



**HAL**  
open science

# New light on the Kr(4p55s2) Feshbach resonances: high-resolution electron scattering experiments and B-spline R-matrix calculations

T H Hoffmann, M.-W Ruf, H Hotop, O Zatsarinny, K Bartschat, M Allan

► **To cite this version:**

T H Hoffmann, M.-W Ruf, H Hotop, O Zatsarinny, K Bartschat, et al.. New light on the Kr(4p55s2) Feshbach resonances: high-resolution electron scattering experiments and B-spline R-matrix calculations. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 2010, 43 (8), pp.85206. 10.1088/0953-4075/43/8/085206 . hal-00569907

**HAL Id: hal-00569907**

**<https://hal.science/hal-00569907>**

Submitted on 25 Feb 2011

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# 1 New light on the $\text{Kr}^-(4p^5 5s^2)$ Feshbach resonances: high resolution electron 2 scattering experiments and B-spline R-matrix calculations

3 T. H. Hoffmann<sup>1,2</sup>, M.-W. Ruf<sup>1</sup>, H. Hotop<sup>1</sup>, O. Zatsarinny<sup>3</sup>, K. Bartschat<sup>3</sup> and M. Allan<sup>2</sup>

4 <sup>1</sup>*Fachbereich Physik, Technische Universität KL, 67653 Kaiserslautern, Germany*

5 <sup>2</sup>*Department of Chemistry, University of Fribourg, 1700 Fribourg, Switzerland*

6 <sup>3</sup>*Department of Physics and Astronomy,*

7 *Drake University, Des Moines, Iowa 50311, USA*

8 (Dated: February 11, 2010; submitted to J. Phys. B)

In a joint experimental and theoretical effort, we carried out a detailed study of electron scattering from Kr atoms in the energy range of the low-lying  $\text{Kr}^-(4p^5 5s^2)$  Feshbach resonances. Absolute angle-differential cross sections for elastic electron scattering were measured over the energy range 9.3–10.3 eV with an energy width of about 13 meV at scattering angles between 10° and 180°. Using several sets of elastic scattering phase shifts, a detailed analysis of the sharp  $\text{Kr}^-(4p^5 5s^2 \ ^2P_{3/2})$  resonance was carried out, resulting in a resonance width of  $\Gamma_{3/2} = 3.6(2)$  meV. By direct comparison with the position of the  $\text{Ar}^-(3p^5 4s^2 \ ^2P_{3/2})$  resonance, the energy for the  $\text{Kr}^-(4p^5 5s^2 \ ^2P_{3/2})$  resonance was determined as  $E_{3/2} = 9.489(3)$  eV. A Fano-type fit of the higher-lying  $\text{Kr}^-(4p^5 5s^2 \ ^2P_{1/2})$  resonance yielded the resonance parameters  $\Gamma_{1/2} = 33(5)$  meV and  $E_{1/2} = 10.126(4)$  eV. In order to obtain additional insight, B-spline R-matrix calculations were performed for both the elastic and the inelastic cross sections above the threshold for  $4p^5 5s$  excitation. They provide the total and angle differential cross sections for excitation of long-lived and short lived levels of the  $4p^5 5s$  configuration in Kr and branching ratios for the decay of the  $\text{Kr}^-(4p^5 5s^2 \ ^2P_{1/2})$  resonance into the three available exit channels. The results are compared with selected experimental data.

## 9 I. INTRODUCTION

10 The lowest Feshbach resonances of the rare gases are among the sharpest features known in  
11 electron scattering. They may be considered as two spin-paired Rydberg electrons surrounding  
12 a relatively compact positive core. A review of their properties can be found in the article by  
13 Schulz [1], which was later updated by Buckman and Clark [2]. In recent experiments with energy  
14 widths as small as 4 meV, the lowest Feshbach resonances of He [3, 4], Ne [5], and Ar [4] were  
15 studied in unprecedented detail, and more accurate resonance widths and energies than previously  
16 available were determined. These resonances can only decay to the respective ground states and

17 have very small widths ( $\text{He}^- (1s2s^2\ ^2S_{1/2})$ : 10.9(3) meV [3, 4],  $\text{Ne}^- (2p^53s^2\ ^2P_{3/2,1/2})$ : 1.27(7) meV  
 18 [5],  $\text{Ar}^- (3p^54s^2\ ^2P_{3/2,1/2})$ : 2.3(2) meV[4]). For Kr, on the other hand, the fine-structure splitting  
 19 between the two  $\text{Kr}^- (4p^55s^2\ ^2P_{3/2,1/2})$  resonances is much larger than in Ne and Ar, such that  
 20 the higher-lying  $\text{Kr}^- (4p^55s^2\ ^2P_{1/2})$  resonance can decay to three exit channels, namely to the  
 21 ground state  $\text{Kr} (4p^6\ ^1S_0)$  and, in addition, to the two excited  $\text{Kr} (4p^55s\ ^3P_{2,1})$  levels plus a free  
 22 electron (threshold energies 9.915 eV and 10.032 eV, respectively). Correspondingly, the width  
 23 of the  $\text{Kr}^- (4p^55s^2\ ^2P_{1/2})$  resonance is much larger (about 30 meV [6]). It is of obvious interest  
 24 to characterize the size and the resonance shapes in the partial cross sections for the three exit  
 25 channels.

26 The  $\text{Kr}^- (4p^55s^2\ ^2P_{3/2,1/2})$  resonances were first observed (but not characterized) by Schulz [7].  
 27 Kuyatt *et al.* [8] and Sanche and Schulz [9] measured them in improved transmission experiments.  
 28 Angle-differential cross sections at  $45^\circ$  were reported by Swanson *et al.* [10]. From an analysis of  
 29 resonance profiles measured at several angles, Weingartshofer *et al.* [11] deduced a width for the  
 30  $\text{Kr}^- (4p^55s^2\ ^2P_{3/2})$  resonance of 8 meV. Heindorff *et al.* [12] observed the resonance at  $115^\circ$  and  
 31 investigated the angular distribution over the energy range 3.0–10.5 eV. In conjunction with mea-  
 32 surements of the excitation of long-lived Kr levels, Brunt *et al.* [13] gave the energy positions of the  
 33 resonances as 9.484 eV and 10.123 eV, respectively. Using threshold electron spectroscopy, Jureta  
 34 *et al.* [14] obtained the value 10.119(5) eV for the position of the  $\text{Kr}^- (4p^55s^2\ ^2P_{1/2})$  resonance.  
 35 From a consistent analysis of the  $\text{Kr}^- (4p^55s^2\ ^2P_{3/2})$  resonance profile measured at 19 angles, Dubé  
 36 *et al.* [15] deduced a natural width of 3.6(4) meV. Zubek *et al.* [6] observed the resonances at angles  
 37 up to  $180^\circ$  with a magnetic angle changer [16, 17], extracting widths of  $\Gamma_{3/2} = 3.5(10)$  meV and  
 38  $\Gamma_{1/2} = 30(4)$  meV, respectively.

39 In the present paper, we report the results of a joint experimental and theoretical study of  
 40 electron scattering from Kr atoms in the energy range of the low-lying  $\text{Kr}^- (4p^55s^2)$  Feshbach  
 41 resonances with the aim to shed new light on the dynamics of the addressed processes. Two  
 42 different experimental setups were used to study elastic electron scattering from Kr atoms in the  
 43 energy range from 9.3 eV to 10.3 eV with improved energy resolution (13 meV).

44 This paper is organized as follows: In section II we briefly describe the two experiments carried  
 45 out in Kaiserslautern and Fribourg. Section III sketches the analysis of the resonance profiles  
 46 and outlines the *B*-spline *R*-matrix (BSR) method used in the present numerical calculations. In  
 47 section IV we present the experimental results and their analyses and compare them with previous  
 48 measurements and the BSR predictions. Moreover, computed angle-differential cross sections for  
 49 near-threshold excitation of the four levels of the  $\text{Kr}(4p^55s)$  configuration will be compared with

50 experimental results of Phillips [18]. We conclude with a brief summary.

## 51 II. EXPERIMENT

### 52 A. Experiment at Kaiserslautern

53 The electron scattering setup involving a laser photoelectron source was described in detail  
 54 previously [3–5]. Briefly, potassium atoms from an atomic beam source are excited by a Ti:Sa  
 55 laser to the  $K^*$  ( $4p^2P_{3/2}$ ) level that is ionized at threshold with a focused blue intracavity dye  
 56 laser. The photoelectrons are extracted by a weak electric field ( $\approx 10$  V/m) and imaged onto the  
 57 atomic target beam. Five retarding-field electron detectors at fixed angles count the elastically  
 58 scattered electrons. The triply differentially pumped supersonic target beam nearly eliminates  
 59 Doppler broadening [3, 5]. For Kr, problems associated with cluster formation occur at the usual  
 60 nozzle temperature of 300 K (see also [4]). To reduce clustering, the nozzle was heated up to  
 61 470 K. Unfortunately, the heating reduced the energy resolution (energy width around 10 meV)  
 62 as a result of quickly varying surface potentials, presumably due to fluctuations in the potassium  
 63 coverage of the surfaces. As a consequence, the photoelectron apparatus was mainly used for an  
 64 energy calibration of the  $Kr^-$  ( $4p^55s^2^2P_{3/2}$ ) resonance.

### 65 B. Experiment at Fribourg

66 Electrons emitted from a hot filament are energy-selected by a double hemispherical monochro-  
 67 mator and focused onto an effusive beam target, introduced by a 0.25 mm nozzle kept at about  
 68  $30^\circ\text{C}$ . A double hemispherical analyzer for detection of elastically or inelastically scattered elec-  
 69 trons ensures background-free signals [19]. Absolute cross sections are determined by comparison  
 70 against He using a relative-flow method [20]. A specially designed magnetic angle changer allows  
 71 for measurements up to  $180^\circ$  scattering angle [21]. For the present measurements of elastic scat-  
 72 tering at energies around 10 eV, the angular acceptance amounts to  $3^\circ$  full width at half maximum  
 73 (FWHM); the uncertainty of the angular position is estimated as  $\pm 1^\circ$ . Procedures for ensuring  
 74 reliable cross sections were described in detail elsewhere [22, 23]. The confidence limit (two stan-  
 75 dard deviations) for the absolute cross sections is about  $\pm 15\%$ . The incident electron resolution  
 76 was about 13 meV at a beam current of about 400 pA.

### III. THEORY

#### A. Phase-shift analysis of resonance scattering profiles

Elastic scattering of electrons from a heavy rare gas atom can be treated as potential scattering in the presence of spin-orbit coupling. The differential cross section  $d\sigma(\theta)/d\Omega$  then depends upon both the direct scattering amplitude  $f(E, \theta)$  and the spin-flip amplitude  $g(E, \theta)$  [24] according to

$$\frac{d\sigma}{d\Omega}(E, \theta) = |f(E, \theta)|^2 + |g(E, \theta)|^2. \quad (1)$$

These amplitudes can be written as partial-wave sums

$$f(E, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \left[ (l+1) \left( e^{2i\delta_l^+} - 1 \right) + l \left( e^{2i\delta_l^-} - 1 \right) \right] P_l(\cos \theta) \quad (2)$$

and

$$g(E, \theta) = \frac{1}{2ik} \sum_{l=1}^{\infty} \left( e^{2i\delta_l^+} - e^{2i\delta_l^-} \right) P_l^1(\cos \theta), \quad (3)$$

where the wave vector of the electron is given by  $k = \sqrt{2mE}/\hbar$  while  $P_l(\cos \theta)$  and  $P_l^1(\cos \theta)$  ( $l \geq 1$ ) denote the standard and associated Legendre polynomials, respectively. For partial waves with orbital angular momentum  $l \geq 1$ , the total angular momenta  $J^+ = l + 1/2$  and  $J^- = l - 1/2$  experience different phase shifts  $\delta_l^+$  and  $\delta_l^-$ . The influence of the resonances can be described by additional phase shifts

$$\delta_{res}^{\pm} = -\text{arccot} \frac{2(E - E_{res}^{\pm})}{\Gamma_{\pm}} \quad (4)$$

that change by  $\pi$  over an interval given by the natural width  $\Gamma_{\pm}$ . For higher partial waves  $l > l_c$  (with typical values of  $l_c \approx 3$ ), the interaction is dominated by the long-range polarization potential.

An expression due to Thompson [25],

$$f_{l>l_c} = \frac{\pi\alpha k}{a_0} \left( \frac{1}{3} - \frac{1}{2} \sin \frac{\theta}{2} - \sum_{l=1}^{l_c} \frac{P_l(\cos \theta)}{(2l-1)(2l+3)} \right) \quad (5)$$

with  $\alpha$  denoting the static dipole polarizability ( $2.4844(12) \times 10^{-30} \text{ m}^3$  [26]) allows for calculating their influence.

#### B. BSR calculations

The present calculations were performed with the semi-relativistic (Breit-Pauli)  $B$ -spline  $R$ -matrix (BSR) (close-coupling) program of Zatsarinny [27], as well as a recently developed fully

97 relativistic version [28]. An important feature of this code is the ability to define non-orthogonal  
 98 sets of one-electron orbitals, which generally allow for a highly accurate target description with rel-  
 99 atively small (compared to standard approaches with orthogonal orbitals) configuration-interaction  
 100 expansions. Below we will present results from a semi-relativistic 47-state model (BSR47), which  
 101 was already successfully applied to studying the excitation of metastable levels in Kr [29], and  
 102 from a fully relativistic model with 32 states. Of the latter, 31 are physical states (the same as  
 103 the lowest 31 states of the BSR47 model) plus a pseudo-state that was constructed to ensure the  
 104 correct dipole polarizability of the ground state. This model will be denoted as DBSR31p below.

105

### 1. The BSR47 model

106 The target description used for Kr is based on the same philosophy as those described in detail  
 107 for Ne [30] and Ar [31]. We started by generating the  $1s - 4p$  core orbitals from a Hartree-Fock  
 108 calculation for  $\text{Kr}^+$ . Important correlation effects, which should be included in the calculation of  
 109 the excited states of Kr, are the significant core-valence correlation and the strong term-dependence  
 110 of the valence orbitals. There is also very strong configuration mixing between the  $4p^4(n+1)s$  and  
 111  $4p^4nd$  states and, finally, one may want to account for inner-core correlation effects.

112 In the present approach, we treat the core-valence correlation *ab initio* by adding target config-  
 113 urations with an excited core. Standard multi-configuration expansions, however, can become very  
 114 large and are hardly employable in subsequent scattering calculations. For this reason, we used  
 115 the *B*-spline box-based close-coupling method described by Zatsarinny and Froese Fischer [32] to  
 116 generate the target states.

117 Only the  $(4s^24p^5^2P_{3/2,1/2})$  states were used as target states in the *B*-spline bound-state ex-  
 118 pansion. In order to account for the core-valence correlation, the close-coupling expansion for the  
 119 target states also included configurations with an excited core,  $4p^4\bar{5}\ell\bar{5}\ell'$ , where the  $\bar{5}\ell$  ( $\ell = 0, 1, 2, 3$ )  
 120 correlation orbitals were optimized in separate multi-configuration Hartree-Fock calculations for  
 121 each term. In order to limit the bound-state expansions to an acceptable size, we only kept config-  
 122 urations with expansion coefficients greater than 0.01. The above procedure allowed us to reduce  
 123 the error in the binding energies for the lowest  $4p^55s$  and  $4p^54d$  states from 0.35 eV to 0.13 eV,  
 124 indicating that we indeed included a substantial amount of core-valence correlation.

125 Core correlation effects were included by single and double promotion of the  $4s$  and  $4p$  orbitals to  
 126  $\bar{4}\ell$  correlation orbitals, but we only kept configurations with expansion coefficients larger than 0.025.  
 127 The main contributions come from the  $4s4p^5\bar{4}d$ ,  $4s^24p^3\bar{4}d^2$ , and  $4s^24p^4\bar{4}f$  configurations. These are

128 considered sufficient to include the most important inner-core correlation effects with a minimum  
 129 number of correlation configurations.

130 The number of physical states that we can generate by this method depends on the radius  $a$   
 131 of the  $R$ -matrix box. Our choice of  $a = 50 a_0$ , where  $a_0 = 0.529 \times 10^{-10}$  m denotes the Bohr ra-  
 132 dius, yields a good description for the 31 spectroscopic states with dominant configurations  $4p^5 5s$ ,  
 133  $4p^5 5p$ ,  $4p^5 4d$  and  $4p^5 6s$ , respectively. The 16 additional states with dominant configurations  
 134  $4p^5 [J=3/2] 5d, 6p, 7s$  are also described fairly well, but one would generally not expect coupling to  
 135 these target states to be very important for the energy range considered for this work. Instead,  
 136 coupling to the ionization continuum may be important (see below), but performing such calcu-  
 137 lations with a large number of pseudo-states goes beyond our currently available computational  
 138 resources.

139 We emphasize that the above procedure generates *non-orthogonal, term-dependent* sets of radial  
 140 functions for each individual state, also accounting for term mixing due to the spin-orbit interaction.  
 141 In the present calculations, the atomic Hamiltonian includes all one-electron Breit-Pauli operators  
 142 plus the two-electron spin-other-orbit interaction. The relativistic corrections are very important in  
 143 Kr, which is already too heavy to expect excellent *ab initio* results in a perturbative approach with  
 144 non-relativistic orbitals. Consequently, in order to reproduce the correct term mixing we used the  
 145 experimental value of  $\zeta(4p) = 0.666$  eV as the spin-orbit parameter for the 4p orbital. In contrast,  
 146 the non-relativistic wavefunction for the  $4s^2 4p^5$  core yields  $\zeta(4p) = 0.602$  eV, thus requiring a 10%  
 147 adjustment.

## 148 2. The DBSR31p model

149 Here we started by generating the core orbitals (spinors) from a  $\text{Kr}^+$  Dirac-Fock calculation using  
 150 the GRASP2K relativistic atomic-structure package [33]. Next, the valence 5s and 4d orbitals in the  
 151  $4p^4 5s$  and  $4p^4 4d$  configurations were generated in a frozen-core calculation for  $\text{Kr}^+$  in the average-  
 152 term approximation. All these states of  $\text{Kr}^+$  were then used as target states in  $B$ -spline bound-state  
 153 close-coupling calculations to generate the low-lying states of atomic Kr. The corresponding close-  
 154 coupling expansion had the structure

$$\begin{aligned} \Phi(5p^5 nl, J\pi) = & \mathcal{A} \sum_i \{ \varphi(4p^5) \phi(n_i l_i) \}^{J\pi} \\ & + \mathcal{A} \sum_i \{ \varphi(4p^4 5s) \phi(n_i l_i) \}^{J\pi} \end{aligned}$$

$$\begin{aligned}
& + \mathcal{A} \sum_i \{ \varphi(4p^4 4d) \phi(n_i l_i) \}^{J\pi} \\
& + \mathcal{A} \sum_i \{ \varphi(4s 4p^6) \phi(n_i l_i) \}^{J\pi} \\
& + a \varphi(4p^6)
\end{aligned} \tag{6}$$

155 where  $\mathcal{A}$  denotes the anti-symmetrization operator. The unknown large and small radial com-  
156 ponents for the outer valence electron,  $\phi(n\ell)$ , were expanded in individual  $B$ -spline bases. The  
157 coefficients of these expansions were found by diagonalizing the Dirac-Coulomb hamiltonian with  
158 the additional requirement that the wavefunctions vanish at the boundary. Note that we require  
159 orthogonality of the physical  $\phi(n\ell)$  orbitals only to the core orbitals  $1s - 4p$ , but not to the  $5s$  and  
160  $4d$  orbitals of  $\text{Kr}^+$  that are considered here as correlation orbitals. More details of this procedure  
161 can be found in [28].

162 The first sum in Eqn. (6) represents the physical valence states under consideration, while  
163 the next three sums were included to describe the core-valence correlation. Although the above  
164 close-coupling expansion can also generate the  $4p^6$  ground state, we explicitly added the initial one-  
165 configuration wavefunction of this state for a more extended description of the relaxation effects  
166 in the  $4s$  and  $4p$  orbitals for this case. As mentioned above, for an accurate calculation of term  
167 mixing in Kr it is crucial to use the correct value of the spin-orbit parameter for the  $4p$  orbital. In  
168 contrast to the Breit-Pauli approach, the Dirac-Coulomb method yields  $\zeta(4p) = 0.665$  eV. This is  
169 very close to the experimental value of  $0.666$  eV, and hence we do not need an adjustment in this  
170 case. Consequently, the present structure model is indeed fully *ab initio*.

171 The above scheme again yields non-orthogonal, term-dependent orbitals  $\phi(n\ell)$  for each Kr state.  
172 However, the present Dirac-Coulomb approach differs from our Breit-Pauli calculations for noble-  
173 gas atoms regarding the description of the core-valence correlation. Instead of employing specially  
174 designed correlation orbitals (see previous subsection) for this purpose, using the box-based close-  
175 coupling ansatz directly to account for the various terms and the interaction between them in the  
176  $jj$ -coupling scheme resulted in 37 core states in the expansion (6). This scheme yields a relatively  
177 small (up to 120 terms) configuration-interaction expansions for the final target states of Kr. On  
178 the other hand, it produced a very large number of different non-orthogonal orbitals (about 3,000),  
179 which were then employed in the description of all target states. As in BSR47, the size of the  
180  $R$ -matrix box was chosen as  $a = 50 a_0$ , and we obtained a good description of the physical states  
181 with  $n \leq 6$ .

182 In contrast to previous work, however, we then constructed one more odd-parity pseudo-state



183 with total electronic angular momentum  $J = 1$ . This state was designed to ensure that its  
 184 coupling to the ground state produced the correct dipole polarizability. Since most of the dipole  
 185 polarizability of the noble-gas ground states originates from coupling to the continuum, this is the  
 186 simplest and widely used method of accounting for this effect in a coupled-channel calculation.  
 187 [In single-channel calculations, a popular alternative method is to add a polarization term to the  
 188 scattering potential.]

189 The present method reproduced the binding energies with an accuracy of better than 80 meV for  
 190 all states in neutral Kr. We consider this highly accurate, given the complete *ab initio* character of  
 191 these calculations and the relatively small size of the configuration expansions. In the subsequent  
 192 scattering calculations, however, we used the experimental excitation energies. This allowed us  
 193 to compare directly with experiment, especially regarding the near-threshold resonance structure.  
 194 It is worth noting that our procedure of adjusting the target energies effectively corresponds to  
 195 small stretches or contractions of the energy scale between the various thresholds [27]. Since we  
 196 do not force orthogonality between the target and the projectile orbitals (see next subsection), we  
 197 do not have to include  $(N + 1)$ -electron “bound-bound” terms in the close-coupling expansion of  
 198 the collision problem. As a result, using the experimental thresholds does not carry the danger  
 199 of otherwise possible inconsistencies in the relative positions of the  $N$ -electron target and the  
 200  $(N + 1)$ -electron resonance states.

201 Before we describe the collision calculations, it is important to note that the structure models  
 202 described above are not quite as sophisticated as those generated in the structure-only mode of the  
 203 BSR and DBSR codes [34]. This is due to the fact that the projectile electron has to be coupled  
 204 in as well, and hence a compromise has to be made in the number of target configurations that  
 205 can be included in a practical collision calculation. Nevertheless, the accuracy did not deteriorate  
 206 substantially, and we believe that the current target descriptions are an adequate basis for the  
 207 scattering calculations. Also, while they should describe very similar physics (except for the ad-  
 208 ditional pseudo-state in the DBSR31p model), the details of the calculations, including the codes  
 209 used, are very different. Hence, they provide a valuable cross-check between the two approaches  
 210 and the associated computer programs.

### 211 3. Collision Calculations

212 We used the published BSR code [27] and our newly developed DBSR version [28] to solve the  
 213  $(N + 1)$ -electron collision problem. The essential idea is to expand the basis of continuum orbitals

214 used to describe the projectile electron inside the  $R$ -matrix box, i.e., the region where the problem  
 215 is most complicated due to the highly correlated motion of  $N + 1$  electrons, also in terms of a  
 216  $B$ -spline basis. A semi-exponential grid for the  $B$ -spline knot sequence was set up to cover the  
 217 inner region up to the  $R$ -matrix radius. We used the same grid for the structure and the collision  
 218 calculations. For  $a = 50 a_0$ , we employed 82 splines in the Breit-Pauli model and 111 in the Dirac  
 219 approach for the Kr target. The latter increase was necessary to correctly describe the finite-size  
 220 nuclear model with a Fermi potential adopted in the present work.

221 Note that the DBSR calculations lead to significantly larger interaction matrices in the internal  
 222 region compared to the BSR calculations, due to the additional treatment of the small spinor com-  
 223 ponents. In the DBSR31p calculations, which included up to 124 scattering channels, interaction  
 224 matrices with dimensions of about 25,000 needed to be diagonalized. In order to perform those  
 225 calculations we had to parallelize the DBSR code and also used parallelized linear-algebra libraries  
 226 such as `SCALAPACK`.

227 We calculated partial-wave contributions up to  $J = 51/2$  numerically. No extrapolation scheme  
 228 to account for even higher partial waves was necessary for all observables presented in this paper.  
 229 The cross sections of interest were then calculated in the same way as in the standard  $R$ -matrix  
 230 approach. We employed an updated version [35] of the flexible asymptotic  $R$ -matrix (`FARM`) package  
 231 by Burke and Noble [36] to solve the problem in the asymptotic region and to obtain the transition  
 232 matrix elements of interest. After transforming the latter from the present  $jj$ -coupling to the  $jlK$ -  
 233 coupling scheme and also accounting for the appropriate phase convention of the reduced matrix  
 234 elements, we employed the program `MJK` of Grum-Grzhimailo [37] to calculate the angle-differential  
 235 cross sections shown below.

## 236 IV. EXPERIMENTAL RESULTS AND DISCUSSION

### 237 A. Nonresonant elastic scattering

238 The differential cross sections for elastic electron scattering from Kr, measured at an energy of  
 239 9.8 eV, are compared with selected calculated DCS in figure 1. The full circles with error bars  
 240 indicate the experimental absolute measurements at several discrete angles, the open circles result  
 241 from magnetic scans with  $1^\circ$  increment, recorded at three fixed detector positions ( $45^\circ$ ,  $90^\circ$ ,  $135^\circ$ )  
 242 and normalized as described in [4, 22]. The largest (relative) deviations occur at angles around  
 243 the minimum near  $117^\circ$ , where the experimental data are best reproduced when the phase shifts of

244 Sauter and Meyer [45] and Fon *et al.* [42] are used. The optical potential calculations of McEachran  
 245 and Stauffer [46] at 10 eV (not shown in the figure) yield the minimum at  $118^\circ$ , but their minimum  
 246 DCS (obtained from figure 1 of [46]) is almost a factor of 2 higher than our measured value.

247 At forward and backward angles, deviations of up to 20% are observed between the various  
 248 data sets. The BSR47 results for angles up to  $30^\circ$  suffer from the fact that coupling to just  
 249 discrete states only accounts for 30% of the dipole polarizability of the ground state. As mentioned  
 250 above, this problem can be fixed by adding specially constructed pseudo-states to the  $R$ -matrix  
 251 (close-coupling) expansion, as done by Fon *et al.* [42] and Bell *et al.* [43] who concentrated on  
 252 elastic scattering, and also in our DBSR31p model as described above. Clearly, including for the  
 253 polarization of the ground state in the DBSR31p model considerably improves the agreement with  
 254 experiment.

255 The absolute values of our DCS are listed in table I, which also contains the results of four  
 256 previous measurements at an energy of 10 eV [38–41]. A graphical comparison between the earlier  
 257 results can be found in [38]. According to BSR calculations carried out at 9.8 eV and 10.0 eV,  
 258 the DCS at small and large angles vary little with energy ( $<3\%$ ) while the DCS at the minimum  
 259 increases by 18% towards higher energy. Except in the angular range around the minimum of the  
 260 DCS, good to excellent agreement is found between our data and those of Cho *et al.* [39] and Linert  
 261 *et al.* [38]. At small angles, our DCS agree best with those of Danjo [40], whose values become  
 262 progressively too large at angles above  $70^\circ$ . The data of Srivastava *et al.* [41] are 10% to 30%  
 263 smaller than our results at angles below  $110^\circ$ , and 15% to 87% larger at higher angles.

264 The influence of the finite angular resolution on the measured depth of the minimum DCS  
 265 is such that the apparent cross section in the minimum is raised by 13%, 29%, and 51% when  
 266 the theoretical DCS, calculated by the DBSR31p method, is convoluted with a Gaussian angular  
 267 resolution profile of  $4^\circ$ ,  $6^\circ$ , and  $8^\circ$  FWHM, respectively. Since all experiments were carried out  
 268 with an angular acceptance width lower than  $\pm 3^\circ$  (FWHM  $< 6^\circ$ ), the observed differences in the  
 269 apparent cross section close to the minimum are too large to be accounted for solely by angular  
 270 resolution effects. The deeper minimum of our data may be due to the especially low background  
 271 of the Fribourg apparatus.

## 272 B. Characterization of the $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2,1/2})$ resonances

273 The  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance below the excitation threshold is much sharper and more  
 274 prominent than the higher-lying  $\text{Kr}^- (4p^5 5s^2 {}^2P_{1/2})$  resonance that can decay into three exit chan-

275 nels. The properties of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance, which is only coupled to the elastic  
 276 scattering channel, can be accurately determined through a standard partial-wave analysis, once  
 277 reliable phase shifts are known. New energy-dependent spectra of this resonance, measured in  
 278 Fribourg at seven different angles, are shown in figure 2 as open circles. The absolute scale is  
 279 fixed with reference to the experimental angular distribution. The measured data were fitted by  
 280 a resonance profile calculated from a few sets of phase shifts (see table II) and adjustable values  
 281 of the resonance width  $\Gamma_{3/2}$  and of the experimental energy width  $\Delta E$  (full width half maximum  
 282 of a Gaussian function) common to all angles. Small deviations between the experimental and the  
 283 calculated non-resonant cross sections were compensated by angle-dependent correction factors.  
 284 For the fits in figure 2, these factors differed from unity by less than 7%. The optimal values  $\Gamma_{3/2}$   
 285 and  $\Delta E$  thus obtained are summarized in table III.

286 The quality of the fit was judged by the sum of the squared residuals (SSR); the numerical  
 287 quality factor Q of a fit was obtained by dividing the minimal SSR through the SSR resulting from  
 288 a given set of phase shifts. Thus, a Q of 1.0 was assigned to the fit based on the phase shifts of Sauter  
 289 and Meyer [45], which yielded the best agreement. The phase shifts by Fon *et al.* [42] resulted in a  
 290 higher, those by Bell *et al.* [43] and Sienkiewicz and Baylis [44] in a smaller width. The weighted  
 291 mean of the different fits results in a value of 3.58(20) meV for the width of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$   
 292 resonance. Using the phase shifts of Sauter and Meyer [45], fits at individual angles were carried  
 293 out for comparison; for each angle, we give the natural width  $\Gamma$  and experimental energy width  $\Delta E$   
 294 (Angle:  $\Gamma$  (meV) /  $\Delta E$  (meV)):  $10^\circ$ : 3.62 / 12.1;  $22.5^\circ$ : 3.68 / 11.6;  $45^\circ$ : 3.64/12.1;  $90^\circ$ : 3.40/11.6;  
 295  $112.5^\circ$ : 2.62/12.0;  $135^\circ$ : 3.71/11.9;  $180^\circ$ : 3.77/13.6. Since the angular distributions for Kr and Ar  
 296 in the vicinity of the resonance positions are similar, the very small natural width at  $112.5^\circ$  comes  
 297 as no surprise. It shows the influence of remaining uncertainties in the differential cross section  
 298 around the minimum, as already discussed for Ar by Franz *et al.* [4].

299 Our experimental value for the width of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance is compared with  
 300 previous results in table IV. Excellent agreement with the values of Dubé *et al.* [15] and Zubek *et*  
 301 *al.* [6] is observed. The widths of 2.9 meV obtained in the DBSR31p model and the even smaller  
 302 value of 2.7 meV from the BSR47 calculation show consistency between two very independent  
 303 calculations, but these widths appear to be too small. Unfortunately, it looks as if the apparent  
 304 improvement achieved in the BSR47 model in the target description and the angle-integrated  
 305 metastable excitation function [29] does not carry over to the details of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2,1/2})$   
 306 resonances.

307 The position of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance was determined relative to that of the

308  $\text{Ar}^- (3p^5 4s^2 {}^2P_{3/2})$  resonance in the photoelectron setup using a mixed supersonic Ar-Kr beam.  
 309 From a fit to the measured line profiles, we obtain a resonance energy of 9.489(3) eV. Within the  
 310 mutual uncertainties, this value agrees with the results of Brunt *et al.* [13], Jureta *et al.* [14] and  
 311 Zubek *et al.* [6] (see table V).

312 In figure 3, we present the measured energy dependence of the DCS over a broader energy range  
 313 (9.3–10.3 eV), encompassing the higher-lying  $\text{Kr}^- (4p^5 5s^2 {}^2P_{1/2})$  resonance as well. As mentioned  
 314 previously, the latter can also decay into the two nearby excited levels  $\text{Kr} (4p^5 5s^3 P_{2,1})$ . Since this  
 315 decay is almost ten times more rapid than that to the ground state, it leads to a total width of  
 316 33(5) meV. This width is the average value, as determined from fits to the profiles measured at the  
 317 angles  $10^\circ$ ,  $22.5^\circ$ ,  $45^\circ$ ,  $135^\circ$  and  $180^\circ$ . For these fits, Shore profiles [47, 48] were used and convoluted  
 318 with a Gaussian function to account for the experimental resolution of about 13 meV. The observed  
 319 angular variation of the line profiles for both resonances is in good agreement with that reported  
 320 by Weingartshofer *et al.* [11] at an energy width of 30 meV. Once again the BSR47 model gives  
 321 a significantly smaller total width for this resonance (15.4 meV) than the DBSR31p calculation  
 322 (31.9 meV), with the latter being in better agreement with experiment. The large difference in the  
 323 widths predicted by the BSR47 and DBSR31p models indicates a strong sensitivity of the results  
 324 on the details of the model. This makes a theoretical description very challenging.

325 In figure 4, results of the DBSR31p and BSR47 calculations for the angular dependence of  
 326 the resonance profiles are presented and compared with the lineshapes derived from the fits to  
 327 the experimental data. Note that all profiles are shown *without* convolution with the Gaussian  
 328 resolution function. The variation of the experimentally deduced lineshapes with angle is well  
 329 recovered by the BSR calculations with a preference for the BSR47 results while the DBSR31p  
 330 results yield resonance widths closer to the experimental values (see Table IV).

### 331 C. Differential cross sections for electron-impact excitation of Krypton to the $4p^5 5s$ levels

332 In a forthcoming paper [29], BSR calculations of the total cross sections for excitation of the  
 333 metastable  $\text{Kr} (4p^5 5s^3 P_{2,0})$  and of the VUV-emitting  $\text{Kr} (4p^5 5s^3 P_1, {}^1P_1)$  levels are reported and  
 334 found to be in good agreement with experimental data of the Manchester group [13, 51, 52]. A more  
 335 sensitive test of the BSR description for electron scattering from Kr is provided by angle-differential  
 336 cross sections for inelastic processes near threshold. Phillips [18] reported such measurements for  
 337 excitation of the four levels in the  $\text{Kr}(4p^5 5s)$  configuration at three angles ( $30^\circ$ ,  $55^\circ$ ,  $90^\circ$ ) from  
 338 threshold up to about 14 eV. Her absolute cross sections, measured with an energy width of 35 meV,

339 were extracted in digitized form from the respective figures in [18] and are shown in figures 5, 6,  
340 and 7.

341 Comparison with the results from both the DBSR31p and BSR47 calculations shows encour-  
342 aging qualitative agreement with respect to the position and energy dependence of the principal  
343 features up to incident energies of about 12.5 eV. The models do not contain a sufficient number  
344 of states to expect such agreement for higher energies. Both the experimental and the calculated  
345 angle-differential cross sections in figures 5-7 (and also the angle-integrated cross section [29, 51])  
346 for formation of the VUV emitting Kr ( $4p^5 5s^3 P_1$ ) level demonstrate a strong enhancement of this  
347 inelastic channel through the decay from the Kr $^-$  ( $4p^5 5s^2 \ ^2P_{1/2}$ ) resonance. In contrast, production  
348 of the Kr ( $4p^5 5s^3 P_2$ ) level via this resonance is much less pronounced. This different behavior is  
349 explained by the fact that the  $\ ^2P_{1/2}$  resonance can decay to the barrier-free Kr( $\ ^3P_1$ )+e $^-$  ( $l = 0$ )  
350 s-wave channel, but not to the Kr( $\ ^3P_2$ )+e $^-$  ( $l = 0$ ) channel. In agreement with these considera-  
351 tions, the DBSR31p (BSR47) calculations predict angle-integrated relative partial widths of about  
352 8%, 6%, and 86% (20%, 9%, 71%) for the decay of the  $\ ^2P_{1/2}$  resonance to the ground and the  
353 Kr ( $4p^5 5s^3 P_2$ ) and Kr ( $4p^5 5s^3 P_1$ ) states, respectively. These partial widths were calculated with  
354 the time-delay method of Smith [53] for obtaining the decay probabilities of a given resonance into  
355 different final channels.

356 Below the Kr( $\ ^3P_1$ ) threshold, at about 10.01 eV, another sharp resonance feature shows up in the  
357 calculated DCS for the inelastic Kr( $\ ^3P_2$ ) channel, which is expected to be due to a (shape) resonance  
358 with the configuration  $4p^5(\ ^2P_{3/2})5s5p(\ ^3P)$  [2]. In the review of Buckman and Clark, the position  
359 of the lowest resonance with the configuration  $4p^5(\ ^2P_{3/2})5s5p(\ ^3P)$  is given as 10.039(10) eV; this  
360 value was derived from the appearance of a peak labeled “b” in the metastable Kr excitation  
361 function just above the Kr( $\ ^3P_2$ ) threshold.

362 There are clearly problems with the magnitude of the cross-section values, particularly at a  
363 scattering angle of  $55^\circ$ . These problems could be related to the angular dependence of the cross  
364 sections, i.e., a comparison at the nominal scattering without accounting for the angular resolution  
365 in the experiment may be misleading. Further work will need to be done to analyze the remaining  
366 discrepancies.

## 367 V. CONCLUSIONS

368 The Kr $^-$  ( $4p^5 5s^2 \ ^2P_{3/2,1/2}$ ) resonances in elastic electron scattering from Kr atoms were mea-  
369 sured at an improved energy resolution (13 meV). For the Kr $^-$  ( $4p^5 5s^2 \ ^2P_{3/2}$ ) resonance, a nat-

370 ural width of 3.6(2) meV was deduced from a partial-wave analysis of the angle-dependent reso-  
 371 nance profiles. The resonance energy was determined as 9.489(3) eV with reference to the posi-  
 372 tion of the sharp  $\text{Ar}^- (3p^5 4s^2 {}^2P_{3/2})$  Feshbach resonance (11.103(1) eV [4, 50]). The higher-lying  
 373  $\text{Kr}^- (4p^5 5s^2 {}^2P_{1/2})$  resonance (position 10.126(4) eV) was analyzed by Fano-type fits to the mea-  
 374 sured profiles, resulting in a width of 33(5) meV. This much larger value results from the strong  
 375 decay of this resonance to the excited  $\text{Kr} (4p^5 5s {}^3P_1)$  level. Both the DBSR31p and the BSR47  
 376 calculations predict that the  ${}^2P_{1/2}$  resonance decays predominantly to the nearby  $\text{Kr} (4p^5 5s {}^3P_1)$   
 377 +  $e^-$  channel.

378 The variation of the experimental lineshapes with angle is well recovered by the BSR calcu-  
 379 lations. However, the width of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance is predicted about 20%–25%  
 380 smaller than our experimental result of  $3.6 \pm 0.2$  meV, which is in good agreement with previous  
 381 measurements. Regarding the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{1/2})$  resonance, the fully relativistic DBSR31p model,  
 382 which accounts for long-range polarization effects, predicts a width of  $\approx 32$  meV, in good agreement  
 383 with experiment ( $33 \pm 5$  meV). On the other hand, the BSR47 model (a slightly different structure  
 384 description, more coupled states, but without accounting for polarization effects due to coupling  
 385 to the target continuum) predicts a much smaller width of only  $\approx 15$  meV for this resonance.

386 Unfortunately, it is currently not possible for us to pin down a single reason for the remaining  
 387 discrepancies between experiment and theory in the resonance widths and the apparently high  
 388 sensitivity of the theoretical results for the width of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{1/2})$  resonance. We suspect it  
 389 to be a combination of the background description and the fact that the latter resonance position is  
 390 so close to threshold that any small difference in the predicted position will also affect the calculated  
 391 width very strongly. This becomes even more important due to the fact that the theoretical  
 392 excitation thresholds need to be adjusted to reproduce the experimental energy splittings and thus  
 393 to allow for a direct comparison between experiment and theory. While these adjustments are very  
 394 small in the present case and the BSR approach due to the lack of  $(N + 1)$ -electron terms in the  
 395 close-coupling expansion is generally much less sensitive to this adjustment procedure than the  
 396 standard Belfast  $R$ -matrix approach, we cannot rule out that it is at least partially responsible for  
 397 the sensitivity seen in our results. These findings, as well as the comparison with the angle- and  
 398 final-state-resolved cross sections of Phillips [18], emphasize the need for further high-resolution  
 399 precision experiments as well as continued theoretical efforts to fully understand the intricacies of  
 400 these collision processes.



## Acknowledgments

401

402 This work was supported by the Deutsche Forschungsgemeinschaft (grant HO427/28), by the  
 403 “Forschungszentrum Optische Technologien und Lasergesteuerte Prozesse”, by the European Sci-  
 404 ence Foundation through the network EIPAM (“Electron-Induced Processing At the Molecular  
 405 level” Exchange Grant No. 1288), by the Swiss National Science Foundation (project No. 200020-  
 406 121841), and the United States National Science Foundation under grants #PHY-0757755 and  
 407 #PHY-0903818, as well as the Teragrid allocation MCA08X034. We thank K. Franz for exper-  
 408 imental support in the early phase of the project. We gratefully acknowledge W. Meyer and  
 409 G. Sauter for providing their scattering phase shifts for Kr and M. Zubek for sending a preprint of  
 410 ref. [38].

- 
- 411 [1] G. J. Schulz, *Rev. Mod. Phys.* **45**, 378 (1973).  
 412 [2] S. J. Buckman and C. W. Clark, *Rev. Mod. Phys.* **66**, 539 (1994).  
 413 [3] A. Gopalan, J. Bömmels, S. Götte, A. Landwehr, K. Franz, M. W. Ruf, H. Hotop, and K. Bartschat,  
 414 *Eur. Phys. J. D* **22**, 17 (2003).  
 415 [4] K. Franz, T. H. Hoffmann, J. Bömmels, A. Gopalan, G. Sauter, W. Meyer, M. Allan, M.-W. Ruf, and  
 416 H. Hotop, *Phys. Rev. A* **78**, 012712 (2008).  
 417 [5] J. Bömmels, K. Franz, T. H. Hoffmann, A. Gopalan, O. Zatsarinny, K. Bartschat, M.-W. Ruf, and  
 418 H. Hotop, *Phys. Rev. A* **71**, 012704 (2005).  
 419 [6] M. Zubek, B. Mielewska, J. Channing, G. C. King, and F. H. Read, *J. Phys. B: At. Mol. Opt. Phys.*  
 420 **32**, 1351 (1999).  
 421 [7] G. J. Schulz, *Phys. Rev.* **136**, A650 (1964).  
 422 [8] C. E. Kuyatt, J. A. Simpson, and S. R. Mielczarek, *Phys. Rev.* **138**, A385 (1965).  
 423 [9] L. Sanche and G. J. Schulz, *Phys. Rev. A* **5**, 1672 (1972).  
 424 [10] N. Swanson, J. W. Cooper, and C. E. Kuyatt, *Phys. Rev. A* **8**, 1825 (1973).  
 425 [11] A. Weingartshofer, K. Willmann, and E. M. Clarke, *J. Phys. B: At. Mol. Phys.* **7**, 79 (1974).  
 426 [12] T. Heindorff, J. Hofftt, and P. Dabkiewicz, *J. Phys. B: At. Mol. Phys.* **9**, 89 (1976).  
 427 [13] J. N. H. Brunt, G. C. King, and F. H. Read, *J. Phys. B: At. Mol. Phys.* **9**, 2195 (1976).  
 428 [14] J. Jureta, S. Cvejanovic, J. N. H. Brunt, and F. H. Read, *J. Phys. B: At. Mol. Phys.* **11**, L347 (1978).  
 429 [15] D. Dubé, D. Tremblay, and D. Roy, *Phys. Rev. A* **47**, 2893 (1993).  
 430 [16] F. H. Read and J. M. Channing, *Rev. Sci. Instrum.* **67**, 2372 (1996).  
 431 [17] M. Zubek, N. Gulley, G. C. King, and F. H. Read, *J. Phys. B: At. Mol. Opt. Phys.* **29**, L239 (1996).  
 432 [18] J. M. Phillips, *J. Phys. B: At. Mol. Phys.* **15**, 4259 (1982).



- 433 [19] M. Allan, *J. Phys. B: At. Mol. Opt. Phys.* **25**, 1559 (1992).
- 434 [20] J. C. Nickel, P. W. Zetner, G. Shen, and S. Trajmar, *J. Phys. E: Sci. Instrum.* **22**, 730 (1989).
- 435 [21] M. Allan, *J. Phys. B: At. Mol. Opt. Phys.* **33**, L215 (2000).
- 436 [22] M. Allan, *J. Phys. B: At. Mol. Opt. Phys.* **38**, 3655 (2005).
- 437 [23] M. Allan, *J. Phys. B: At. Mol. Opt. Phys.* **40**, 3531 (2007).
- 438 [24] N. F. Mott and H. S. W. Massey, *The theory of atomic collisions* (Oxford University Press, Oxford,  
439 1965), 3rd ed.
- 440 [25] D. G. Thompson, *Proc. Roy. Soc. A, Math. and Phys. Sci.* **294**, 160 (1966).
- 441 [26] D. R. Lide, ed., *T. M. Miller in CRC Handbook of Chemistry and Physics* (CRC Press (Taylor &  
442 Francis), Boca Raton, 2008), 88th ed.
- 443 [27] O. Zatsarinny, *Comp. Phys. Commun.* **174**, 273 (2006).
- 444 [28] O. Zatsarinny and K. Bartschat, *Phys. Rev. A* **77**, 062701 (2008).
- 445 [29] O. Zatsarinny and K. Bartschat, *J. Phys. B: At. Mol. Opt. Phys.* **43**, in press (2010).
- 446 [30] O. Zatsarinny and K. Bartschat, *J. Phys. B: At. Mol. Opt. Phys.* **37**, 2173 (2004).
- 447 [31] O. Zatsarinny and K. Bartschat, *J. Phys. B: At. Mol. Opt. Phys.* **37**, 4693 (2004).
- 448 [32] O. Zatsarinny and C. F. Fischer, *J. Phys. B: At. Mol. Opt. Phys.* **35**, 4669 (2002).
- 449 [33] P. Jönsson, X. He, C. F. Fischer, and I. P. Grant, *Comp. Phys. Commun.* **177**, 597 (2007).
- 450 [34] O. Zatsarinny and K. Bartschat, *Phys. Scr.* **T134**, 014020 (2009).
- 451 [35] C. J. Noble, private communication (2008).
- 452 [36] V. M. Burke and C. J. Noble, *Comp. Phys. Commun.* **85**, 471 (1995).
- 453 [37] A. N. Grum-Grzhimailo, *Comp. Phys. Commun.* **152**, 101 (2003).
- 454 [38] I. Linert, B. Mielewska, G. C. King, and M. Zubek, *Phys. Rev. A* **81**, 012706 (2010).
- 455 [39] H. Cho, R. J. Gulley, and S. J. Buckman, *J. Kor. Phys. Soc.* **42**, 71 (2003).
- 456 [40] A. Danjo, *J. Phys. B: At. Mol. Opt. Phys.* **21**, 3759 (1988).
- 457 [41] S. K. Srivastava, H. Tanaka, A. Chutjian, and S. Trajmar, *Phys. Rev. A* **23**, 2156 (1981).
- 458 [42] W. C. Fon, K. A. Berrington, and A. Hibbert, *J. Phys. B: At. Mol. Phys.* **17**, 3279 (1984).
- 459 [43] K. L. Bell, K. A. Berrington, and A. Hibbert, *J. Phys. B: At. Mol. Opt. Phys.* **21**, 4205 (1988).
- 460 [44] J. E. Sienkiewicz and W. E. Baylis, *J. Phys. B: At. Mol. Opt. Phys.* **24**, 1739 (1991).
- 461 [45] G. Sauter and W. Meyer, private communication of preliminary data (2009).
- 462 [46] R. P. McEachran and A. D. Stauffer, *J. Phys. B: At. Mol. Opt. Phys.* **36**, 3977 (2003).
- 463 [47] B. W. Shore, *Phys. Rev.* **171**, 43 (1968).
- 464 [48] I. D. Petrov, V. L. Sukhorukov, and H. Hotop, *J. Phys. B: At. Mol. Opt. Phys.* **41**, 065205 (2008).
- 465 [49] F. M. J. Pichanick and J. A. Simpson, *Phys. Rev.* **168**, 64 (1968).
- 466 [50] P. Hammond, *J. Phys. B: At. Mol. Opt. Phys.* **29**, L231 (1996).
- 467 [51] J. N. H. Brunt, G. C. King, and F. H. Read, *J. Phys. B: At. Mol. Phys.* **10**, 3781 (1977).
- 468 [52] S. J. Buckman, P. Hammond, G. C. King, and F. H. Read, *J. Phys. B: At. Mol. Phys.* **16**, 4219 (1983).
- 469 [53] F. T. Smith, *Phys. Rev.* **118**, 349 (1960).

TABLE I: Absolute angle-differential cross sections for elastic e–Kr scattering (in  $10^{-20} \text{m}^2/\text{sr}$ ). Comparison of different experimental data measured at 10 eV: Linert *et al.* [38], angular acceptance  $\Delta\theta \pm 2^\circ$ , uncertainty  $\pm 15\%$ ; Cho *et al.* [39],  $\Delta\theta \pm 1.5^\circ$ , uncertainty  $\pm (7 - 15)\%$ ; Danjo [40],  $\Delta\theta \pm 2^\circ$ , uncertainty  $\pm 20\%$ ; Srivastava *et al.* [41],  $\Delta\theta \pm 1.8^\circ$ , uncertainty  $\pm 20\%$ ; present work (measured at 9.8 eV),  $\Delta\theta \pm 1.5^\circ$ , uncertainty  $\pm 15\%$ .

angle ( $^\circ$ )	this work	Linert <i>et al.</i>	Cho <i>et al.</i>	Danjo	Srivastava <i>et al.</i>
10	13.00			13.6	
15	11.02			11.6	
20	9.31		10.637	9.8	7.1
25	7.57		8.659	7.6	5.8
30	6.11	6.246	6.916	6.6	4.6
35	4.88		5.110	5.4	3.8
40	3.84	3.778	3.917	4.4	3.1
45	3.01		2.922	3.2	2.3
50	2.39	2.364	2.400	2.8	1.8
55	1.96		1.928	2.3	1.5
60	1.64	1.568	1.640	1.9	1.3
65	1.45		1.480	1.6	1.2
70	1.33	1.393	1.399	1.6	1.1
75	1.25		1.325	1.8	1.1
80	1.20	1.242	1.220	1.6	1.1
85	1.09		1.112	1.4	1.0
90	0.946	0.907	0.939	1.2	0.84
95	0.783		0.788	1.1	0.68
100	0.559	0.489	0.612	0.79	0.46
105	0.317		0.406	0.54	0.28
110	0.144	0.162	0.218	0.30	0.10
115	0.071	0.136	0.131	0.18	0.084
117	0.063				
120	0.080	0.213	0.142	0.38	0.15
125	0.216		0.278	0.72	0.36
130	0.499	0.613	0.597		0.70
135	0.912		1.344		
140	1.41	1.577	1.781		
145	2.00		2.353		
150	2.64	3.095	2.921		
155	3.30		3.271		
160	3.97	4.377	3.695		
165	4.71		4.098		
170	5.23	4.926	4.325		
175	5.59		4.586		
180	5.72	5.882	4.688		

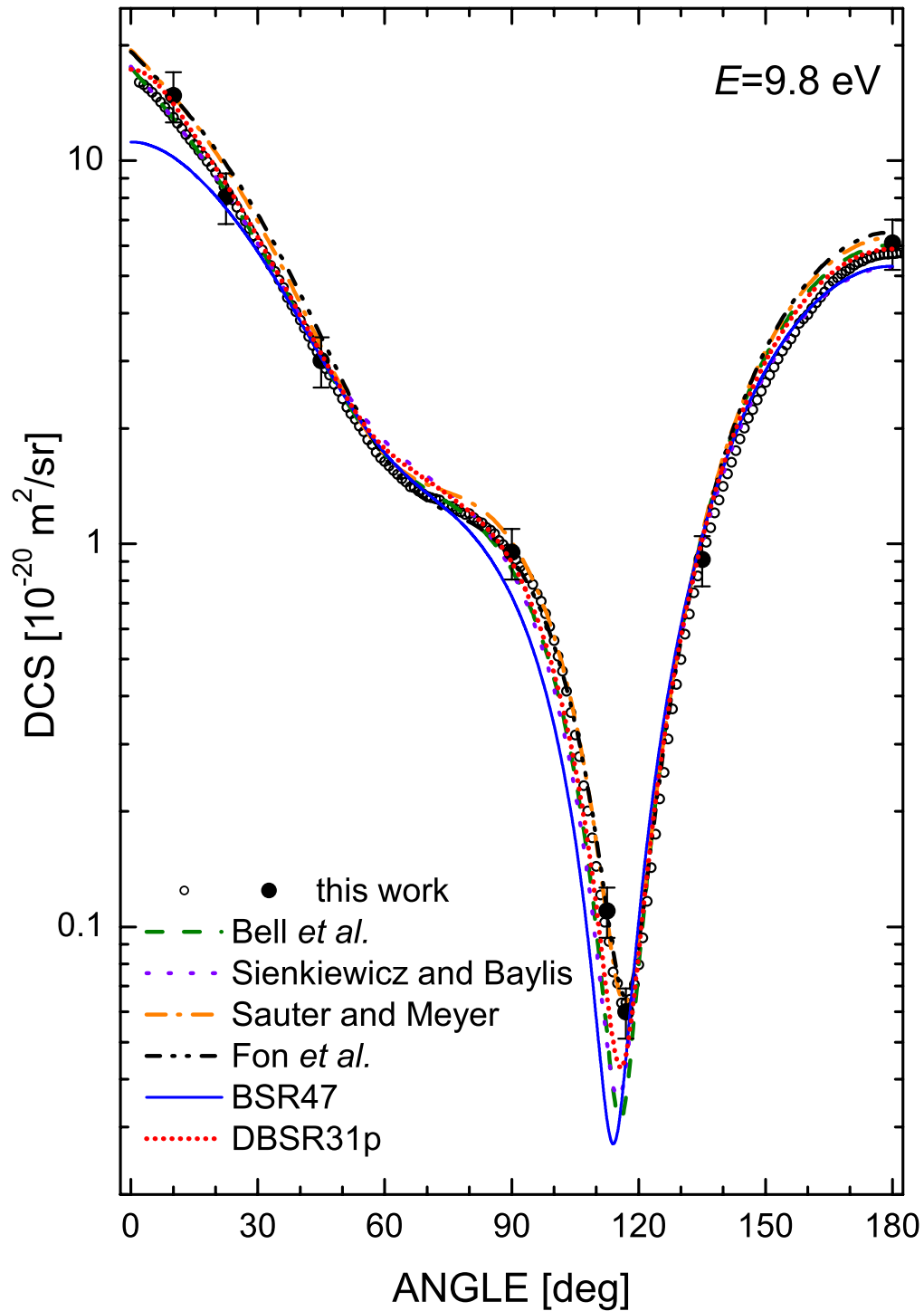


FIG. 1: Differential cross section for elastic e–Kr scattering, measured in Fribourg at an electron energy of 9.8 eV, compared to angular distributions calculated with theoretical phase shifts due to Fon *et al.* [42], Bell *et al.* [43], Sienkiewicz and Baylis [44], and Sauter and Meyer [45]. The full circles with error bars indicate the experimental absolute measurements at several discrete angles, the open circles were obtained from magnetic scans with  $1^\circ$  increment, recorded at three fixed detector positions ( $45^\circ$ ,  $90^\circ$ ,  $135^\circ$ ) and normalized as described in [22]. The predictions of the DBSR31p and the BSR47 model are also included. (colour online)

TABLE II: Comparison of phase shifts for elastic e–Kr scattering from different authors (in rad).

Phases from	$\delta_0(9.5\text{eV})$	$\delta_1(9.5\text{eV})$	$\delta_2(9.5\text{eV})$	$\delta_3(9.5\text{eV})$
	$\delta_0(9.8\text{eV})$	$\delta_1(9.8\text{eV})$	$\delta_2(9.8\text{eV})$	$\delta_3(9.8\text{eV})$
Bell <i>et al.</i> [43]	-1.260	-0.687	+0.865	+0.132
	-1.283	-0.705	+0.894	+0.137
Fon <i>et al.</i> [42]	-1.250	-0.736	+0.955	+0.130
	-1.274	-0.753	+0.986	+0.134
Sienkiewicz and Baylis $\delta^+$ [44]	-1.244	-0.732	+0.825	+0.144
	-1.267	-0.751	+0.854	+0.149
Sienkiewicz and Baylis $\delta^-$		-0.691	+0.828	+0.143
		-0.710	+0.857	+0.148
Sauter and Meyer [45]	-1.182	-0.667	+0.986	+0.155
	-1.206	-0.683	+1.016	+0.162

TABLE III: Width of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance when analyzed using different phase shifts (Q: quality factor, see text).

Phases from	$\Gamma$ (meV)	$\Delta E$ (meV)	Q
Bell <i>et al.</i> [43]	3.31	12.3	0.32
Fon <i>et al.</i> [42]	3.74	12.2	0.52
Sienkiewicz and Baylis [44]	3.30	12.4	0.34
Sauter and Meyer [45]	3.67	12.3	1.00

TABLE IV: Natural width of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2,1/2})$  resonances.

	$\Gamma_{3/2}$ (meV)	$\Gamma_{1/2}$ (meV)
Swanson <i>et al.</i> [10]	3.8–6.0	
Weingartshofer <i>et al.</i> [11]	8	
Dubé <i>et al.</i> [15]	3.6(4)	
Zubek <i>et al.</i> [6]	3.5(1.0)	30(4)
this work (exp.)	3.6(2)	33(5)
this work (DBSR31p)	2.9	31.9
this work (BSR47)	2.7	15.4

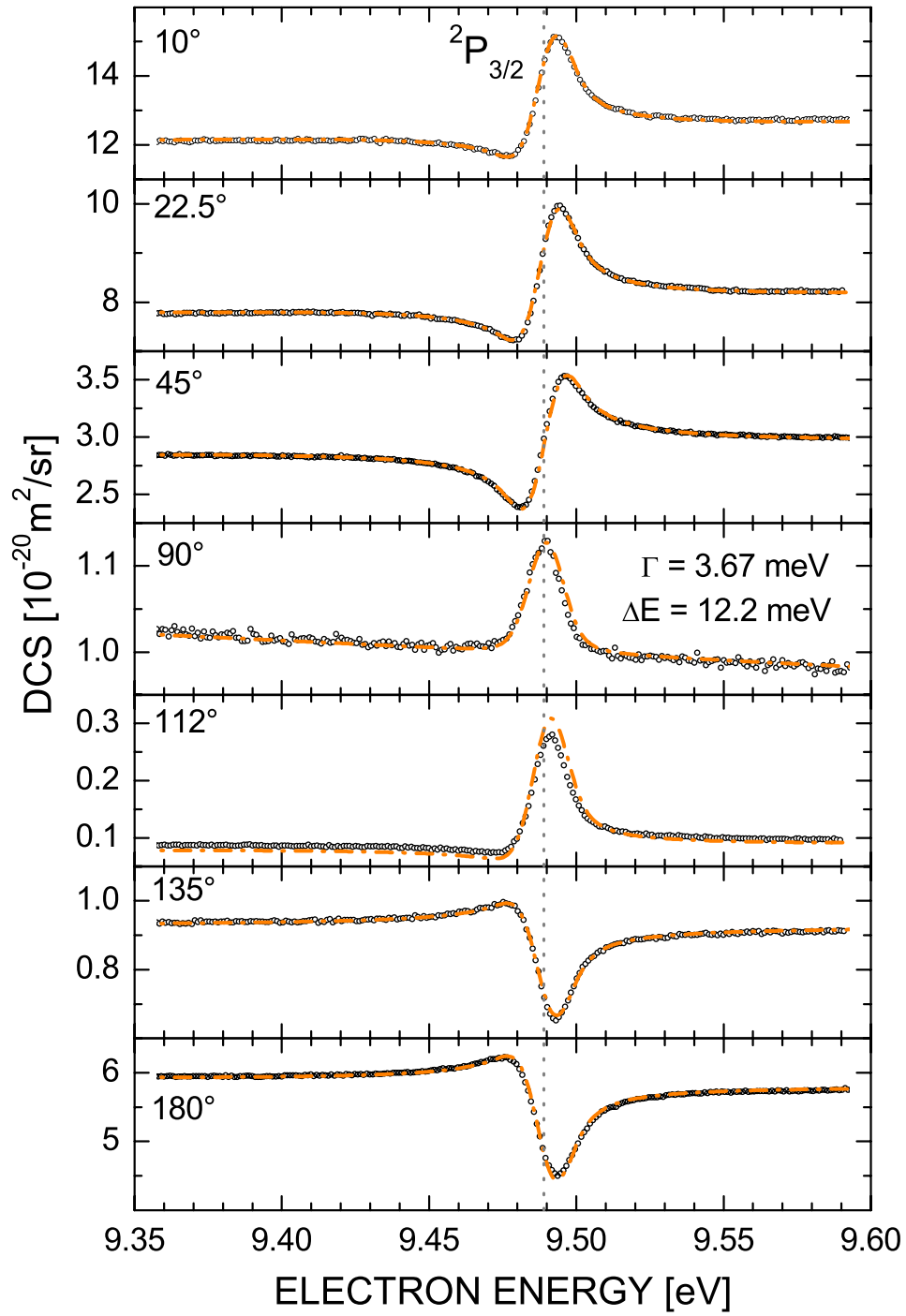


FIG. 2: Differential cross section for elastic e–Kr scattering in the vicinity of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2})$  resonance (open circles: experiment). The line profiles (chain orange curves) were calculated from the phases of Sauter and Meyer [45]. (colour online)

TABLE V: Energy position and fine-structure splitting of the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2,1/2})$  resonances.

	Energy [eV]		$\Delta_{\text{FS}}$ [meV]
	${}^2P_{3/2}$	${}^2P_{1/2}$	
Kuyatt <i>et al.</i> [8]	9.45 – 9.48(1)	10.10(1)	640(10)
Pichanick and Simpson [49]		10.05	
Sanche and Schulz [9]	9.50 – 9.53(3)	10.16 – 10.19(3)	660
Swanson <i>et al.</i> [10] <sup>a</sup>	9.515	10.155	640
Weingartshofer <i>et al.</i> [11] <sup>b</sup>	9.525(10)	10.162	637(10)
Brunt <i>et al.</i> [13]	9.484(10)	10.123	639(3)
Jureta <i>et al.</i> [14]	9.490(12)	10.119(5)	
Zubek <i>et al.</i> [6] <sup>c</sup>	9.485(12)	10.121(15)	636
this work (BSR47)	9.489	10.126	637
this work (BSR31p)	9.488	10.128	640

<sup>a</sup> position of the first resonance by Sanche and Schulz [9] taken as reference

<sup>b</sup> recalibrated values, using 19.365 eV [3] as the energy for the  $\text{He}^- (1s2s^2 {}^2S_{1/2})$  resonance

<sup>c</sup> relative to the position for the  $\text{Ar}^- (3p^5 4s^2 {}^2P_{3/2})$  resonance: 11.103 eV [4, 50]

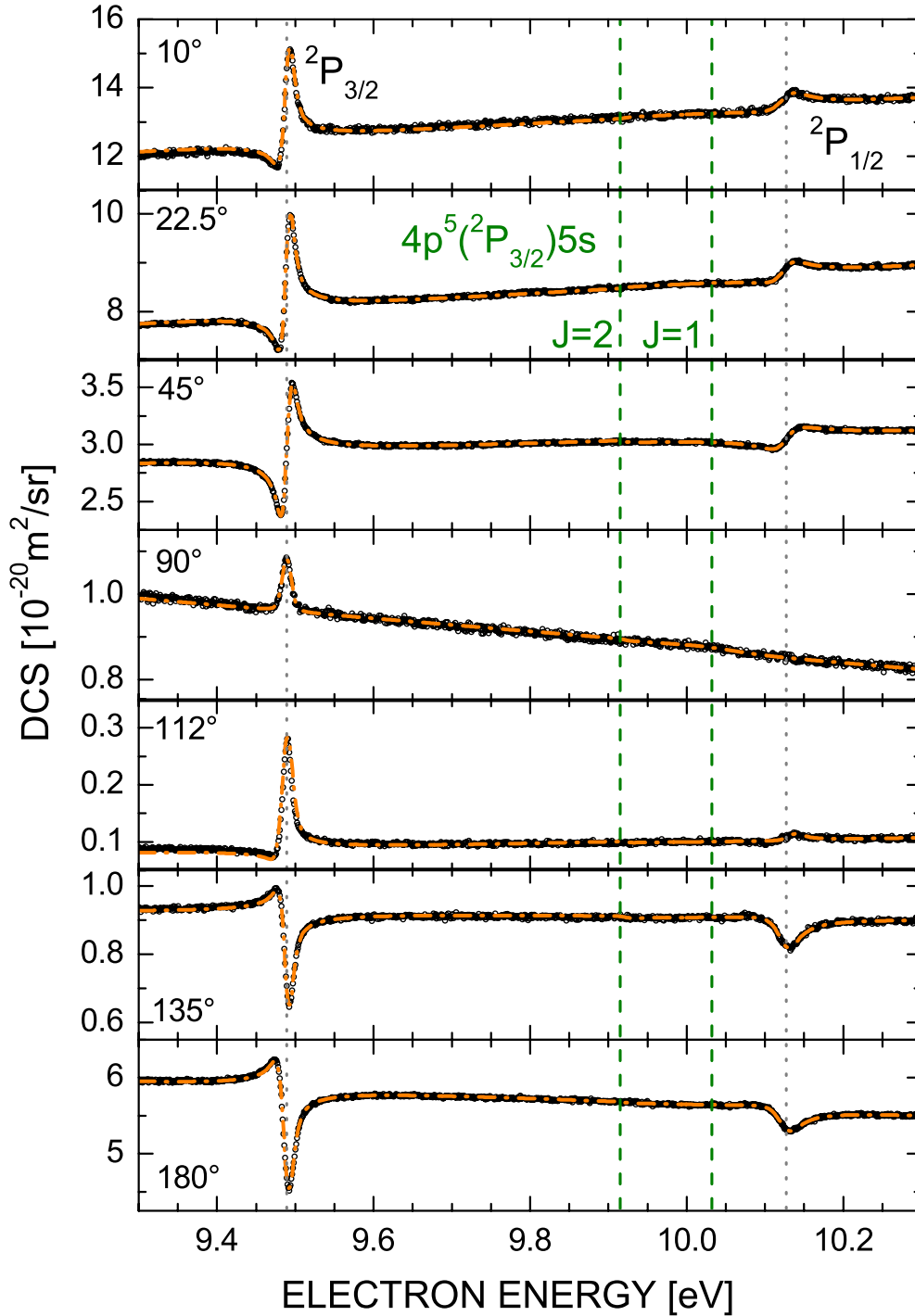


FIG. 3: Differential cross section for elastic e–Kr scattering in the vicinity of the  $\text{Kr}^- (4p^5 5s^2 \ ^2P_{3/2,1/2})$  resonances (open circles: experiment). The chain orange curves represent the result of a phase-shift analysis for the  $\text{Kr}^- (4p^5 5s^2 \ ^2P_{3/2})$  resonance and Fano-type profiles with appropriate background (see text) for the  $\text{Kr}^- (4p^5 5s^2 \ ^2P_{1/2})$  resonance. The broken vertical lines indicate the thresholds for the  $\text{Kr} (4p^5 5s^2 \ ^3P_{2,1})$  levels while the dotted vertical lines represent the positions of the  $^2P_{3/2}$  and  $^2P_{1/2}$  resonances. (colour online)

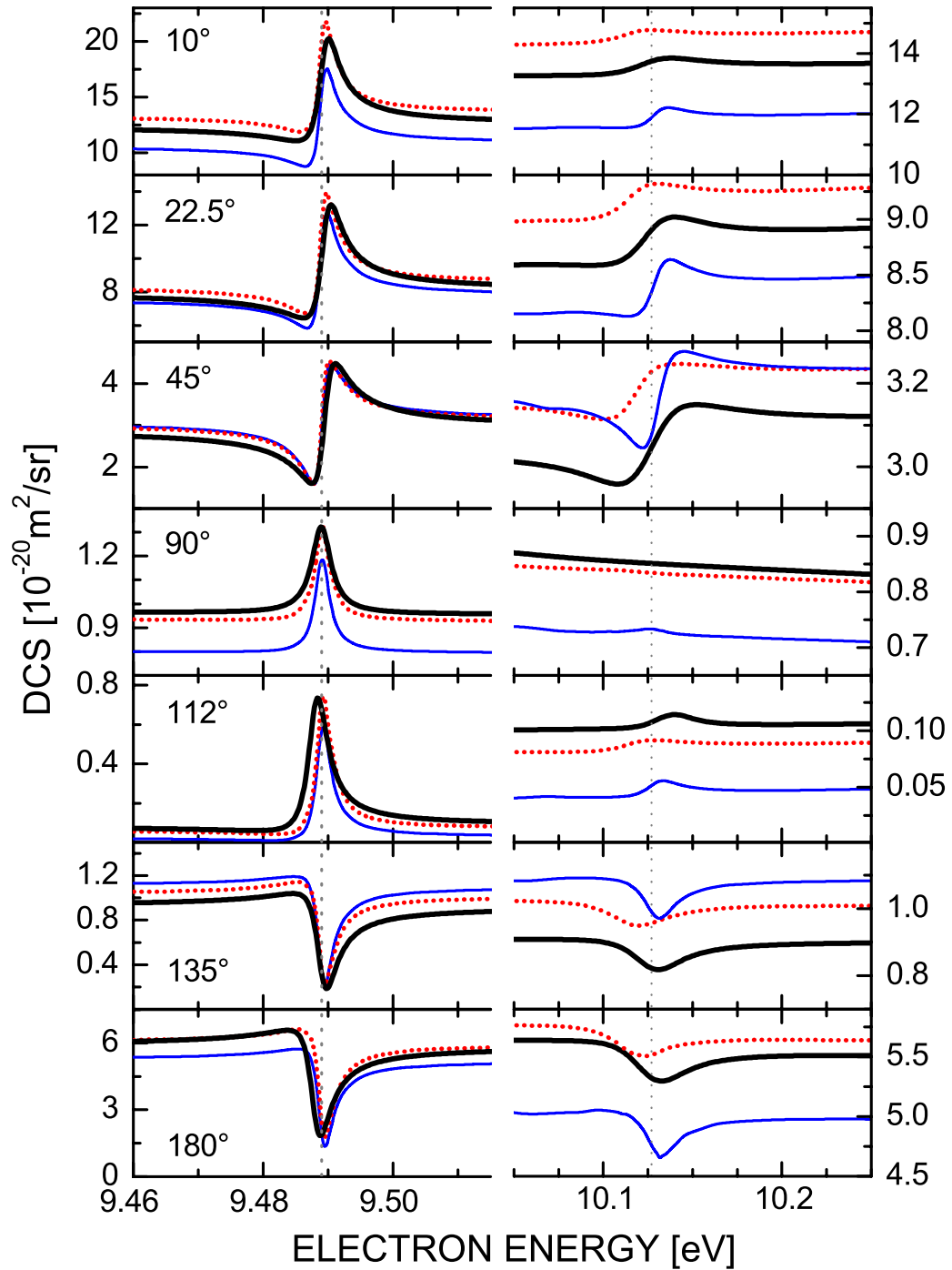


FIG. 4: Differential cross section for elastic  $e$ -Kr scattering around the  $\text{Kr}^- (4p^5 5s^2 {}^2P_{3/2,1/2})$  resonances. The unconvoluted line shapes, deduced from the fits to the experimental data, are shown as thick black curves and compared with theoretical results obtained from the DBSR31p (dotted red curves) and BSR47 (full blue curves) models (colour online). The dotted vertical lines represent the positions of the  ${}^2P_{3/2}$  and  ${}^2P_{1/2}$  resonances.



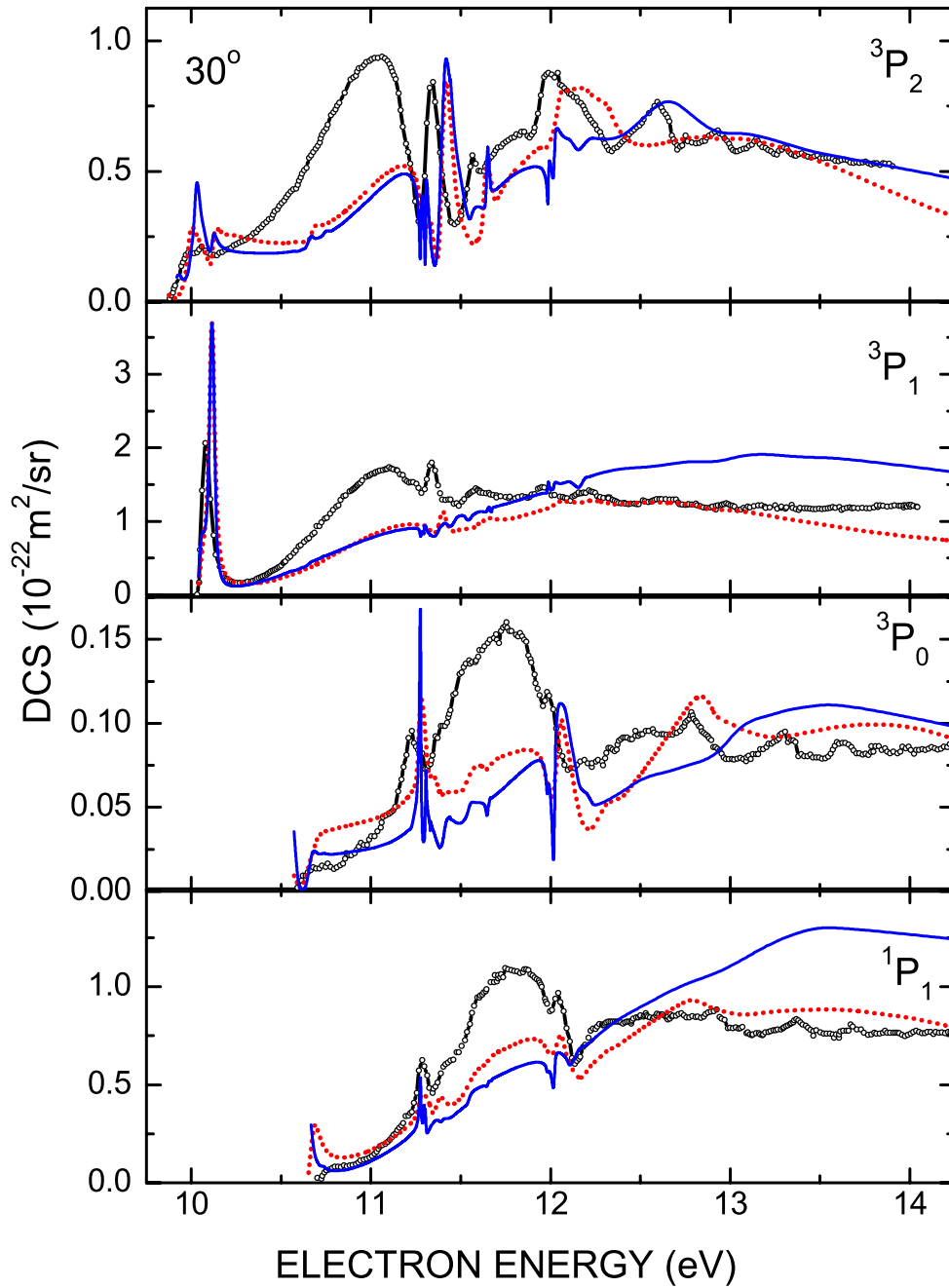


FIG. 5: Differential cross section for electron-impact excitation of Kr at a scattering angle of  $30^\circ$ . The experimental data (open circles; resolution 35 meV) are taken from Phillips by digitizing the data in figure 5 of [18]. They are compared with theoretical results obtained from the DBSR31p (dotted red curves) and BSR47 (full blue curves) models (colour online).

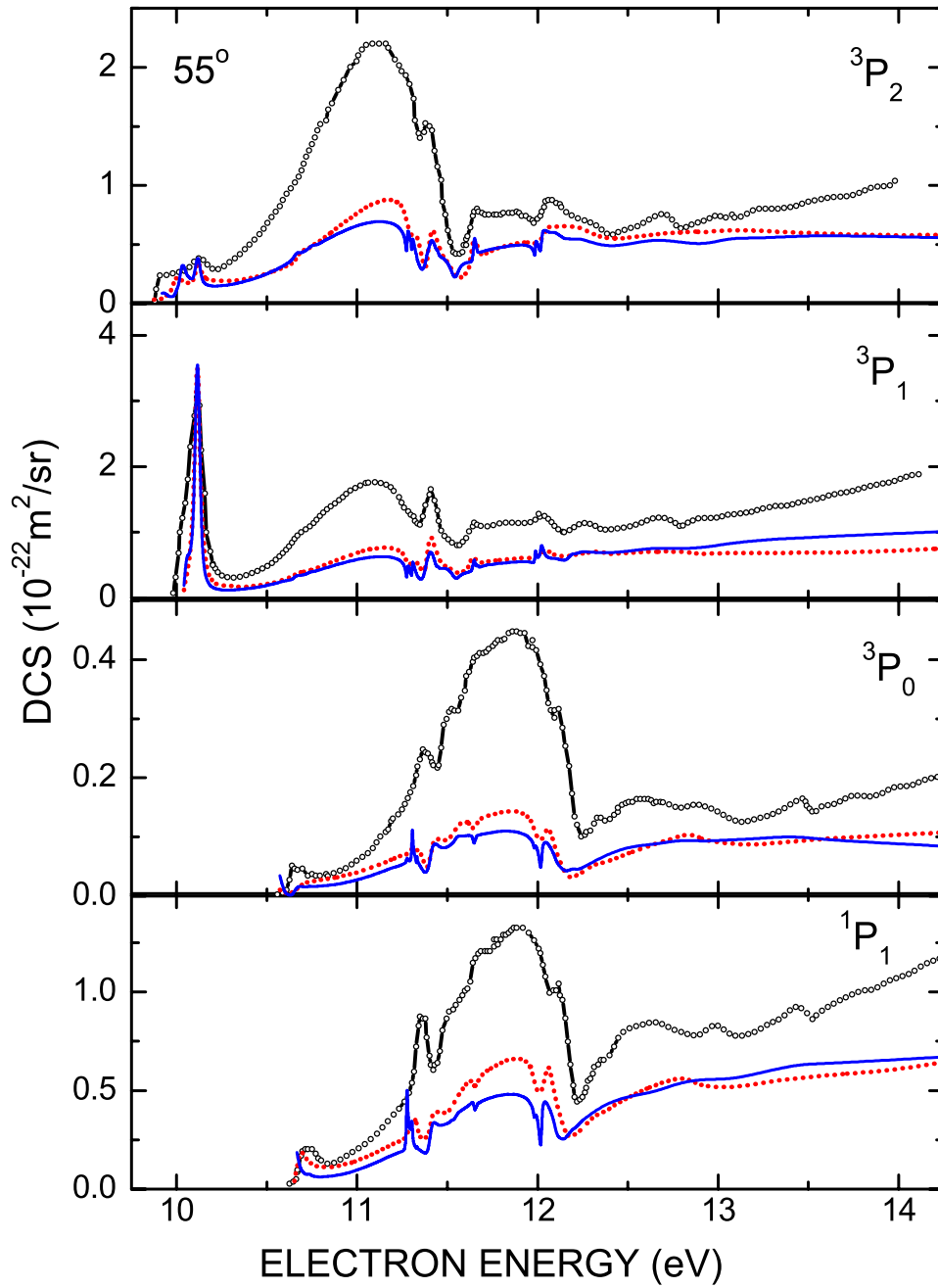


FIG. 6: Differential cross section for electron-impact excitation of Kr at a scattering angle of  $55^\circ$ . The experimental data (open circles; resolution 35 meV) are taken from Phillips by digitizing the data in figure 4 of [18]. They are compared with theoretical results obtained from the DBSR31p (dotted red curves) and BSR47 (full blue curves) models (colour online).

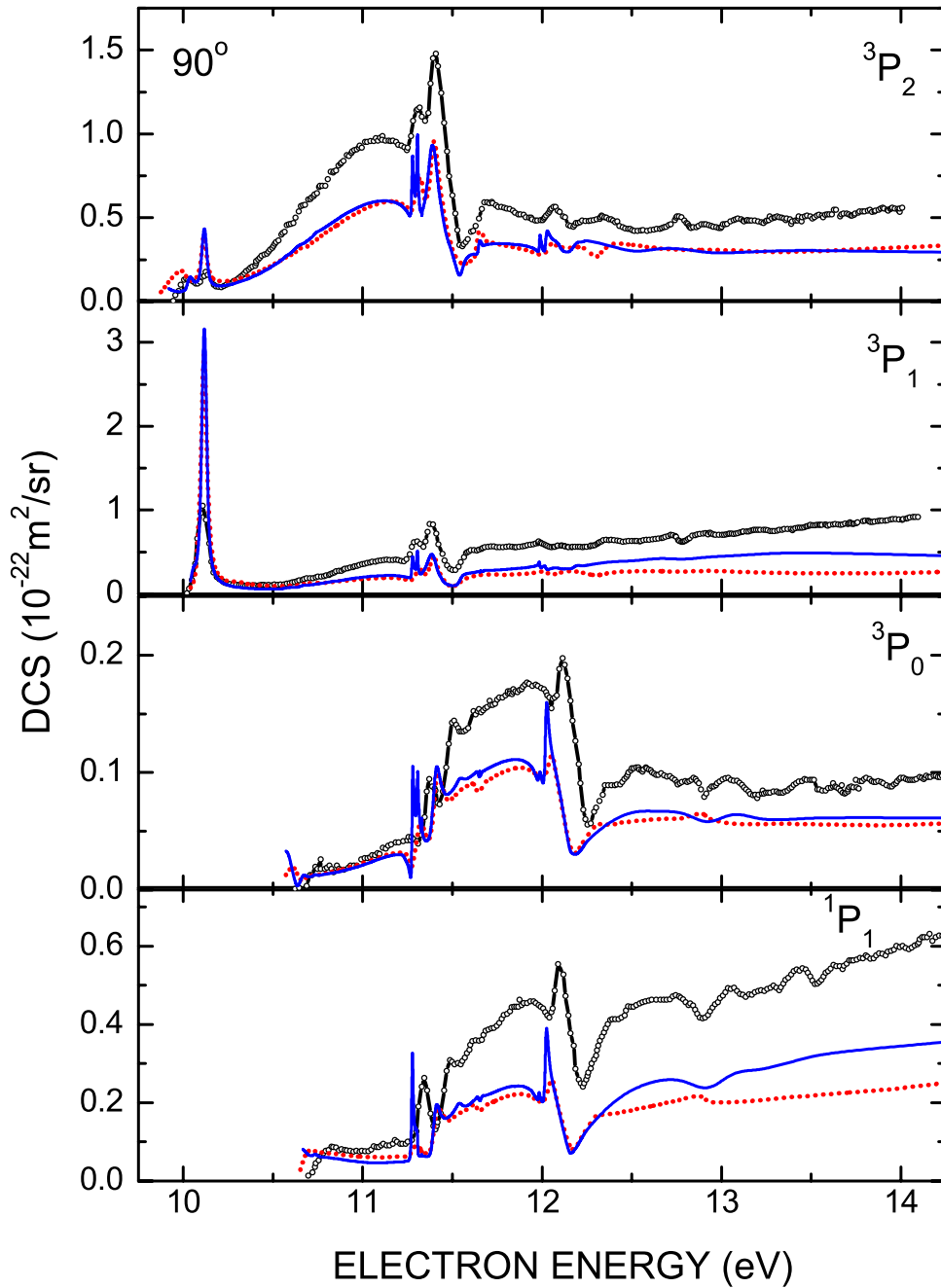


FIG. 7: Differential cross section for electron-impact excitation of Kr at a scattering angle of  $90^\circ$ . The experimental data (open circles; resolution 35 meV) are taken from Phillips by digitizing the data in figure 3 of [18]. They are compared with theoretical results obtained from the DBSR31p (dotted red curves) and BSR47 (full blue curves) models (colour online).