-4-N_2^+(S) + e = Pyrazole-4-N_2•(D)	-666.95	-674.17	-0.300790	-0.072240	0.0010	0.0002	178	125	1.3493	1.4248	1.1171	1.1891
54	Pyrazole-4-N_2^+(T) + e = Pyrazole-4-N_2•(D)	-916.54	-907.78	-0.421350	-0.072240	0.0001	0.0002	121	125	1.3881	1.4248	1.2077	1.1891
55	Pyrazole-5-N_2^+(S) + e = Pyrazole-5-N_2•(D)	-716.13	-721.30	-0.320440	-0.091860	0.0010	0.0002	180	124	1.3486	1.4168	1.1191	1.1913
56	Pyrazole-5-N_2^+(T) + e = Pyrazole-5-N_2•(D)	-925.62	-914.96	-0.426750	-0.091860	0.0001	0.0002	121	124	1.3944	1.4168	1.2049	1.1913
57	1,3,5-$(CH_3)_3$-Pyrazole-4-N_2^+(S) + e =	-611.85	-618.02	-0.269760	-0.052490	0.0001	0.0054	178	126	1.3370	1.4151	1.1219	1.1927

№	Reaction	ΔE, kJ/mol	ΔG, kJ/mol	LUMO, Eh		Ring Deviation *, Å		Angle C-N-N		Dist. C-N *, Å		Dist. N-N *, Å	
				R-N_2+	R-N_2•	R-N_2+	R-N_2•	R-N_2+	R-N_2•	R-N_2+	R-N_2•	R-N_2+	R-N_2•
	1,3,5-$(CH_3)_3$-Pyrazole-4-N_2•(D)												
58	1,3,5-$(CH_3)_3$-Pyrazole-4-N_2^+(T) + e = 1,3,5-$(CH_3)_3$-Pyrazole-4-N_2•(D)	-837.17	-826.80	-0.375320	-0.052490	0.0034	0.0054	124	126	1.4357	1.4151	1.1864	1.1927
63	Imidazole-2-N_2^+(S) + e = Imidazole-2-N_2•(D)	-703.86	-709.57	-0.312960	-0.087810	0.0019	0.0001	178	124	1.3516	1.4166	1.1200	1.1909
64	Imidazole-2-N_2^+(T) + e = Imidazole-2-N_2•(D)	-877.63	-871.00	-0.406660	-0.087810	0.0002	0.0001	121	124	1.3975	1.4166	1.2034	1.1909
65	Imidazole-4-N_2^+(S) + e = Imidazole-4-N_2•(D)	-657.31	-665.10	-0.299360	-0.068230	0.0003	0.0007	179	125	1.3619	1.4292	1.1151	1.1879
66	Imidazole-4-N_2^+(T) + e = Imidazole-4-N_2•(D)	-878.12	-871.57	-0.407200	-0.068230	0.0119	0.0007	121	125	1.4083	1.4292	1.1963	1.1879
67	Imidazole-5-N_2^+(S) + e = Imidazole-5-N_2•(D)	-693.64	-699.70	-0.308350	-0.082000	0.0003	0.0003	177	126	1.3387	1.4106	1.1225	1.1923
68	Imidazole-5-N_2^+(T) + e = Imidazole-5-N_2•(D)	-879.20	-872.44	-0.408500	-0.082000	0.0003	0.0003	121	126	1.3947	1.4106	1.2038	1.1923
69	1H-1,2,3-Triazole-4-N_2^+(S) + e = 1H-1,2,3-Triazole-4-N_2•(D)	-710.85	-717.17	-0.321380	-0.085180	0.0013	0.0004	177	124	1.3588	1.4257	1.1143	1.1879
70	1H-1,2,3-Triazole-4-N_2^+(T) + e = 1H-1,2,3-Triazole-4-N_2•(D)	-967.83	-956.28	-0.439210	-0.085180	0.0002	0.0004	121	124	1.3841	1.4257	1.2080	1.1879
71	1H-1,2,3-Triazole-5-N_2^+(S) + e = 1H-1,2,3-Triazole-5-N_2•(D)	-756.78	-761.88	-0.340350	-0.104100	0.0013	0.0002	178	124	1.3472	1.4167	1.1186	1.1905
72	1H-1,2,3-Triazole-5-N_2^+(T) + e = 1H-1,2,3-Triazole-5-N_2•(D)	-980.36	-965.25	-0.440580	-0.104100	0.0590	0.0002	126	124	1.3931	1.4167	1.1941	1.1905
73	1H-1,2,4-Triazole-3-N_2^+(S) + e = 1H-1,2,4-Triazole-3-N_2•(D)	-712.63	-721.20	-0.328560	-0.084900	0.0004	0.0003	179	124	1.3825	1.4355	1.1101	1.1867
74	1H-1,2,4-Triazole-3-N_2^+(T) + e = 1H-1,2,4-Triazole-3-N_2•(D)	-975.27	-969.37	-0.440390	-0.084900	0.0200	0.0003	126	124	1.3858	1.4355	1.1955	1.1867
75	1H-1,2,4-Triazole-5-N_2^+(S) + e = 1H-1,2,4-Triazole-5-N_2•(D)	-764.53	-769.49	-0.344420	-0.108080	0.0003	0.0001	179	123	1.3654	1.4252	1.1151	1.1887
76	1H-1,2,4-Triazole-5-N_2^+(T) + e = 1H-1,2,4-Triazole-5-N_2•(D)	-981.58	-971.29	-0.446480	-0.108080	0.0000	0.0001	121	123	1.3926	1.4252	1.2063	1.1887
77	2H-1,2,3-Triazole-4-N_2^+(S) + e = 2H-1,2,3-Triazole-4-N_2•(D)	-717.73	-725.09	-0.327940	-0.089140	0.0011	0.0005	178	125	1.3651	1.4282	1.1130	1.1884
78	2H-1,2,3-Triazole-4-N_2^+(T) + e = 2H-1,2,3-Triazole-4-N_2•(D)	-1048.50	-1039.09	-0.429380	-0.089140	0.4585	0.0005	178	125	1.3256	1.4282	1.1393	1.1884
79	4H-1,2,4-Triazole-3-N_2^+(S) + e = 4H-1,2,4-Triazole-3-N_2•(D)	-753.37	-759.17	-0.337800	-0.099240	0.0021	0.0007	175	124	1.3551	1.4220	1.1173	1.1900

№	Reaction	ΔE, kJ/mol	ΔG, kJ/mol	LUMO, Eh		Ring Deviation *, Å		Angle C-N-N		Dist. C-N *, Å		Dist. N-N *, Å	
				R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•	R-N_2^+	R-N_2•
80	4H-1,2,4-Triazole-3-N_2^+(T) + e = 4H-1,2,4-Triazole-3-N_2•(D)	-965.81	-957.31	-0.439450	-0.099240	0.0399	0.0007	121	124	1.3841	1.4220	1.2062	1.1900
81	Tetrazole-5-N_2^+(S) + e = Tetrazole-5-N_2•(D)	-815.73	-820.97	-0.368930	-0.120520	0.0010	0.0001	177	123	1.3642	1.4246	1.1139	1.1891
82	Tetrazole-5-N_2^+(T) + e = Tetrazole-5-N_2•(D)	-1067.13	-1053.06	-0.473020	-0.120520	0.0003	0.0001	121	123	1.3767	1.4246	1.2129	1.1891
83	Furan-2-N_2^+(S) + e = Furan-2-N_2•(D)	-691.07	-697.50	-0.312500	-0.086320	0.0002	0.0013	179	125	1.3428	1.4051	1.1209	1.1930
84	Furan-2-N_2^+(T) + e = Furan-2-N_2•(D)	-875.86	-869.92	-0.409290	-0.086320	0.0010	0.0013	123	125	1.3808	1.4051	1.2070	1.1930
85	Furan-3-N_2^+(S) + e = Furan-3-N_2•(D)	-674.26	-682.32	-0.308260	-0.077560	0.0004	0.0003	179	125	1.3556	1.4318	1.1157	1.1881
86	Furan-3-N_2^+(T) + e = Furan-3-N_2•(D)	-884.76	-878.81	-0.410160	-0.077560	0.0201	0.0003	124	125	1.4155	1.4318	1.1903	1.1881
87	Thiophene-2-N_2^+(S) + e = Thiophene-2-N_2•(D)	-670.17	-676.91	-0.304400	-0.089890	0.0003	0.0005	179	127	1.3457	1.4122	1.1204	1.1896
88	Thiophene-2-N_2^+(T) + e = Thiophene-2-N_2•(D)	-869.28	-863.08	-0.400140	-0.089890	0.0000	0.0005	123	127	1.3917	1.4122	1.2005	1.1896
89	Thiophene-3-N_2^+(S) + e = Thiophene-3-N_2•(D)	-659.01	-666.73	-0.300420	-0.081680	0.0004	0.0001	179	125	1.3654	1.4444	1.1162	1.1860
90	Thiophene-3-N_2^+(T) + e = Thiophene-3-N_2•(D)	-878.71	-872.16	-0.402750	-0.081680	0.0262	0.0001	124	125	1.4221	1.4444	1.1905	1.1860

* Ring Deviation - суммарное отклонение атомов от плоскости цикла (ангстрем); ** Break - разрыв цикла или связи C-NN;

1. Присоединение электрона к диазониевому катиону характеризуется значениями энергии Гиббса от -600 до -1200 кДж/моль.
2. В случаях нарушения плоскости цикла в катионах, при присоединении электрона приводит восстановление плоской структуры.
3. При присоединении электрона к диазониевому катиону в синглетном состоянии происходит изменение угла связи C-N-N со 180° до 125°, за исключением: 1,2,3-Triazine-5-N_2^+, N-O-Pyridine-4-N_2^+, 4-NO_2-Ph-N_2^+. Вероятно это связано с тем, что для этих катионов при синглет-триплетном переходе угол связи не меняется и остается равным 180°.
4. Для исходных диазониевых катионов в триплетном состоянии изменение угла связи C-N-N происходит в случае, если он близок к 180°. При углах близких к 122° изменений не происходит.
5. После присоединения электронов нейтральные частицы имеют невысокие отрицательные значения LUMO, т.е. практически теряют способность к присоединению второго электрона.