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K lines in the sulphur isonuclear sequence

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Abstract

Accurate and complete sets of atomic data are being computed for the radiative and Auger processes giving rise to K lines in ions of sulphur. AUTOSTRUCTURE, HFR and BPRM codes are used, taking into account configuration interaction, core relaxation and relativistic effects so as to generate data following an approach used in our previous studies on iron and oxygen. Level energies, wavelengths, A-values and Auger rates are compared with available measurements and previous calculations.
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1. Introduction

Impetus of accurate atomic data production relevant to X-ray astronomy comes from current developments in instrumentation, which has seen dramatic improvements in sensitivity, spatial and spectral resolution, since the launch of the *Chandra* and *XMM-Newton* satellites. They provide spectra of resolving power $\sim 300-1000$ in the energy range $0.2-8$ keV in contrast with the previous *ASCA* satellite (resolving power ~ 20). The next launch of the *Astro-E2* satellite will further improve the situation with its fixed 6 eV resolution XRS spectrometer.

Line features involving the K shell of all the ions of medium Z elements fall within the above-mentioned spectral region. As few accurate data were available for modelling those lines, we have begun to calculate them starting with the most cosmically abundant among them, i.e. iron (Kallman et al., 2004) and oxygen (García

et al., 2005). In the present paper, we give sample results of our calculations for the other abundant elements comparing them with other theoretical and experimental data.

2. Calculations

We have used the multiplatform approach described in detail elsewhere (Bautista et al., 2003). It briefly consists in using different standard atomic codes assessing accuracy rankings of the calculated atomic parameters (level energies, wavelengths, A-values and Auger rates).

The HFR code implements the pseudo-relativistic Hartree–Fock method of Cowan (1981). AUTOSTRUCTURE (AST) (Badnell, 1986, 1997) constructs atomic state functions from an orbital basis generated in a statistical Thomas–Fermi–Dirac potential (Eissner and Nussbaumer, 1969). It also provides the necessary target atomic orbitals for solving the close-coupling equations (Burke and Seaton, 1971) implemented in the Breit–Pauli

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R-matrix (BPRM) package (Burke and Berrington, 1993) in order to compute the scattering data (collision strengths and photoionisation cross sections).

As the atomic orbitals between the initial 1*s*-hole and final valence configurations are significantly different due to the difference in the nuclear charge screening, core relaxation effects have to be taken into account alongside the configuration interaction (CI) and relativistic effects. In order to do so, both structure codes, i.e. HFR and AST, use non-orthogonal orbital basis. CI were included within the $n = 3$ complex and the relativistic corrections were introduced solving the Breit–Pauli Hamiltonian.

3. Results

A comparison of the available experimental level energies with our eigenvalues computed in the sulphur isonuclear sequence by both HFR and AST codes is given in Table 1 showing a good agreement with experiment. Fig. 1 shows the wavelength differences (in mÅ) between HFR values and others as function of the HFR wavelength. In Fig. 2, ratios of calculated radiative transition probabilities with respect to HFR values are presented as function of the HFR A-value (in s^{-1}). Fig. 3 is the equivalent of Fig. 2 but for the Auger widths (in s^{-1}).

Table 1
Comparison between the experimental and our calculated level energies in the sulphur isonuclear sequence

Ion	Level designation	Energy (eV)		
		Expt[a]	AST[b]	HFR[c]
S XV	$1s^2\ ^1S_0$	0.0000	0	0
	$1s2s\ ^3S_1$	2430.3475	2429.3	2430.1
	$1s2p\ ^3P^o_0$	2446.7429	2446.0	2446.2
	$1s2p\ ^3P^o_1$	2447.1406	2446.4	2446.9
	$1s2s\ ^1S_0$	2448.1265	2447.9	2448.2
	$1s2p\ ^3P^o_2$	2460.6256	2460.3	2460.9
S XIV	$1s^22s\ ^2S_{1/2}$	0.0000	0	0
	$1s^22p\ ^2P^o_{1/2}$	27.8178	28.7	27.8
	$1s^22p\ ^2P^o_{3/2}$	29.6854	30.6	29.7
	$1s2s^2\ ^2S^o_{1/2}$	2408.02	2408.6	2408.0
	$1s(^2S)2s2p(^3P^o)\ ^4P^o_{1/2}$	2415.26	2415.5	2414.7
	$1s(^2S)2s2p(^3P^o)\ ^4P^o_{3/2}$	2415.77	2416.0	2415.4
	$1s(^2S)2s2p(^3P^o)\ ^4P^o_{5/2}$	2417.00	2417.2	2416.7
	$1s(^2S)2s2p(^3P^o)\ ^2P^o_{1/2}$	2437.05	2438.2	2437.3
	$1s(^2S)2p^2(^3P)\ ^4P_{1/2}$	2445.13	2445.5	2444.7
	$1s(^2S)2p^2(^3P)\ ^4P_{3/2}$	2445.95	2446.3	2445.5
	$1s(^2S)2p^2(^3P)\ ^4P_{5/2}$	2446.87	2447.2	2446.7
	$1s(^2S)2s2p(^1P^o)\ ^2P^o_{1/2}$	2447.05	2449.0	2447.8
	$1s(^2S)2s2p(^1P^o)\ ^2P^o_{3/2}$	2447.55	2449.3	2448.3
	$1s(^2S)2p^2(^1D)\ ^2D_{5/2}$	2459.62	2461.2	2460.4
	$1s(^2S)2p^2(^1D)\ ^2D_{3/2}$	2459.72	2461.3	2460.1
	$1s(^2S)2p^2(^3P)\ ^2P_{1/2}$	2462.82	2464.4	2463.4
	$1s(^2S)2p^2(^3P)\ ^2P_{3/2}$	2464.62	2466.2	2465.2
	$1s(^2S)2p^2(^1S)\ ^2S_{1/2}$	2478.96	2481.1	2480.1
S I	$[1s]3p^5\ ^3P^o_2$	2472.0[d]	2468.4	2468.7

[a]NIST Atomic Spectra Database (http://physics.nist.gov/PhysRefData/ASD).
[b]AUTOSTRUCTURE calculations (this work).
[c]HFR calculations (this work).
[d]Photoabsorption measurement of S$_2$ vapour (Durand et al., 1996).