

THE FIRST IONIZATION ENERGY, ELECTRON AFFINITY AND ELECTRONEGATIVITY CALCULATED BY THE $X\alpha$ METHOD WITH AB INITIO SELF-CONSISTENT EXCHANGE PARAMETER

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Ab initio self-consistent exchange parameters α_{SCF} have been introduced into the $X\alpha$ method. Slater's transition-state method and the definition of electronegativity given by Iczkowski and Margrave have been applied. First ionization energy, electron affinity and electronegativity have been calculated.

Introduction

Important development has been made in the theory of the $X\alpha$ method since it was first advanced by Slater [1]. All the same it is still not precisely known how the exchange parameter α is to be determined. In 1976 Gopinathan, Whitehead and Bogdanovic [2] derived an analytical expression for the α parameter assuming a linear variation of the Fermi-hole density. However, they applied an adjusting parameter, too.

Earlier, in 1974, one of the authors [3] proposed a method to determine ab initio exchange parameters in the $X\alpha$ method. Recently a comparison has been presented [4] for the spin orbitals of a few atoms calculated by the $X\alpha$ method with several values of exchange parameters.

Here, the first ionization energy, electron affinity, electronegativity and chemical potential calculated by the $X\alpha$ method using ab initio self-consistent exchange parameter are presented. Slater's transition-state method has been applied.

The electronegativity determined by the formula of Mulliken [5] and the transition-state method is equal to the one obtained using the definition of electronegativity by Iczkowski and Margrave [6] disregarding the third order terms.

The $X\alpha$ method with self-consistent ab initio exchange parameters

One of the authors has suggested a method [3] which rests on the free-electron gas theory. The exchange potential of an electron with spin up can be written in the form [7]

$$V_{X\uparrow}(1) = -8F(\eta) \left[\frac{3}{4\pi} \rho_{\uparrow}(1) \right]^{1/3}, \quad (1)$$

where

$$F(\eta) = \frac{1}{2} + \frac{1-\eta^2}{4\eta} \ln \left| \frac{1+\eta}{1-\eta} \right|. \quad (2)$$

ρ_{\uparrow} is the total electron density of the electrons with spin up and

$$\eta = \frac{p}{p_F}, \quad (3)$$

where p is the momentum of the electron considered and p_F is the Fermi momentum. (Energies are in Rydbergs, other quantities are in atomic units.) This exchange potential can be averaged in the momentum space near the Fermi surface for a thin shell containing ν_{\uparrow} electrons in the unit volume, where

$$\nu_{\uparrow}(1) = u_i^*(1)u_i(1) \quad (4)$$

is the density of the electron considered. We then find for the exchange potential the following

$$V_{X\alpha_{\uparrow\text{shell}}} = -6\alpha_{\uparrow\text{shell}} \left[\frac{3}{4\pi} \rho_{\uparrow}(1) \right]^{1/3}, \quad (5)$$

where

$$\alpha_{\uparrow\text{shell}} = \frac{\rho_{\uparrow}}{\nu_{\uparrow}} \left[1 - \frac{1}{2}\eta - \frac{1}{2}\eta^3 + \frac{1}{4}(\eta^2 - 1)^2 \ln \left| \frac{1+\eta}{1-\eta} \right| \right] \quad (6)$$

and

$$\eta = \left(1 - \frac{\nu_{\uparrow}}{\rho_{\uparrow}} \right)^{1/3}. \quad (7)$$

As this exchange potential is different for the different spin orbitals, i.e. for different shells, it is averaged over the shells

$$\alpha_{\uparrow}(r) = \frac{\sum_{j\uparrow} n_j \alpha_{\uparrow\text{shell}}}{\sum_{j\uparrow} n_j}. \quad (8)$$

This exchange parameter $\alpha_{\uparrow}(r)$ is still a function. To get a constant parameter α_{\uparrow} the mean squared deviation of the original $X\alpha$ exchange potential

$$V_{X\alpha_{\uparrow}}(1) = -6\alpha_{\uparrow} \left[\frac{3}{4\pi} \rho_{\uparrow}(1) \right]^{1/3} \quad (9)$$

and the exchange potential

$$V_{X\alpha_{\uparrow}(1)}(1) = -6\alpha_{\uparrow}(1) \left[\frac{3}{4\pi} \rho_{\uparrow}(1) \right]^{1/3} \quad (10)$$

with the exchange parameter (8) is minimised. This exchange parameter α_{\uparrow} can be determined self-consistently. That is why the method is denoted by $X\alpha_{\text{SCF}}$.

**Calculation of ionization energy, electron affinity
and chemical potential in the $X\alpha$ method**

The first ionization energies of atoms have been calculated by the Slater's transition-state method [8]. The ionization energy can be given by the negative of the corresponding orbital energy with an occupation number reduced by half

$$I = -\epsilon_{X\alpha} \left(n - \frac{1}{2} \right). \quad (11)$$

Similarly, the electron affinity is

$$A = -\epsilon_{X\alpha} \left(n + \frac{1}{2} \right). \quad (12)$$

The electronegativity was given by Mulliken [5] with the expression

$$\chi = \frac{A + I}{2}. \quad (13)$$

As the ionization energy of an atom with N electrons is

$$I = \langle EX\alpha(N-1) \rangle - \langle EX\alpha(N) \rangle \quad (14)$$

and the electron affinity is

$$A = \langle EX\alpha(N) \rangle - \langle EX\alpha(N+1) \rangle, \quad (15)$$

for the electronegativity we get

$$\chi = \frac{1}{2} \{ \langle EX\alpha(N-1) \rangle - \langle EX\alpha(N+1) \rangle \}. \quad (16)$$

Two cases are treated. First, the electron leaves the same shell (i) as it enters in case of ionization. Expanding around the neutral atomic state (as a transition-state) the total $X\alpha$ energy is given by

$$\langle EX\alpha(N-1) \rangle = \langle EX\alpha(N) \rangle - \left. \frac{\partial \langle EX\alpha \rangle}{\partial n_i} \right|_0 + \frac{1}{2} \left. \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_i^2} \right|_0 - \frac{1}{3!} \left. \frac{\partial^3 \langle EX\alpha \rangle}{\partial n_i^3} \right|_0 + \dots \quad (17)$$

and

$$\langle EX\alpha(N+1) \rangle = \langle EX\alpha(N) \rangle + \left. \frac{\partial \langle EX\alpha \rangle}{\partial n_i} \right|_0 + \frac{1}{2} \left. \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_i^2} \right|_0 + \frac{1}{3!} \left. \frac{\partial^3 \langle EX\alpha \rangle}{\partial n_i^3} \right|_0 + \dots \quad (18)$$

For the electronegativity we get

$$\chi = -\frac{\partial \langle EX\alpha \rangle}{\partial n_i} \Big|_0 - \frac{1}{3!} \frac{\partial^3 \langle EX\alpha \rangle}{\partial n_i^3} \Big|_0 \approx -\epsilon_{iX\alpha} \quad (19)$$

using the well-known

$$\epsilon_{iX\alpha} = \frac{\partial \langle EX\alpha \rangle}{\partial n_i} \quad (20)$$

formula of the $X\alpha$ method.

Secondly, the electron leaves the i th shell forming a positive ion and enters the k th shell forming a negative ion. The occupation numbers of the i th shell are denoted by n_i^{N-1} , and n_i^{N+1} and n_i^0 for the negative and positive ions and for a suitably chosen transition-state, respectively. The same notation is used for the k th shell.

$$\begin{aligned} \langle EX\alpha(N-1) \rangle &= \langle EX\alpha \rangle_0 + \frac{\partial \langle EX\alpha \rangle}{\partial n_i} \Big|_0 (n_i^{N-1} - n_i^0) + \\ &+ \frac{\partial \langle EX\alpha \rangle}{\partial n_k} \Big|_0 (n_k^{N-1} - n_k^0) + \frac{1}{2} \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_i^2} \Big|_0 (n_i^{N-1} - n_i^0)^2 + \\ &+ \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_i \partial n_k} \Big|_0 (n_i^{N-1} - n_i^0)(n_k^{N-1} - n_k^0) + \frac{1}{2} \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_k^2} \Big|_0 (n_k^{N-1} - n_k^0)^2 + \dots, \end{aligned} \quad (21)$$

$$\begin{aligned} \langle EX\alpha(N-1) \rangle &= \langle EX\alpha \rangle_0 + \frac{\partial \langle EX\alpha \rangle}{\partial n_i} \Big|_0 (n_i^{N+1} - n_i^0) + \\ &+ \frac{\partial \langle EX\alpha \rangle}{\partial n_k} \Big|_0 (n_k^{N+1} - n_k^0) + \frac{1}{2} \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_i^2} \Big|_0 (n_i^{N+1} - n_i^0)^2 + \\ &+ \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_i \partial n_k} \Big|_0 (n_i^{N+1} - n_i^0)(n_k^{N+1} - n_k^0) + \frac{1}{2} \frac{\partial^2 \langle EX\alpha \rangle}{\partial n_k^2} \Big|_0 (n_k^{N+1} - n_k^0)^2 + \dots \end{aligned} \quad (22)$$

The third-order terms are neglected. If the transition-state is given by

$$n_i^0 = (n_i^{N+1} + n_i^{N-1})/2$$

and

$$n_k^0 = (n_k^{N+1} + n_k^{N-1})/2 \quad (23)$$

the second-order terms will vanish in the expression of electronegativity. Taking into consideration that

$$n_i^{N-1} - n_i^{N+1} = n_k^{N-1} - n_k^{N+1} = -1, \quad (24)$$

we arrive at the results

$$\chi \approx -\frac{1}{2} \epsilon_{iX\alpha}^0 - \frac{1}{2} \epsilon_{kX\alpha}^0, \quad (25)$$

where the superscript 0 shows that the one-electron energies are calculated for the transition-state.

Recently the electronegativity χ of an atom has been defined by the formula [7]

$$\chi = -\mu = -\frac{\partial E}{\partial N}\Big|_Z, \quad (26)$$

where E is the total energy of the atom, N is the number of electrons and Z is the atomic number. So the electronegativity is the negative of the chemical potential μ . The partial derivative of the $X\alpha$ total energy with respect to the number of electrons is given by

$$\begin{aligned} \frac{\partial \langle EX\alpha \rangle}{\partial N}\Big|_Z &= \sum_j \int \left\{ \frac{\partial \langle EX\alpha \rangle}{\partial u_j^*}\Big|_Z \frac{\partial u_j^*}{\partial N}\Big|_Z + \frac{\partial \langle EX\alpha \rangle}{\partial u_j}\Big|_Z \frac{\partial u_j}{\partial N}\Big|_Z \right\} dv + \\ &+ \sum_j \frac{\partial \langle EX\alpha \rangle}{\partial n_j}\Big|_Z \frac{\partial n_j}{\partial N}. \end{aligned} \quad (27)$$

The summation goes for the spin orbitals with the occupation number n_j . The first term in Eq. (27) containing the partial derivative of the spin orbitals vanishes as the $X\alpha$ one-electron equations come from the variation principle. We have

$$\begin{aligned} &\sum_j \int \left\{ \frac{\partial \langle EX\alpha \rangle}{\partial u_j^*}\Big|_Z \frac{\partial u_j^*}{\partial N}\Big|_Z + \frac{\partial \langle EX\alpha \rangle}{\partial u_j}\Big|_Z \frac{\partial u_j}{\partial N}\Big|_Z \right\} dv = \\ &= \sum_j \int (n_j \epsilon_j u_j \frac{\partial u_j^*}{\partial N}\Big|_Z + n_j \epsilon_j u_j^* \frac{\partial u_j}{\partial N}\Big|_Z) dv = \sum_j n_j \epsilon_j \frac{\partial}{\partial N} \int u_j^* u_j dv = 0, \end{aligned} \quad (28)$$

because the spin orbitals are normalised.

To evaluate the second term of expression (27), two cases are considered. Provided only one spin orbital (i) changes its occupation number when going from the negative ion to the positive one, we have

$$\sum_j \frac{\partial \langle EX\alpha \rangle}{\partial n_j}\Big|_Z \frac{\partial n_j}{\partial N} = \epsilon_i X\alpha. \quad (29)$$

So the electronegativity equals the negative of the highest occupied orbital energy, i.e.,

$$\chi = -\mu = -\epsilon_i X\alpha. \quad (30)$$

In the second case two spin orbitals (i and k) change their occupation numbers during a transition from the negative to the positive ion. These occupation numbers n_i and n_k are not a continuous function of N at the ground state of the atom and hence the formula (29) cannot be applied. As it has been shown the Slater's

transition-state method can be used in this case, too. Nevertheless, it is worth mentioning that the formula (25) obtained by the transition-state method contains derivatives at the transition-state which differ from the derivatives calculated at the ground state of the atom.

It is easy to calculate the difference between the Mulliken's expression of electronegativity and the formula given by Margrave and Iczkowski. The electron affinity and the first ionization energy ($I = I_1$) can be written in the power series of N

$$A = \langle EX\alpha(N) \rangle - \langle EX\alpha(N+1) \rangle = - \left. \frac{\partial \langle EX\alpha \rangle}{\partial N} \right|_Z - \frac{1}{2} \left. \frac{\partial^2 \langle EX\alpha \rangle}{\partial N^2} \right|_Z - \frac{1}{3!} \left. \frac{\partial^3 \langle EX\alpha \rangle}{\partial N^3} \right|_Z + \dots, \quad (31)$$

$$I = I_1 = \langle EX\alpha(N-1) \rangle - \langle EX\alpha(N) \rangle = - \left. \frac{\partial \langle EX\alpha \rangle}{\partial N} \right|_Z + \frac{1}{2} \left. \frac{\partial^2 \langle EX\alpha \rangle}{\partial N^2} \right|_Z - \frac{1}{3!} \left. \frac{\partial^3 \langle EX\alpha \rangle}{\partial N^3} \right|_Z + \dots \quad (32)$$

Similarly, the second ionization energy is given by

$$I_2 = \langle EX\alpha(N-2) \rangle - \langle EX\alpha(N-1) \rangle = -I_1 + \langle EX\alpha(N-2) \rangle - \langle EX\alpha(N) \rangle = -I_1 - 2 \left. \frac{\partial \langle EX\alpha \rangle}{\partial N} \right|_Z + 2 \left. \frac{\partial^2 \langle EX\alpha \rangle}{\partial N^2} \right|_Z + \frac{4}{3} \left. \frac{\partial^3 \langle EX\alpha \rangle}{\partial N^3} \right|_Z + \dots \quad (33)$$

Combining the formulae (31), (32) and (33) the electronegativity is given by

$$\chi = - \left. \frac{\partial E}{\partial N} \right|_Z = \frac{1}{2}(I_1 + A) - \frac{A + I_2 - 2I_1}{6}. \quad (34)$$

Results and discussion

The first ionization energies have been determined by the transition-state method using the formula (11). Though, in the case of a few atoms the occupation number of two shells changes during the ionization. (For example the electron configuration for Ni is $4s^2 3d^8$ and for Ni^+ $3d^9$, so the transition-state is $4s^1 3d^{8.5}$.) Denoting the occupation numbers of these two shells in the initial state by n_1^i, n_2^i , in the final state by n_1^f, n_2^f and in the transition-state by n_1^0, n_2^0 , the expansion of

the total energy around the transition-state is given by

$$\begin{aligned} \langle EX\alpha(n_1^i, n_2^i) \rangle = & \langle EX\alpha(n_1^0, n_2^0) \rangle + \frac{\partial \langle EX\alpha \rangle}{\partial n_1} \Big|_0 (n_1^i - n_1^0) + \\ & + \frac{\partial \langle EX\alpha \rangle}{\partial n_2} \Big|_0 (n_2^i - n_2^0) + \dots, \end{aligned} \quad (35)$$

$$\begin{aligned} \langle EX\alpha(n_1^f, n_2^f) \rangle = & \langle EX\alpha(n_1^0, n_2^0) \rangle + \frac{\partial \langle EX\alpha \rangle}{\partial n_1} \Big|_0 (n_1^f - n_1^0) + \\ & + \frac{\partial \langle EX\alpha \rangle}{\partial n_2} \Big|_0 (n_2^f - n_2^0) + \dots. \end{aligned} \quad (36)$$

Neglecting the third-order terms we arrive at the ionization energy

$$\begin{aligned} \langle EX\alpha(n_1^f, n_2^f) \rangle - \langle EX\alpha(n_1^i, n_2^i) \rangle = & \frac{\partial \langle EX\alpha \rangle}{\partial n_1} \Big|_0 (n_1^f - n_1^i) + \\ & + \frac{\partial \langle EX\alpha \rangle}{\partial n_2} \Big|_0 (n_2^f - n_2^i). \end{aligned} \quad (37)$$

For example the ionization energy of the Ni is given by

$$I = \epsilon_{3d}^0 - 2\epsilon_{4s}^0, \quad (38)$$

where ϵ_{3d}^0 and ϵ_{4s}^0 are the 3d and 4s one-electron energies in the transition-state mentioned above. The same expression has been used for V and Co.

Table I contains the ionization energies calculated by the $X\alpha$ method with the exchange parameters $\alpha = 1$, α_{vt} [9] and α_{SCF} . For comparison the experimental [10] and the Hartree-Fock data [11] are also presented. Of course, the Hartree-Fock ionization energies are the closest to the experimental data. The $X\alpha$ results with $\alpha = 1$ are the furthest from the experimental ionization energies. The $X\alpha$ ionization energies gained by α_{vt} and α_{SCF} are often very close together, though sometimes there is considerable difference between them.

Table II contains the electronegativity of atoms calculated by the $X\alpha$ method with the exchange parameters α_{SCF} and α_{vt} [12]. The expressions (19) and (25) are used for this calculation. Generally, there is only small difference between the results gained by the exchange parameter α_{SCF} and α_{vt} .

Table III includes the electron affinity of atoms calculated by the $X\alpha$ method with the exchange parameters α_{SCF} and α_{vt} [12]. The electron affinity may be given by the Mulliken formula (13)

$$A = 2\chi - I. \quad (39)$$

Table I
 First ionization energies of atoms calculated by the Hartree-Fock and the $X\alpha$ methods with $\alpha = 1$ [9] and α_{vt} [9] and the self-consistently determined exchange parameters α_{SCF} . Experimental ionization energies are also presented [10] (in Rydbergs)

Z	HF	$\alpha = 1$	$X\alpha$ α_{vt}	α_{SCF}	Exp
3	0.392	0.434	0.370	0.318	0.396
4	0.619	0.811	0.675	0.638	0.685
5	0.620	0.750	0.582	0.471	0.610
6	0.814	0.992	0.781	0.809	0.828
7	1.017	1.255	0.984	1.012	1.069
8	1.233	1.522	1.194	1.223	1.000
9	1.460	1.798	1.412	1.442	1.280
10	1.701	2.086	1.635	1.671	1.585
11	0.365	0.430	0.345	0.338	0.378
12	0.500	0.683	0.547	0.547	0.562
13	0.420	0.519	0.384	0.378	0.440
14	0.557	0.699	0.528	0.525	0.599
15	0.701	0.881	0.673	0.747	0.775
16	0.853	1.068	0.824	0.818	0.761
17	1.013	1.260	0.979	0.973	0.956
18	1.182	1.458	1.140	1.280	1.158
19	0.295	0.362	0.286	0.279	0.319
20	0.391	0.540	0.427	0.417	0.449
21	0.420	0.584	0.467	0.310	0.482
22	0.444	0.620	0.499	0.493	0.502
23	0.466	0.406	0.474	0.475	0.495
24	0.415	0.553	0.464	0.463	0.497
25	0.503	0.711	0.572	0.477	0.546
26	0.520	0.738	0.594	0.588	0.514
27	0.537	0.293	0.400	0.403	0.578
28	0.553	0.266	0.383	0.386	0.561
29	0.477	0.660	0.542	0.646	0.567
30	0.585	0.836	0.670	0.664	0.690
31	0.417	0.523	0.377	0.521	0.441
32	0.539	0.681	0.503	0.495	0.579
33	0.660	0.834	0.625	0.616	0.721
34	0.785	0.986	0.747	0.737	0.717
35	0.914	1.140	0.872	0.859	0.870
36	1.048	1.296	0.997	0.984	1.029

Table II
 Electronegativity of atoms calculated by the $X\alpha$ method with the
 exchange parameters α_{SCF} and α_{vt} [12] (in Rydbergs)

Z	α_{SCF}	α_{vt}
3	0.165	0.190
4	0.253	0.279
5	0.264	0.250
6	0.399	0.377
7	0.535	0.512
8	0.680	0.656
9	0.836	0.808
10	0.791	0.758
11	0.164	0.171
12	0.223	0.223
13	0.160	0.165
14	0.262	0.265
15	0.365	0.368
16	0.474	0.479
17	0.590	0.596
18	0.519	0.523
19	0.135	0.141
20	0.128	0.137
21	0.209	0.185
22	0.217	0.224
23	0.299	0.245
24	0.314	0.254
25	0.311	0.318
26	0.338	0.346
27	0.351	0.276
28	0.362	0.284
29	0.373	0.290
30	0.228	0.269
31	0.149	0.155
32	0.241	0.248
33	0.332	0.340
34	0.425	0.434
35	0.521	0.532

Table III
 Electron affinity of atoms calculated by the $X\alpha$ method with the exchange parameter α_{SCF} and α_{vt} [12] using the formula (13) and (12). In a few cases the Hartree-Fock [14] and the experimental [13] electron affinities are also presented (in Rydbergs)

Z	$X\alpha$				Exp	HF
	α_{SCF} Eq. (39)	α_{SCF} Eq. (12)	α_{vt} Eq. (39)	α_{vt} Eq. (12)		
3	0.012		0.009			0.043
4	-0.132		-0.115			
5	0.057		-0.082			0.022
6	-0.010	0.065	-0.027	0.050	0.092	0.086
7	0.058	0.135	0.040	0.118		-0.020
8	0.137	0.216	0.118	0.198	0.108	0.090
9	0.229	0.309	0.206	0.287	0.253	0.248
10	-0.089		-0.120			
11	-0.010	0.017	-0.004			0.057
12	-0.101		-0.101			
13	-0.057		-0.053			0.036
14	-0.001	0.082	0.001	0.041		0.102
15	-0.017	0.142	0.063	0.101		0.057
16	0.130	0.167	0.134	0.171	0.152	0.156
17	0.208	0.244	0.213	0.248	0.266	0.262
18	-0.242		-0.095			
19	-0.010	0.012	-0.004			
20	-0.161		-0.153			
21	0.108		-0.097			
22	-0.059		-0.051			
23	0.123		0.016			
24	0.150		0.043			
25	0.144	0.097	0.065	0.107		
26	0.088		0.099	0.142		
27	0.094		0.154	0.176		
28	0.339		0.185	0.210		
29	0.101		0.038			
30	-0.209		-0.132			
31	0.066	0.061	-0.067			
32	-0.013		-0.007			
33	0.048	0.083	0.054			
34	0.113		0.121			
35	0.182	0.213	0.193			

Table IV
The electron affinity, the first and second ionization energies
and the chemical potential for a few atoms (in Rydbergs)

Z	A Eq. (12)	I_1 Eq. (11)	I_2 Eq. (11)	χ Eq. (30)	$\chi_M = \frac{1}{2}(I_1 + A)$	χ Eq. (34)
6	0.065	0.809	1.817	0.399	0.437	0.393
9	0.309	1.442	2.872	0.836	0.876	0.826
17	0.244	0.973	1.827	0.590	0.609	0.588
35	0.213	0.860	1.608	0.521	0.536	0.519

In a few cases the electron affinity has been determined by using the expression (12), too. For comparison the experimental [13] and Hartree-Fock [14] data are also presented for a few atoms. With a few exceptions there is quite good agreement between the experimental and the $X\alpha$ data. In the majority of the results the electron affinities determined by the exchange parameter α_{SCF} and α_{ut} are close together. There is considerable disagreement between them in a few cases. However, it is not surprising that there is a difference between the electron affinity calculated by expressions (12) and (39). The Eq. (34) presents a more precise expression. To illustrate the correctness of Eq. (34), the electronegativity has been calculated using the expressions (30) and (34) for a few atoms. Table IV presents the electron affinity calculated by Eq. (12), the first and second ionization energies calculated by Eq. (11), the electronegativity using the expression (30), the Mulliken's electronegativity and the electronegativity given by Eq. (34).

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