IOCAT 2026 Conference

The 1st International Online Conference on Atoms

29–30 January 2026 | Online

MDPI

Critically evaluated atomic data of Kr V-VI relevant to the hot DO-type white dwarf RE0503-289

Aftab Alam, Abid Husain,M.Sahama,K.Harish

Department of Physics,Aligarh Muslim University,Aligarh 202002,India

INTRODUCTION

Spectral lines of krypton (Kr V–VII) have been observed in the UV spectrum of the hot DO-type white dwarf RE 0503–289. About ten spectral lines of Kr V and fourteen lines of Kr VI have been used to determine the krypton abundance of it [1]. Rauch et al[1]. provided extensive atomic data (Kr IV–VII) without any uncertainty estimates. However, reliable and evaluated atomic data of these ions are essential for abundance determination. Recently, we evaluated transition probabilities for Kr VI. In this work, we intended to perform the same for the Kr V spectrum and its detailed comparison with the literature data.In the present study,we have calculated the weighted transition probability(gA) for the ten spectral lines oberved in the UV spectrum of DO-type white dwarf RE0503-289 using relativistic Hartree-Fock method.And a critical analysis of (gA) values of these lines were caried out as discussed in Result and discussion section.

METHOD

The atomic structure and radiative parameters of Kr V were calculated using the Cowan suite of codes, based on the pseudo-relativistic Hartree–Fock (HFR) method (window-based version). The computational procedure follows Ref. [2]. Transition probabilities were evaluated using multiple comparison schemes.

Two atomic models were considered:

- HFR-A: Configuration set identical to that used by Rauch et al. [1] for Kr V.
- HFR-B: Expanded configuration basis, providing an improved treatment of valence–valence (VV) correlation effects (Ref. [3]).

The model of Rauch et al. [1] includes a core-polarization (CPOL) correction to account for core–valence (CV) interactions, whereas CPOL was not included in the present models. A comparison between HFR-A and HFR-B therefore allows assessment of the impact of configuration interaction on the calculated gA-values. ***For both models, Slater parameters were initially scaled to 85% of the HFR values for F^k and 75% for G^k and R^k. The average energies E_av and spin–orbit parameters ζ_(n,l) were fixed at their HFR values***. A least-squares fitting (LSF) procedure was applied to minimize deviations between calculated and experimental energy levels.

The fitting used experimentally established levels from Ref. [4], together with levels newly identified in the present work.***The Standard deviation of the fit for both parity cames out to be less than 400cm^{-1}***.The optimized models were then used to compute radiative transition probabilities.

Table 1:Critically evaluated Kr V lines detected in UVS of RE0503-289

W_obs (Å)	Lower level	Upper level	log(gf)_ Raineri[4]	log(gf)_ Rauch[1]	log(gf)_ TW	CF_TW	Acc.
1384.59	$4s^24p4d\ ^3P^\circ_2$	$4s^24p5p\ ^1P_1$	−1.19	−0.59	−0.80	−0.18	D+
1387.95	$4s^24p4d\ ^3P^\circ_1$	$4s^24p5p\ ^3P_0$	−0.75	−0.65	−0.75	−0.23	D+
1392.63	$4s^24p4d\ ^1D^\circ_2$	$4s^24p5p\ ^3P_1$	−0.42	−0.70	−0.53	−0.44	D+
1393.61	$4s^24p4d\ ^3D^\circ_3$	$4s^24p5p\ ^3P_2$	−0.22	−0.16	−0.19	−0.40	D+
1515.64	$4s^24p5p\ ^3D_1$	$4s^24p5d\ ^3F^\circ_2$	−0.61	+0.39	+0.43	+0.67	D+
1566.03	$4s^24p4d\ ^3D^\circ_2$	$4s^24p5p\ ^3D_2$	−1.78	−2.42	−1.57	+0.04	E
1581.27	$4s4p^24d\ ^1D_2$	$4s^24p5d\ ^1D^\circ_2$	−3.11	−1.42	−1.31	+0.15	E
1589.22	$4s^24p5p\ ^3D_2$	$4s^24p5d\ ^3F^\circ_3$	+0.71	+0.68	+0.68	+0.69	D+
1591.87	$4s^24p5p\ ^3P_2$	$4s^24p5d\ ^3D^\circ_3$	+0.41	+0.49	+0.47	+0.56	D+
1764.47	$4s^24p5s\ ^1P^\circ_1$	$4s^24p5p\ ^1S_0$	−0.17	−0.17	−0.26	−0.57	D+

RESULTS & DISCUSSION

The accuracy of the calculated weighted transition probabilities (gA) and line strengths (S) in atomic units (a.u.) has been evaluated through a comparative analysis with the established literature of Raineri[4] and Rauch[1]. As illustrated in the comparison plots (Raineri vs. Rauch and This Work vs. Rauch), the results are categorized into two primary accuracy grades based on their percentage uncertainty: Grade D+, representing transitions with an uncertainty ≤ 31.

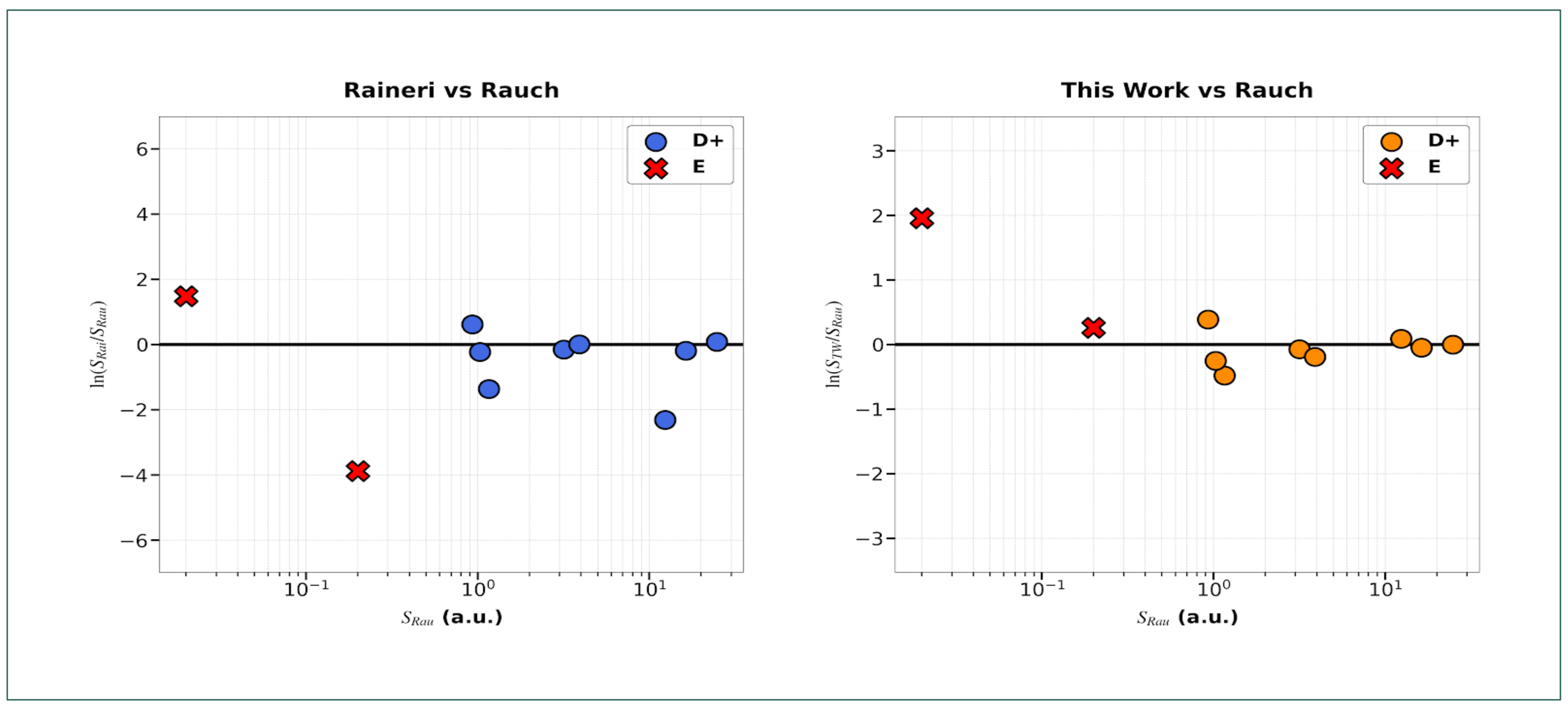

Fig 1. Line strength(S) comparisions calculated from different HFR Models

The primary driver of high uncertainty in the Grade E transitions, which are highlighted in the This Work vs. Rauch graph as red X markers, is the Cancellation Factor (CF). When the CF is low (CF < 0.1), the transition probability becomes exceptionally sensitive to the specific Configuration Interaction (CI) expansion and Core Polarization (CP) treatments used in the model. In these cases, the transition integral suffers from extreme destructive interference, where the final value of S is the small difference between large competing terms. As observed in the ln (S_W /S_{Rau}) vs. S_{Rau} plot, the logarithmic deviation spikes significantly for weak lines (e.g., S ≈ 0.02 a.u. at CF = 0.04), resulting in the Grade E classification. This instability occurs because minor variations in the calculation of mixing coefficients (ci) can lead to massive percentage changes in the resulting gA value. Conversely, transitions with CF ≥ 0.1 remain robust and well-aligned with literature values, appearing as large solid circles near the zero-scale baseline. This graphical analysis confirms that while our model is highly reliable for the majority of transitions, those characterized by strong cancellation effects require cautious interpretation in spectroscopic applications due to their inherent numerical sensitivity.Main critically evaluated results are given in **Table 1.**

CONCLUSION

Calculated transition probabilities (gA) and line strengths (S) show high reliability when benchmarked against Raineri and Rauch. Transitions with a Cancellation Factor (CF)>0.1 achieve Grade D+ accuracy (≤ 31%), making them suitable for precise spectroscopic modeling.

Conversely, transitions with CF < 0.1 fall into Grade E (>50% uncertainty). These weak lines are hypersensitive to Configuration Interaction and Core Polarization, where destructive interference causes numerical instability. While our methodology is robust for most transitions, low-CF lines require cautious interpretation in astrophysical and plasma applications.

REFERENCES

[1] Rauch T, Quinet P, Hoyer D, Werner K, Richter P, Kruk JW, et al. Stel_x0002_lar laboratories. VII. New Kr IV – VII oscillator strengths and an improved spectral analysis of the hot, hydrogen-deficient DO-type white dwarf RE 0503-289. Astron Astrophys 2016;590:A128. http://dx.doi.org/10.1051/0004-6361/201628131, arXiv:1603.00701.

[2] Kramida A. A suite of atomic structure codes originally developed by R. D. Cowan adapted for Windows-based personal computers. National Institute of Standardsand Technology; 2021, http://dx.doi.org/10.18434/T4/15025

[3] Marcinek R, Migdalek J. Oscillator strengths for some systems with the ns2np ground-state configuration. II. Gallium isoelectronic sequence. J Phys B At Mol Phys 1993;26(8):1403–14. http://dx.doi.org/10.1088/0953-4075/26/8/008.

[4] M.Raineri,M.Gallardo,C.J.B.Pagan,et al,Life times and transition probabilities in Kr V.JQSRT 113(2012) 1612-1627,http://dx.doi.org/10.1016/j.jqsrt.2012.03.022