Сродство к электрону и структурные параметры $Ar^+ + e = Ar•$

№	Reaction	ΔE, kJ/mol	ΔG, kJ/mol	LUMO, Eh		Ring Deviation *, Å	
				Ar^+	Ar•	Ar^+	Ar•
1	CH_3^+(S) + e = CH_3•(D)	-954.08	-959.69	-0.486590	-0.080600		
2	CH_3^+(T) + e = CH_3•(D)	-1293.77	-1278.87	-0.544280	-0.080600		
3	$C_2H_5^+$(S) + e = C_2H_5•(D)	-788.09	-796.17	-0.324030	-0.060550		
4	$C_2H_5^+$(T) + e = C_2H_5•(D)	-1141.40	-1119.17	-0.496720	-0.060550		
5	1-CH_3-$C_2H_4^+$(S) + e = 1-CH_3-C_2H_4•(D)	-709.39	-714.86	-0.347960	-0.048460		
6	1-CH_3-$C_2H_4^+$(T) + e = 1-CH_3-C_2H_4•(D)	-1078.45	-1059.04	-0.466640	-0.048460		
7	1,1-$(CH_3)_2$-$C_2H_3^+$(S) + e = 1,1-$(CH_3)_2$-C_2H_3•(D)	-650.04	-648.74	-0.321560	-0.042240		
8	1,1-$(CH_3)_2$-$C_2H_3^+$(T) + e = 1,1-$(CH_3)_2$-C_2H_3•(D)	-1030.07	-1014.97	-0.428030	-0.042240		
9	Pyridine-2$^+$(S) + e = Pyridine-2•(D)	-756.19	-757.17	-0.343690	-0.084630	0.0005	0.0012
10	Pyridine-2$^+$(T) + e = Pyridine-2•(D)	-927.48	-919.04	-0.430750	-0.084630	0.0012	0.0012
11	Pyridine-3$^+$(S) + e = Pyridine-3•(D)	-807.61	-805.95	-0.341510	-0.109400	0.0011	0.2607
12	Pyridine-3$^+$(T) + e = Pyridine-3•(D)	-910.16	-903.99	-0.416460	-0.109400	0.2607	0.2607
13	Pyridine-4$^+$(S) + e = Pyridine-4•(D)	-823.98	-817.41	-0.368060	-0.110460	0.0005	0.0002
14	Pyridine-4$^+$(T) + e = Pyridine-4•(D)	-910.17	-904.32	-0.411220	-0.110460	0.0002	0.0002
15	Pyrazine-2$^+$(S) + e = Pyrazine-2•(D)	-782.24	-783.30	-0.355910	-0.102310	0.0007	0.2523
16	Pyrazine-2$^+$(T) + e = Pyrazine-2•(D)	-956.78	-950.21	-0.435720	-0.102310	0.2523	0.2523
17	Pyrimidine-2$^+$(S) + e = Pyrimidine-2•(D)	-778.73	-780.86	-0.342040	-0.088310	0.0003	0.0019
18	Pyrimidine-2$^+$(T) + e = Pyrimidine-2•(D)	-913.56	-911.73	-0.413720	-0.088310	0.0019	0.0019
19	Pyrimidine-4$^+$(S) + e = Pyrimidine-4•(D)	-788.46	-788.72	-0.360100	-0.102340	0.0026	0.0000
20	Pyrimidine-4$^+$(T) + e = Pyrimidine-4•(D)	-965.69	-961.19	-0.434950	-0.102340	0.0000	0.0000
21	Pyrimidine-5$^+$(S) + e = Pyrimidine-5•(D)	-868.71	-862.32	-0.381390	-0.126980	0.0004	0.0002

22	Pyrimidine-5^{+}(T) + e = Pyrimidine-5•(D)	-903.43	-899.43	-0.413310	-0.126980	0.0002	0.0002
23	1,2,3-Triazine-4^{+}(S) + e = 1,2,3-Triazine-4•(D)	-629.02	-623.69	-0.365020	-0.125580	**Break****	0.0000
24	1,2,3-Triazine-4^{+}(T) + e = 1,2,3-Triazine-4•(D)	-933.56	-935.55	-0.422920	-0.125580	0.0000	0.0000
25	1,2,3-Triazine-5^{+}(S) + e = 1,2,3-Triazine-5•(D)	-864.29	-864.07	-0.393150	-0.145990	0.0029	0.0001
26	1,2,3-Triazine-5^{+}(T) + e = 1,2,3-Triazine-5•(D)	-964.03	-955.53	-0.439120	-0.145990	0.0001	0.0001
27	1,2,4-Triazine-3^{+}(S) + e = 1,2,4-Triazine-3•(D)	-842.93	-843.39	-0.368740	-0.112240	0.0001	0.0009
28	1,2,4-Triazine-3^{+}(T) + e = 1,2,4-Triazine-3•(D)	-901.18	-902.46	-0.414170	-0.112240	0.0009	0.0009
29	1,2,4-Triazine-5^{+}(S) + e = 1,2,4-Triazine-5•(D)	-802.17	-804.47	-0.369260	-0.121030	0.0003	0.0012
30	1,2,4-Triazine-5^{+}(T) + e = 1,2,4-Triazine-5•(D)	-954.04	-952.29	-0.440980	-0.121030	0.0012	0.0012
31	1,2,4-Triazine-6^{+}(S) + e = 1,2,4-Triazine-6•(D)	-850.63	-851.87	-0.389840	-0.126990	0.0015	0.0016
32	1,2,4-Triazine-6^{+}(T) + e = 1,2,4-Triazine-6•(D)	-916.84	-916.00	-0.420710	-0.126990	0.0016	0.0016
33	1,3,5-Triazine-2^{+}(S) + e = 1,3,5-Triazine-2•(D)	-819.21	-820.19	-0.365090	-0.107680	0.0001	0.0003
34	1,3,5-Triazine-2^{+}(T) + e = 1,3,5-Triazine-2•(D)	-979.83	-976.66	-0.440040	-0.107680	0.0003	0.0003
35	N-O-Pyridine-2^{+}(S) + e = N-O-Pyridine-2•(D)	-901.33	-898.11	-0.387160	-0.133710	0.4951	0.0012
36	N-O-Pyridine-2^{+}(T) + e = N-O-Pyridine-2•(D)	-809.49	-808.69	-0.385440	-0.133710	0.0012	0.0012
37	N-O-Pyridine-3^{+}(S) + e = N-O-Pyridine-3•(D)	-867.63	-863.47	-0.377790	-0.127120	0.2439	0.0009
38	N-O-Pyridine-3^{+}(T) + e = N-O-Pyridine-3•(D)	-817.79	-816.32	-0.388810	-0.127120	0.0009	0.0009
39	N-O-Pyridine-4^{+}(S) + e = N-O-Pyridine-4•(D)	-878.27	-874.03	-0.382040	-0.123720	0.4161	0.0000
40	N-O-Pyridine-4^{+}(T) + e = N-O-Pyridine-4•(D)	-799.60	-798.52	-0.381640	-0.123720	0.0000	0.0000
41	Ph^{+}(S) + e = Ph•(D)	-801.48	-796.11	-0.353450	-0.093480	0.0000	0.0000
42	Ph^{+}(T) + e = Ph•(D)	-881.18	-875.48	-0.410940	-0.093480	0.0000	0.0000
43	4-NO_2-Ph^{+}(S) + e = 4-NO_2-Ph•(D)	-874.23	-867.56	-0.375810	-0.121220	0.0002	0.0037
44	4-NO_2-Ph^{+}(T) + e = 4-NO_2-Ph•(D)	-942.43	-931.54	-0.422680	-0.121220	0.0037	0.0037
45	4-CH_3O-Ph^{+}(S) + e = 4-CH_3O-Ph•(D)	-789.57	-783.50	-0.341610	-0.090990	0.2471	0.0000

46	4-CH_3O-Ph^+(T) + e = 4-CH_3O-Ph•(D)	-773.62	-772.26	-0.361220	-0.090990	0.0000	0.0000
47	Pyrrole-2^+(S) + e = Pyrrole-2•(D)	-842.68	-842.45	-0.376060	-0.120070	0.5921	0.0002
48	Pyrrole-2^+(T) + e = Pyrrole-2•(D)	-783.45	-783.74	-0.377920	-0.120070	0.0002	0.0002
49	Pyrrole-3^+(S) + e = Pyrrole-3•(D)	-850.31	-850.30	-0.368370	-0.101530	0.4555	0.0006
50	Pyrrole-3^+(T) + e = Pyrrole-3•(D)	-794.98	-792.93	-0.382350	-0.101530	0.0006	0.0006
51	Pyrazole-3^+(S) + e = Pyrazole-3•(D)	-912.78	-908.18	-0.409800	-0.111880	0.0012	0.0017
52	Pyrazole-3^+(T) + e = Pyrazole-3•(D)	-920.95	-916.53	-0.429440	-0.111880	0.0017	0.0017
53	Pyrazole-4^+(S) + e = Pyrazole-4•(D)	-913.31	-910.37	-0.397020	-0.121700	0.0041	0.0002
54	Pyrazole-4^+(T) + e = Pyrazole-4•(D)	-890.89	-886.99	-0.419130	-0.121700	0.0002	0.0002
55	Pyrazole-5^+(S) + e = Pyrazole-5•(D)	-950.19	-944.90	-0.410820	-0.141420	0.4261	0.0005
56	Pyrazole-5^+(T) + e = Pyrazole-5•(D)	-898.78	-890.72	-0.424260	-0.141420	0.0005	0.0005
57	1,3,5-$(CH_3)_3$-Pyrazole-4^+(S) + e = 1,3,5-$(CH_3)_3$-Pyrazole-4•(D)	-816.19	-813.79	-0.342360	-0.106170	0.2741	0.0001
58	1,3,5-$(CH_3)_3$-Pyrazole-4^+(T) + e = 1,3,5-$(CH_3)_3$-Pyrazole-4•(D)	-784.33	-781.81	-0.361090	-0.106170	0.0001	0.0001
59	$C13H18N_6^+$(S) + e = $C13H18N_6$•(D)						
60	$C13H18N_6^+$(T) + e = $C13H18N_6$•(D)						
61	$C13H18N_4^+$(S) + e = $C13H18N_4$•(D)						
62	$C13H18N_4^+$(T) + e = $C13H18N_4$•(D)						
63	Imidazole-2^+(S) + e = Imidazole-2•(D)	-906.49	-903.91	-0.402920	-0.129270	0.5496	0.0003
64	Imidazole-2^+(T) + e = Imidazole-2•(D)	-856.35	-854.45	-0.406700	-0.129270	0.0003	0.0003
65	Imidazole-4^+(S) + e = Imidazole-4•(D)	-885.71	-884.48	-0.406090	-0.103340	0.0023	0.0012
66	Imidazole-4^+(T) + e = Imidazole-4•(D)	-846.49	-843.53	-0.403750	-0.103340	0.0012	0.0012
67	Imidazole-5^+(S) + e = Imidazole-5•(D)	-912.43	-908.20	-0.389650	-0.136600	0.0298	0.0007
68	Imidazole-5^+(T) + e = Imidazole-5•(D)	-846.80	-843.74	-0.403480	-0.136600	0.0007	0.0007
69	1H-1,2,3-Triazole-4^+(S) + e = 1H-1,2,3-Triazole-4•(D)	-971.75	-968.65	-0.429960	-0.132350	0.0003	0.0010

70	1H-1,2,3-Triazole-4^{+}(T) + e = 1H-1,2,3-Triazole-4•(D)	-952.94	-945.01	-0.443080	-0.132350	0.0010	0.0010
71	1H-1,2,3-Triazole-5^{+}(S) + e = 1H-1,2,3-Triazole-5•(D)	-1007.38	-1002.41	-0.431980	-0.164600	0.0004	0.0000
72	1H-1,2,3-Triazole-5^{+}(T) + e = 1H-1,2,3-Triazole-5•(D)	-819.33	-792.92	-0.401420	-0.164600	**Break****	0.0000
73	1H-1,2,4-Triazole-3^{+}(S) + e = 1H-1,2,4-Triazole-3•(D)	-960.45	-958.43	-0.425940	-0.124090	0.0002	0.0013
74	1H-1,2,4-Triazole-3^{+}(T) + e = 1H-1,2,4-Triazole-3•(D)	-973.92	-969.08	-0.451180	-0.124090	0.0013	0.0013
75	1H-1,2,4-Triazole-5^{+}(S) + e = 1H-1,2,4-Triazole-5•(D)	-1009.64	-1002.20	-0.440850	-0.153690	0.2600	0.0004
76	1H-1,2,4-Triazole-5^{+}(T) + e = 1H-1,2,4-Triazole-5•(D)	-973.84	-969.10	-0.450940	-0.153690	0.0004	0.0004
77	2H-1,2,3-Triazole-4^{+}(S) + e = 2H-1,2,3-Triazole-4•(D)	-987.79	-984.19	-0.434110	-0.135600	0.0001	0.0006
78	2H-1,2,3-Triazole-4^{+}(T) + e = 2H-1,2,3-Triazole-4•(D)	-989.24	-981.99	-0.461460	-0.135600	0.0006	0.0006
79	4H-1,2,4-Triazole-3^{+}(S) + e = 4H-1,2,4-Triazole-3•(D)	-975.01	-971.41	-0.415010	-0.154050	0.0004	0.0002
80	4H-1,2,4-Triazole-3^{+}(T) + e = 4H-1,2,4-Triazole-3•(D)	-964.44	-957.51	-0.445670	-0.154050	0.0002	0.0002
81	Tetrazole-5^{+}(S) + e = Tetrazole-5•(D)	-790.05	-782.89	-0.365710	-0.183370	**Break****	0.0012
82	Tetrazole-5^{+}(T) + e = Tetrazole-5•(D)	-1072.06	-1063.03	-0.475980	-0.183370	0.0012	0.0012
83	Furan-2^{+}(S) + e = Furan-2•(D)	-915.72	-913.28	-0.401650	-0.130550	0.5993	0.0019
84	Furan-2^{+}(T) + e = Furan-2•(D)	-848.21	-846.11	-0.405900	-0.130550	0.0019	0.0019
85	Furan-3^{+}(S) + e = Furan-3•(D)	-928.03	-925.79	-0.404520	-0.123410	0.4382	0.0003
86	Furan-3^{+}(T) + e = Furan-3•(D)	-859.57	-856.05	-0.410180	-0.123410	0.0003	0.0003
87	Thiophene-2^{+}(S) + e = Thiophene-2•(D)	-878.60	-876.75	-0.371020	-0.132020	0.6611	0.0012
88	Thiophene-2^{+}(T) + e = Thiophene-2•(D)	-841.34	-839.11	-0.395210	-0.132020	0.0012	0.0012
89	Thiophene-3^{+}(S) + e = Thiophene-3•(D)	-852.03	-847.77	-0.367640	-0.116430	0.0000	0.0003
90	Thiophene-3^{+}(T) + e = Thiophene-3•(D)	-857.20	-853.14	-0.401770	-0.116430	0.0003	0.0003

* Ring Deviation - суммарное отклонение атомов от плоскости цикла (ангстрем)

** Break - разрыв цикла

Присоединение электрона к карбкатиону характеризуется:

1. Сродство к электрону для большинства карбкатионов от -650 до -1300 кДж/моль.

2. В случаях нарушения плоскости цикла в исходных карбкатионах происходит восстановление плоской структуры при присоединении электрона. Исключением являются карбкатионы пиридина и пиразина, где восстановление не происходит, либо происходит потеря плоского строения цикла.
3. После присоединения электронов, нейтральные частицы имеют невысокие отрицательные значения LUMO, т.е. практически теряют способность к присоединению второго электрона.