

Сродство к электрону и структурные параметры $R^+ + e = R\bullet$

| № | Reaction | ΔE , kJ/mol | ΔG , kJ/mol | LUMO, Eh | | Ring Deviation *, Å | |
|----|--|---------------------|---------------------|-----------|------------|---------------------|------------|
| | | | | R^+ | $R\bullet$ | R^+ | $R\bullet$ |
| 1 | $CH_3^+(S) + e = CH_3\bullet(D)$ | -954.08 | -959.69 | -0.486590 | -0.080600 | | |
| 2 | $CH_3^+(T) + e = CH_3\bullet(D)$ | -1293.77 | -1278.87 | -0.544280 | -0.080600 | | |
| 3 | $C_2H_5^+(S) + e = C_2H_5\bullet(D)$ | -788.09 | -796.17 | -0.324030 | -0.060550 | | |
| 4 | $C_2H_5^+(T) + e = C_2H_5\bullet(D)$ | -1141.40 | -1119.17 | -0.496720 | -0.060550 | | |
| 5 | $1-CH_3-C_2H_4^+(S) + e = 1-CH_3-C_2H_4\bullet(D)$ | -709.39 | -714.86 | -0.347960 | -0.048460 | | |
| 6 | $1-CH_3-C_2H_4^+(T) + e = 1-CH_3-C_2H_4\bullet(D)$ | -1078.45 | -1059.04 | -0.466640 | -0.048460 | | |
| 7 | $1,1-(CH_3)_2-C_2H_3^+(S) + e = 1,1-(CH_3)_2-C_2H_3\bullet(D)$ | -650.04 | -648.74 | -0.321560 | -0.042240 | | |
| 8 | $1,1-(CH_3)_2-C_2H_3^+(T) + e = 1,1-(CH_3)_2-C_2H_3\bullet(D)$ | -1030.07 | -1014.97 | -0.428030 | -0.042240 | | |
| 9 | $Pyridine-2^+(S) + e = Pyridine-2\bullet(D)$ | -756.19 | -757.17 | -0.343690 | -0.084630 | 0.0005 | 0.0012 |
| 10 | $Pyridine-2^+(T) + e = Pyridine-2\bullet(D)$ | -927.48 | -919.04 | -0.430750 | -0.084630 | 0.0012 | 0.0012 |
| 11 | $Pyridine-3^+(S) + e = Pyridine-3\bullet(D)$ | -807.61 | -805.95 | -0.341510 | -0.109400 | 0.0011 | 0.2607 |
| 12 | $Pyridine-3^+(T) + e = Pyridine-3\bullet(D)$ | -910.16 | -903.99 | -0.416460 | -0.109400 | 0.2607 | 0.2607 |
| 13 | $Pyridine-4^+(S) + e = Pyridine-4\bullet(D)$ | -823.98 | -817.41 | -0.368060 | -0.110460 | 0.0005 | 0.0002 |
| 14 | $Pyridine-4^+(T) + e = Pyridine-4\bullet(D)$ | -910.17 | -904.32 | -0.411220 | -0.110460 | 0.0002 | 0.0002 |
| 15 | $Pyrazine-2^+(S) + e = Pyrazine-2\bullet(D)$ | -782.24 | -783.30 | -0.355910 | -0.102310 | 0.0007 | 0.2523 |
| 16 | $Pyrazine-2^+(T) + e = Pyrazine-2\bullet(D)$ | -956.78 | -950.21 | -0.435720 | -0.102310 | 0.2523 | 0.2523 |
| 17 | $Pyrimidine-2^+(S) + e = Pyrimidine-2\bullet(D)$ | -778.73 | -780.86 | -0.342040 | -0.088310 | 0.0003 | 0.0019 |
| 18 | $Pyrimidine-2^+(T) + e = Pyrimidine-2\bullet(D)$ | -913.56 | -911.73 | -0.413720 | -0.088310 | 0.0019 | 0.0019 |
| 19 | $Pyrimidine-4^+(S) + e = Pyrimidine-4\bullet(D)$ | -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 | $4\text{-CH}_3\text{O-Ph}^+(\text{S}) + \text{e} = 4\text{-CH}_3\text{O-Ph}\cdot(\text{D})$ | -789.57 | -783.50 | -0.341610 | -0.090990 | 0.2471 | 0.0000 |
| 46 | $4\text{-CH}_3\text{O-Ph}^+(\text{T}) + \text{e} = 4\text{-CH}_3\text{O-Ph}\cdot(\text{D})$ | -773.62 | -772.26 | -0.361220 | -0.090990 | 0.0000 | 0.0000 |
| 47 | $\text{Pyrrole-2}^+(\text{S}) + \text{e} = \text{Pyrrole-2}\cdot(\text{D})$ | -842.68 | -842.45 | -0.376060 | -0.120070 | 0.5921 | 0.0002 |
| 48 | $\text{Pyrrole-2}^+(\text{T}) + \text{e} = \text{Pyrrole-2}\cdot(\text{D})$ | -783.45 | -783.74 | -0.377920 | -0.120070 | 0.0002 | 0.0002 |
| 49 | $\text{Pyrrole-3}^+(\text{S}) + \text{e} = \text{Pyrrole-3}\cdot(\text{D})$ | -850.31 | -850.30 | -0.368370 | -0.101530 | 0.4555 | 0.0006 |
| 50 | $\text{Pyrrole-3}^+(\text{T}) + \text{e} = \text{Pyrrole-3}\cdot(\text{D})$ | -794.98 | -792.93 | -0.382350 | -0.101530 | 0.0006 | 0.0006 |
| 51 | $\text{Pyrazole-3}^+(\text{S}) + \text{e} = \text{Pyrazole-3}\cdot(\text{D})$ | -912.78 | -908.18 | -0.409800 | -0.111880 | 0.0012 | 0.0017 |
| 52 | $\text{Pyrazole-3}^+(\text{T}) + \text{e} = \text{Pyrazole-3}\cdot(\text{D})$ | -920.95 | -916.53 | -0.429440 | -0.111880 | 0.0017 | 0.0017 |
| 53 | $\text{Pyrazole-4}^+(\text{S}) + \text{e} = \text{Pyrazole-4}\cdot(\text{D})$ | -913.31 | -910.37 | -0.397020 | -0.121700 | 0.0041 | 0.0002 |
| 54 | $\text{Pyrazole-4}^+(\text{T}) + \text{e} = \text{Pyrazole-4}\cdot(\text{D})$ | -890.89 | -886.99 | -0.419130 | -0.121700 | 0.0002 | 0.0002 |
| 55 | $\text{Pyrazole-5}^+(\text{S}) + \text{e} = \text{Pyrazole-5}\cdot(\text{D})$ | -950.19 | -944.90 | -0.410820 | -0.141420 | 0.4261 | 0.0005 |
| 56 | $\text{Pyrazole-5}^+(\text{T}) + \text{e} = \text{Pyrazole-5}\cdot(\text{D})$ | -898.78 | -890.72 | -0.424260 | -0.141420 | 0.0005 | 0.0005 |
| 57 | $1,3,5\text{-(CH}_3)_3\text{-Pyrazole-4}^+(\text{S}) + \text{e} = 1,3,5\text{-(CH}_3)_3\text{-Pyrazole-4}\cdot(\text{D})$ | -816.19 | -813.79 | -0.342360 | -0.106170 | 0.2741 | 0.0001 |
| 58 | $1,3,5\text{-(CH}_3)_3\text{-Pyrazole-4}^+(\text{T}) + \text{e} = 1,3,5\text{-(CH}_3)_3\text{-Pyrazole-4}\cdot(\text{D})$ | -784.33 | -781.81 | -0.361090 | -0.106170 | 0.0001 | 0.0001 |
| 63 | $\text{Imidazole-2}^+(\text{S}) + \text{e} = \text{Imidazole-2}\cdot(\text{D})$ | -906.49 | -903.91 | -0.402920 | -0.129270 | 0.5496 | 0.0003 |
| 64 | $\text{Imidazole-2}^+(\text{T}) + \text{e} = \text{Imidazole-2}\cdot(\text{D})$ | -856.35 | -854.45 | -0.406700 | -0.129270 | 0.0003 | 0.0003 |
| 65 | $\text{Imidazole-4}^+(\text{S}) + \text{e} = \text{Imidazole-4}\cdot(\text{D})$ | -885.71 | -884.48 | -0.406090 | -0.103340 | 0.0023 | 0.0012 |
| 66 | $\text{Imidazole-4}^+(\text{T}) + \text{e} = \text{Imidazole-4}\cdot(\text{D})$ | -846.49 | -843.53 | -0.403750 | -0.103340 | 0.0012 | 0.0012 |
| 67 | $\text{Imidazole-5}^+(\text{S}) + \text{e} = \text{Imidazole-5}\cdot(\text{D})$ | -912.43 | -908.20 | -0.389650 | -0.136600 | 0.0298 | 0.0007 |
| 68 | $\text{Imidazole-5}^+(\text{T}) + \text{e} = \text{Imidazole-5}\cdot(\text{D})$ | -846.80 | -843.74 | -0.403480 | -0.136600 | 0.0007 | 0.0007 |
| 69 | $1\text{H-1,2,3-Triazole-4}^+(\text{S}) + \text{e} = 1\text{H-1,2,3-Triazole-4}\cdot(\text{D})$ | -971.75 | -968.65 | -0.429960 | -0.132350 | 0.0003 | 0.0010 |
| 70 | $1\text{H-1,2,3-Triazole-4}^+(\text{T}) + \text{e} = 1\text{H-1,2,3-Triazole-4}\cdot(\text{D})$ | -952.94 | -945.01 | -0.443080 | -0.132350 | 0.0010 | 0.0010 |
| 71 | $1\text{H-1,2,3-Triazole-5}^+(\text{S}) + \text{e} = 1\text{H-1,2,3-Triazole-5}\cdot(\text{D})$ | -1007.38 | -1002.41 | -0.431980 | -0.164600 | 0.0004 | 0.0000 |
| 72 | $1\text{H-1,2,3-Triazole-5}^+(\text{T}) + \text{e} = 1\text{H-1,2,3-Triazole-5}\cdot(\text{D})$ | -819.33 | -792.92 | -0.401420 | -0.164600 | Break** | 0.0000 |
| 73 | $1\text{H-1,2,4-Triazole-3}^+(\text{S}) + \text{e} = 1\text{H-1,2,4-Triazole-3}\cdot(\text{D})$ | -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

1. Сродство к электрону для большинства карбкатионов находится в диапазоне 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.