

## Use of combined Hartree–Fock–Roothaan theory in evaluation of lowest states of $K[Ar]4s^03d^1$ and $Cr^+[Ar]4s^03d^5$ isoelectronic series over noninteger n-Slater type orbitals

II GUSEINOV\*, M ERTURK and E SAHIN

Department of Physics, Faculty of Arts and Sciences, Onsekiz Mart University, Çanakkale, Turkey

\*Corresponding author. E-mail: ihuseyin@comu.edu.tr; iguseinov@cheerful.com

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**Abstract.** By using noninteger n-Slater type orbitals in combined Hartree–Fock–Roothaan method, self-consistent field calculations of orbital and lowest states energies have been performed for the isoelectronic series of open shell systems  $K[Ar]4s^03d^1$  ( $^2D$ ) ( $Z = 19–30$ ) and  $Cr^+[Ar]4s^03d^5$  ( $^6S$ ) ( $Z = 24–30$ ). The results of the calculations for the orbital and total energies obtained by using minimal basis-sets of noninteger n-Slater type orbitals are given in the tables. The results are compared with the extended-basis Hartree–Fock computations. The orbital and total energies are in good agreement with those presented in the literature. The results can be useful in the study of various properties of heavy atomic systems when the combined Hartree–Fock–Roothaan approach is employed.

**Keywords.** Hartree–Fock–Roothaan equations; noninteger n-Slater type orbitals; open shell theory; isoelectronic series.

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### 1. Introduction

The Hartree–Fock–Roothaan (HFR) or basis-set expansion method is a convenient and powerful tool for the study of electronic structure of atoms and molecules [1]. It is well known that the choice of the basis functions is very important when the algebraic approximation is employed, because it determines both the computational efficiency and accuracy of the results obtained within a given approach. The most frequently used basis functions for atomic calculations are Slater type orbitals (STO) defined as [2]

$$\chi_{n^*lm}(\zeta, \vec{r}) = \frac{(2\zeta)^{n^*+1/2}}{[\Gamma(2n^*+1)]^{1/2}} r^{n^*-1} e^{-\zeta r} S_{lm}(\theta, \varphi). \quad (1)$$

Here,  $\Gamma(x)$  and  $S_{lm}(\theta, \varphi)$  are the gamma function and complex or real spherical harmonics, respectively and  $\zeta > 0$  is the orbital exponent. The quantity  $n^*$  occurring in eq. (1) is a positive integer (for  $n^* = n$ ) or a noninteger principal quantum number of STO (ISTO and NISTO). The determination of nonlinear parameters  $n^*$  and  $\zeta$  appearing in eq. (1) is very important for describing the atomic orbitals.

Over the years, much progress has been made in using ISTO and NISTO as atomic basis functions in the electronic structure calculations of atoms [3–15]. The ground-state energies of isoelectronic series with the open shells for first-row transition atoms were calculated by Clementi-Roetti [16] and Fischer [17] using Hartree–Fock limit (HFL) in the ISTO basis-sets and numerical Hartree–Fock (NHF) approaches, respectively. In ref. [18] the combined HFR (CHFR) method, introduced in [19], numerically has been confirmed for some first row atoms in single- and double-zeta approximations using ISTO basis-sets.

To improve the quality of basis-sets, many nonstandard basis functions proposed by different authors have been used in the electronic structure calculations (see refs [20,21] and references therein). To determine physical properties, such as diamagnetic susceptibility, nuclear magnetic shielding, nuclear quadrupole coupling constant, electric field gradient, etc., the high-quality wave functions are of crucial importance. Because of this, in the study of atomic and molecular systems, the use of basis functions with noninteger principal quantum numbers is more convenient than the conventional ones.

Koga and coworkers have shown [9,12–15] that the NISTO basis-sets gave more accurate ground-state total energies and properties of atoms than ISTO in single- and double-zeta approach. Within the minimal basis framework, the efficiency of NISTO was increased significantly when the atomic number increased. In the case of occupied d-orbitals, the conventional ISTO approach gave unphysical positive orbital energies. On the other hand, negative d-orbital energies were obtained by the use of NISTO basis-sets.

It is known that the isoelectronic series of atoms have not been investigated exhaustively using the NISTO basis-sets, particularly for heavy atoms and ions. The purpose of the present paper is to perform the calculations for the lowest states of the isoelectronic series of  $K[Ar]4s^03d^1$  and  $Cr^+[Ar]4s^03d^5$  configurations using NISTO in the CHFR method. To demonstrate the efficiency of NISTO, all the calculations were performed within the minimal basis-sets framework. The computational method is described in the next section. Hartree atomic units are used throughout this work.

## 2. Theory and computational method

It is well known that the total energy functional in HFR method is the average of the energies of all the important symmetry-adapted configuration state functions [22]. The orbitals are optimized so that the energy functional reaches its minimum. According to CHFR theory, the postulated energy for arbitrary number of closed- and open-shell electronic configurations, in the case of atoms is given by [19]

$$E(LS) = 2 \sum_i^n f_i h_i + \sum_{i,j,k,l}^n \left( 2A_{kl}^{ij} J_{kl}^{ij} - B_{kl}^{ij} K_{kl}^{ij} \right). \quad (2)$$

Lowest states of  $K[Ar]4s^03d^1$  and  $Cr^+[Ar]4s^03d^5$  isoelectronic series

Here,  $f_i$  is the fractional occupancy of shell  $i$ .  $h_i$ ,  $J_{kl}^{ij}$  and  $k_{kl}^{ij}$  are the one-electron, and Coulomb and exchange integrals, respectively. The coupling-projection (CP) coefficients  $A_{kl}^{ij}$  and  $B_{kl}^{ij}$  appearing in eq. (2) in closed–closed and closed–open shells interaction are determined as

$$A_{kl}^{ij} = B_{kl}^{ij} = f_i f_k \delta_{ij} \delta_{kl}. \quad (3)$$

The necessity for determining the open–open shell interaction CP coefficients arises from the following relation of the expectation value for the total energy

$$E(^{2S+1}L) = \frac{1}{(2L+1)(2S+1)} \sum_{M_L M_S} \int \Psi_{M_L M_S}^{LS*} \hat{H} \Psi_{M_L M_S}^{LS} d\tau. \quad (4)$$

To find the CP coefficients, we should compare the results obtained from eq. (2) with those in eq. (4) (see refs [18,19] and references therein for more details about these coefficients). The wave functions  $\Psi_{M_L M_S}^{LS}$  occurring in eq. (4) can be constructed by the use of determinantal Slater [23] or determinantal modified Slater methods (see §4 of [19]). We notice that the CP coefficients have the following symmetry properties:

$$A_{kl}^{ij} = A_{ij}^{kl}, \quad A_{kl}^{ij} = A_{lk}^{ji}, \quad (5)$$

$$B_{kl}^{ij} = B_{ij}^{kl}, \quad B_{kl}^{ij} = B_{lk}^{ji}. \quad (6)$$

The CP coefficients for the isoelectronic series  $K[Ar]4s^03d^1$  ( $^2D$ ), which have a single electron in open shell, can be determined by using eq. (3). The values of open–open shell CP coefficients for the lowest state of isoelectronic series  $Cr^+$  are given in table 1. In the table, the Slater atomic orbitals are denoted by

$nlm$ : 100 200 211 210 21–1 300 311 310 31–1 322 321 320 32–1 32–2  
 $i$  : 1 2 3 4 5 6 7 8 9 10 11 12 13 14

**Table 1.** The values of open–open shells coupling-projection coefficients for isoelectronic series of the lowest state electronic configuration  $Cr^+[Ar]4s^03d^5$  ( $^6S$ ).

$i$	$j$	$k$	$l$	$A_{kl}^{ij} = A_{ij}^{kl}$	$B_{kl}^{ij} = B_{ij}^{kl}$
10	10	11	11	1/4	1/2
		12	12	1/4	1/2
		13	13	1/4	1/2
		14	14	1/4	1/2
11	11	12	12	1/4	1/2
		13	13	1/4	1/2
		14	14	1/4	1/2
12	12	13	13	1/4	1/2
		14	14	1/4	1/2
13	13	14	14	1/4	1/2

When we rewrite eq. (2) in terms of the linear combination coefficients  $C$ , then we obtain for the energy functional the following algebraic relation:

$$E = 2 \sum_q (\rho h)_{qq} + \sum_{ij,kl} \sum_{pq} (2C_{ip}^\dagger A_{kl}^{ij} \Gamma_{kl}^{pq} C_{qj} - C_{ip}^\dagger B_{kl}^{ij} \Lambda_{kl}^{pq} C_{qj}), \quad (7)$$

where  $\rho = CfC^\dagger$  and

$$\Gamma_{kl}^{pq} = (C^\dagger I^{pq} C)_{kl} \quad (8)$$

$$\Lambda_{kl}^{pq} = (C^\dagger K^{pq} C)_{kl}. \quad (9)$$

Two electron integrals  $I_{kl}^{pq}$  and  $K_{kl}^{pq}$  occurring in these equations are defined as

$$I_{kl}^{pq} = \iint \chi_p^*(x_1) \chi_k^*(x_2) \frac{1}{r_{21}} \chi_q(x_1) \chi_l(x_2) dv_1 dv_2 \quad (10)$$

$$K_{kl}^{pq} = \iint \chi_p^*(x_1) \chi_k^*(x_2) \frac{1}{r_{21}} \chi_l(x_1) \chi_q(x_2) dv_1 dv_2. \quad (11)$$

In eqs (7)–(11), the NISTO are denoted by the indices  $p, q, k$  and  $l$ .

The Coulomb and exchange integrals defined by eqs (10) and (11), respectively, have the same form except the indices. These one-centre two-electron integrals over the NISTO basis-sets can be evaluated using relations in terms of the gamma and hypergeometric functions given in refs [12,24].

We have constructed a self-consistent field program in *Mathematica* international mathematical software based on the CHFR method using ISTO and NISTO basis sets. All the nonlinear parameters were optimized with the help of quasi-Newton method. Initial values of the nonlinear parameters occurring in NISTO were taken from the ISTO results. The values of nonlinear parameters obtained were used, then, in the optimization of NISTO nonlinear parameters. We observed that the final virial ratios did not deviate from the exact value of  $-2$  by more than  $10^{-7}$ . All the values of parameters tabulated have nine decimals. Because of this, the ratios obtained are much more precise than those of ref. [16]. We notice that our optimizations in all the calculations are sufficiently accurate.

### 3. Results and discussion

The CHFR method described above and developed to date appears to yield good results when applied in atomic systems. The total energies ( $E_{\text{NISTO}}$ ), their differences  $\Delta E_{E_{\text{ISTO}} - E_{\text{NISTO}}}$ ,  $\Delta E_{E_{\text{RNISTO}} - E_{\text{NISTO}}}$  and  $\Delta E_{E_{\text{NISTO}} - E_{\text{HFL}}}$  for the isoelectronic series  $\text{K}[\text{Ar}]4s^0 3d^1$  ( $^2D$ ) and  $\text{Cr}^+[\text{Ar}]4s^0 3d^5$  ( $^6S$ ) configurations are given in tables 2 and 3, respectively. The cusp condition is satisfied if nonlinear parameters  $n^*$  is restricted with  $n^* \geq 1$ . As the optimal noninteger values of the smallest  $n_{1s}$  are smaller than their

Lowest states of  $K[Ar]4s^03d^1$  and  $Cr^+[Ar]4s^03d^5$  isoelectronic series

**Table 2.** The NISTO total energies ( $E_{NISTO}$ ), total energy differences  $\Delta E_{E_{ISTO}-E_{NISTO}}$ ,  $\Delta E_{E_{RNISTO}-E_{NISTO}}$  and  $\Delta E_{E_{NISTO}-E_{HFL}}$  for the isoelectronic series  $K[Ar]4s^03d^1$  ( $^2D$ ).

Atomic number ( $Z$ )	$-E_{NISTO}$	$\Delta E_{E_{ISTO}-E_{NISTO}}$	$\Delta E_{E_{RNISTO}-E_{NISTO}}$	$\Delta E_{E_{NISTO}-E_{HFL}}$
19	598.851382	0.84644960	0.00789662	–
20	676.252721	0.95981275	0.00791816	0.31716869
21	758.849277	1.05639764	0.00792645	0.24291325
22	846.509362	1.11930839	0.00792791	0.23984792
23	939.207319	1.19123486	0.00792097	0.23808065
24	1036.93294	1.27320899	0.00790654	0.23726120
25	1139.68009	1.36531133	0.00788547	0.23641231
26	1247.44456	1.46751099	0.00785857	0.23624026
27	1360.22328	1.57977907	0.00782655	0.23772273
28	1478.01390	1.70210432	0.00779003	–
29	1600.81460	1.83449098	0.00774955	0.23990433
30	1728.62391	1.97695414	0.00770558	0.24079114

nominal value of 1, the restriction of NISTO to  $n_{1s} \geq 1$  is applied to the optimization of total energies for correct electron-nuclear cusp condition. Therefore, we also calculated the restricted NISTO (RNISTO) total energies. It is well known that the improvement of energy deteriorates when the cusp condition in the SCF calculation is incorporated. As we expected, RNISTO total energies lie above the NISTO total energies and the average energy loss ( $\Delta E_{E_{RNISTO}-E_{NISTO}}$ ) is about 8 miliHartree. We see from tables that the total energy difference  $\Delta E_{E_{ISTO}-E_{NISTO}}$  increases as the atomic number  $Z$  increases. We

**Table 3.** The NISTO total energies ( $E_{NISTO}$ ), total energy differences  $\Delta E_{E_{ISTO}-E_{NISTO}}$ ,  $\Delta E_{E_{RNISTO}-E_{NISTO}}$  and  $\Delta E_{E_{NISTO}-E_{HFL}}$  for the isoelectronic series  $Cr^+[Ar]4s^03d^5$  ( $^6S$ ).

Atomic number ( $Z$ )	$-E_{NISTO}$	$\Delta E_{E_{ISTO}-E_{NISTO}}$	$\Delta E_{E_{RNISTO}-E_{NISTO}}$	$\Delta E_{E_{NISTO}-E_{HFL}}$
24	1042.63610	2.12989941	0.00782892	0.50270510
25	1148.63351	2.21472891	0.00778214	0.47479287
26	1260.15639	2.30036178	0.00773398	0.45770857
27	1377.18138	2.39237955	0.00768361	0.44691620
28	1499.69495	2.49254084	0.00763092	0.43955482
29	1627.68816	2.60154709	0.00757602	0.43194206
30	1761.15468	2.71973201	0.00751910	0.43121965

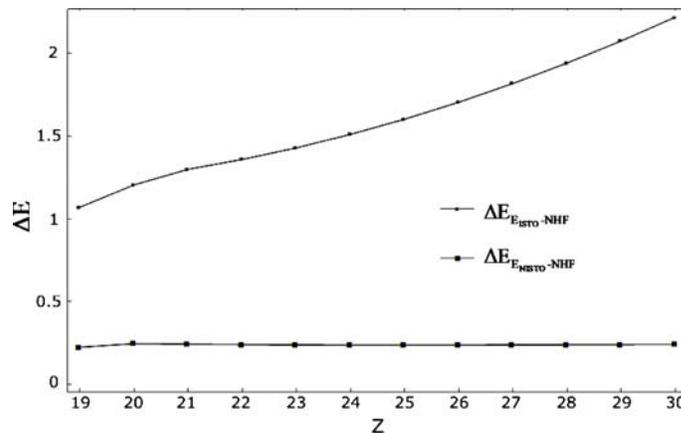
also observed that the efficiency of NISTO increases rapidly with the increased atomic number  $Z$  with respect to the ISTO. The comparison of our results obtained in NISTO basis-sets with the corresponding Clementi-Roetti's HFL energies [16] shows that the energy differences  $\Delta E_{E_{\text{NISTO}}-E_{\text{HFL}}}$  are almost not changed.

The total energy errors for the ISTO and NISTO basis-sets relative to the NHF [17] for the isoelectronic series of K and  $\text{Cr}^{+1}$  are shown in figures 1 and 2, respectively. It should be noted that the total energy errors  $\Delta E_{E_{\text{ISTO}}-E_{\text{NHF}}}$  for the ISTO basis sets increase smoothly with an increase in both the atomic number  $Z$  and the number of electrons. In the NISTO basis sets calculations, on the contrary, the trend of total energy errors  $\Delta E_{E_{\text{NISTO}}-E_{\text{NHF}}}$  is in opposite direction consistently. As seen from figures 1 and 2, the results of NISTO basis-sets calculations are about 3–4 times more accurate than those in ISTO basis-set.

We notice that the Clementi-Roetti HFL energies [16] for  $Z = 28$  in isoelectronic series of configuration  $\text{K}[\text{Ar}]4s^03d^1$  ( $^2D$ ) is incorrect. It should be noted that for  $Z = 20$  in K isoelectronic series, Clementi-Roetti configuration ( $\text{K}[\text{Ar}]4s^13d^0$ ) is different from our configuration ( $\text{K}[\text{Ar}]4s^03d^1$ ).

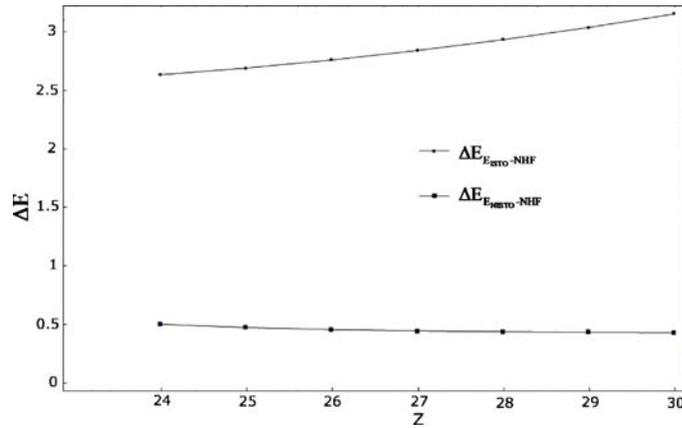
In tables 4 and 5, we present orbital energies obtained from the NISTO basis-sets for the isoelectronic series K and  $\text{Cr}^{+1}$ . For these isoelectronic series, all the orbital energies are improved in NISTO calculations within the minimal basis framework.

Table 6 lists the optimum nonlinear parameters  $n^*$  and  $\zeta$  for  $Z = 25$  in K and  $\text{Cr}^{+1}$  isoelectronic series. It should be noted that the deviation from nominal values of principal quantum numbers is largest for  $3d$  orbital, i.e.,  $1.93 \leq n_{3d}^* \leq 2.51$ . The improvement of the NISTO basis-sets by the extension of the  $n^*$  from integer to noninteger values is due to the fact that these optimal values are significantly different from the nominal values of orbitals.



**Figure 1.** The energy differences  $\Delta E_{E_{\text{ISTO}}-E_{\text{NHF}}}$  and  $\Delta E_{E_{\text{NISTO}}-E_{\text{NHF}}}$  as a function of atomic number  $Z$  for the lowest states ( $^2D$ ) of isoelectronic series K (the results of NHF are obtained from ref. [17]).

Lowest states of  $K[Ar]4s^03d^1$  and  $Cr^+[Ar]4s^03d^5$  isoelectronic series



**Figure 2.** The energy differences  $\Delta E_{E_{ISTO}-E_{NHF}}$  and  $\Delta E_{E_{NISTO}-E_{NHF}}$  as a function of atomic number  $Z$  for the lowest states ( ${}^6S$ ) of isoelectronic series  $Cr^{+1}$  (the results of NHF are obtained from ref. [17]).

The forceful use of the NISTO basis-sets in the calculations of heavy atoms has been studied for isoelectronic series  $K$  and  $Cr^{+1}$ . We showed that the efficiency of the NISTO basis sets is increased especially with increase in the atomic number  $Z$  in isoelectronic series of  $K[Ar]4s^03d^1$  ( ${}^2D$ ) and  $Cr^+[Ar]4s^03d^5$  ( ${}^6S$ ) configurations. NISTO total and orbital energies are closer to the corresponding NHF values than the ISTO ones. The size of the present noninteger  $n$ -Slater orbitals is smaller than that of the usual extended integer  $n$ -Slater orbitals presented in literature. This reduction considerably extends the range of applications of the NISTO in calculations of atomic properties. We plan further to take into account these criteria of atomic orbitals. Work is in progress in our group for the analytical CHFR calculations of ground and excited states of heavy atoms and their ions. It should be noted that the analytical solutions of CHFR eqs (2) and (7) can be performed for the arbitrary states of electronic configurations which have many open shells (whatever their symmetry is). The CHFR method can be of considerable help and importance in the simplification of open-shell atomic structure calculations. This method has, in our opinion, an advantage and an attractive simplicity over standard approaches presented in literature. The CHFR method and a computer code are presented which allow more forceful computation of HFL energies. The resulting wave functions and parameters are available by request through e-mail addresses: ihuseyin@comu.edu.tr or merturk@comu.edu.tr.

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**Table 4.** The NISTO orbital energies ( $\epsilon_{\text{NISTO}}$ ) for the lowest states ( ${}^2D$ ) of isoelectronic series K from  $Z = 19$  to  $Z = 30$ .

$Z$	19	20	21	22	23	24	25	26	27	28	29	30
$-\epsilon_{1s}$	133.603651	149.445801	166.438178	184.487104	203.553606	223.630444	244.714653	266.804426	289.898648	313.996501	339.097386	365.200830
$-\epsilon_{2s}$	14.5271200	16.8493428	19.5794525	22.6275102	25.9478952	29.5317822	33.37535559	37.4762976	41.8331080	46.4446972	51.3102559	56.4291447
$-\epsilon_{2p}$	11.5462001	13.6504007	16.1610087	18.9873563	22.0846383	25.4443114	29.0627522	32.9377803	37.0680125	41.4524535	46.0903690	50.9811827
$-\epsilon_{3s}$	1.82769771	2.31221035	3.09378837	4.04766950	5.12954992	6.33178284	7.65131097	9.08643545	10.6361133	12.2996271	14.0764630	15.9662294
$-\epsilon_{3p}$	1.03513957	1.42459350	2.10644979	2.95431985	3.92843338	5.02210858	6.23267403	7.55861690	8.99899727	10.5531591	12.2206217	14.0010136
$-\epsilon_{3d}$	0.05656511	0.32625429	0.87539364	1.56544744	2.38166858	3.31909000	4.37510673	5.54803983	6.83673303	8.24034080	9.75822290	11.3898659

**Table 5.** The NISTO orbital energies ( $\epsilon_{\text{NISTO}}$ ) for the lowest states ( ${}^6S$ ) of isoelectronic series  $\text{Cr}^{+1}$  from  $Z = 24$  to  $Z = 30$ .

$Z$	24	25	26	27	28	29	30
$-\epsilon_{1s}$	220.595019	241.141102	262.723648	285.326618	308.943014	333.569081	359.202552
$-\epsilon_{2s}$	26.3754099	29.6678636	33.2586824	37.1281325	41.2672189	45.6709245	50.3360942
$-\epsilon_{2p}$	22.3011178	25.3695586	28.7340133	32.3752430	36.2845639	40.4571846	44.8901268
$-\epsilon_{3s}$	3.44460766	4.37116914	5.45028014	6.66312594	8.00149957	9.46104911	11.0391758
$-\epsilon_{3p}$	2.21616782	3.04173312	4.01383525	5.11617625	6.34180379	7.68707500	9.14983056
$-\epsilon_{3d}$	0.52961923	1.18779820	1.98429213	2.90830960	3.95480156	5.12089892	6.40477978

Lowest states of  $K[Ar]4s^03d^1$  and  $Cr^+[Ar]4s^03d^5$  isoelectronic series

**Table 6.** The nonlinear parameters of the NISTO basis sets for the atomic number  $Z = 25$  in isoelectronic series of K and  $Cr^+$ .

Atomic number $Z = 25$	K[Ar]4s <sup>0</sup> 3d <sup>1</sup> ( <sup>2</sup> D)		Cr <sup>+</sup> [Ar]4s <sup>0</sup> 3d <sup>5</sup> ( <sup>6</sup> S)	
	$n^*$	$\zeta$	$n^*$	$\zeta$
$n_{1s}$	0.99645209	24.4941697	0.99647518	24.4960254
$n_{2s}$	2.58563321	11.4888291	2.57937902	11.4418132
$n_{2p}$	1.87783777	9.81200419	1.87618327	9.78391095
$n_{3s}$	3.20237374	4.78380498	2.80189306	4.06524086
$n_{3p}$	2.88256319	4.20480489	2.50296721	3.46031436
$n_{3d}$	2.34009217	3.35812484	2.04264412	2.42127890

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