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RESEARCH ARTICLE

Investigation of Transitions to the Atomic Ground State in Fourier Transform Spectra of Holmium

S. Kröger [1*], Gö. Başar [2], I. K. Öztürk [2], S. K. Barka [3,4], L. Windholz[5] and R. Ferber[6]

[1]Hochschule für Technik und Wirtschaft Berlin, Fachbereich 1, Wilhelminenhofstr. 75A, D-12459 Berlin, Germany
[2]İstanbul University, Faculty of Science, Department of Physics, TR-34134 Vezneciler, İstanbul, Türkiye
[3] İstanbul Technical University, Graduate School, Physics Engineering Program, TR-34469 Maslak, İstanbul, Türkiye
[4] Acıbadem Mehmet Ali Aydinlar University, Vocational School of Health Services, Opticianry Program, TR-34752 Ataşehir, İstanbul, Türkiye
[5]Institut für Experimentalphysik, Technische Universität Graz, Petersgasse 16, Graz A-8010, Austria
[6]Laser Centre, Faculty of Physics, Mathematics and Optometry, University of Latvia, LV-1586 Riga, Latvia

ABSTRACT

The aim of this study was to investigate in more detail some previously published atomic holmium energy levels, which were previously only published with very imprecise values for the level energy E and without total angular momentum quantum number J. By analysing Fourier Transform (FT) spectra in the 317 nm-1750 nm wavelength range using hyperfine structure as a diagnostic tool, we sought to enhance the precision of energy measurements and determine the unknown J values. All levels investigated were initially identified through their transitions to the ground state. We have investigated this transition and, if possible, other additional spectral lines that were classified as transitions to the investigated levels. A total of 13 lines from the FT spectra were analysed leading to results for six energy levels. For these six levels a more precise determination of the energy values could be achieved. With the investigation of the hyperfine structure knowledge on their previously unknown J values could be achieved. Furthermore, hyperfine structure constants of the investigated energy levels were determined for the first time.

Keywords: laser spectroscopy; fine structure; hyperfine structure; holmium

1. INTRODUCTION

The rare earth element holmium (Ho), which has an atomic number of 67 and a single stable isotope, ^{165}Ho, holds significant importance in astrophysics. For example, it is crucial in the study of nucleosynthesis, the process responsible for the formation of heavy elements in stars, and in determining the age of star clusters (see Sneden et al. 2009, and references therein). The nuclear spin of the isotope ^{165}Ho is $I = 7/2$. Its large nuclear magnetic dipole moment of $\mu_I = 4.17(3)\,\mu_N$ and its electric quadrupole moment $Q = 2.7\,\mathrm{b} - 3.6\,\mathrm{b}$ (Stone 2005) result in a widely splitting hyperfine structure (hfs) for most spectral lines. This hfs serves as a good fingerprint when searching for new fine structure energy levels.

This study is a continuation of years of extensive research into the atomic structure of Ho conducted by our research group (Kröger et al. 1997; Al-Labady et al. 2017; Başar et al. 2017; Özdalgiç et al. 2019a,b,c; Başar et al. 2020; Bingol et al. 2023; Barka et al. 2024; Zengin et al. 2024; Windholz et al. 2024). Other research groups have also carried out studies on fine structure, hyperfine structure and the discovery of new experimental fine structure energy levels of holmium in the last decade: (Furmann et al. 2018; Stefanska & Furmann 2018; Stefanska et al. 2018a,b; Furmann et al. 2019a,b; Chomski et al. 2021, 2022, 2023; Furmann et al. 2024). Despite these efforts, significant gaps remain in the experimental knowledge of energetically high-lying energy levels of Ho.

The present work is concerned with some energy levels which are mentioned in a paper by Smirnov (2013). In this reference, it is written: “Asterisks indicate the energies of five levels presented in [7] but not observed in other studies.”, where the reference [7] refers to a work by Gorshkov & Komarovskii (1979)[1].We found no mention of these levels in any other literature. This study aims to investigate these levels in greater detail. We have set our task of investigating these levels more closely. The aim was to determine the energy levels more precisely, to find out the J-values and to determine the hyperfine constants of these levels. For this purpose, we have checked our spectra for lines that include these levels.

[1] The work by Gorshkov & Komarovskii (1979) is published in the journal *Optika i spektroskopija* and is written in Russian language

Corresponding Author: S. Kröger **E-mail:** sophie.kroeger@htw-berlin.de
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2. EXPERIMENT

The experimental spectra used in this study are the same as those analysed in several of our previous studies (Al-Labady et al. 2017; Başar et al. 2017; Özdalgiç et al. 2019a,b,c; Zengin et al. 2024). Thus, only a brief overview of the experimental setup is provided here.

The Ho samples used in our experiment had a purity of 99.9%. The free and excited Ho atoms were generated in a hollow cathode gas discharge running at approximately 60 mA current. Two Ho spectra were recorded with different buffer gases: one with argon (Ar) and the other with neon (Ne). Both spectra were obtained at buffer gas pressure of a few mbar. To minimize Doppler broadening, the hollow cathode was cooled using with liquid nitrogen.

The available spectra cover a range from 317 nm to 1750 nm. The accuracy of the calibrated wavenumber is 0.005 cm^{-1}. Further details can be found in Al-Labady et al. (2017); Başar et al. (2017); Zengin et al. (2024).

3. SELECTION AND ANALYSIS OF SPECTRAL LINES

In the paper of Gorshkov & Komarovskii (1979) 29 spectral lines of Ho I in the wavelength range from 315 nm to 610 nm are given, which are classified as transition to the ground state. For 20 of these 29 lines, the upper levels have been known before. The upper levels for the remaining nine lines have been published for the first time by Gorshkov & Komarovskii (1979) – as far as we know. The energy values in (Gorshkov & Komarovskii 1979) are given without decimal places (in cm^{-1}) and no J-values or information on electron configuration are given. The data from Gorshkov & Komarovskii (1979) for these nine lines are listed in Table 1. In addition, Table 1 shows the corresponding wavelengths from our spectra and the resulting energy values for the levels under investigation. In the last column the signal to noise ratio (SNR) from our spectra recorded with Ar as buffer gas is listed. One of the nine lines, which lies relatively far at the edge of our spectrum, is not visible in our spectra. The line may be likely weak, and the detector's reduced sensitivity in this range results in an insufficient SNR for detection. Two further lines lie below 317 nm and are therefore outside our wavelength range.

Table 1. Lines classified in Gorshkov & Komarovskii (1979) as transitions to the ground state and have an upper level with an unknown J value.

λ (nm)	E_{up} (cm^{-1})	λ (nm)	E_{up} (cm^{-1})	SNR
from reference		from our FT spectra		
357.912	27932	357.914	27 931.68	710
357.044	27999	357.035	28 000.44	190
354.141	28229	354.135	28 229.74	210
345.123	28966	345.121	28 967.07	190
320.617	31181	not seen in our spectra		
320.100	31231	320.099	31 231.24	4
318.637	31375	318.641	31 374.23	22
315.735	31663	not in our wavelength range		
315.382	31698	not in our wavelength range		

The initial step involved calculating all theoretically possible transitions to these six levels within the wavelength range of our FT spectra using the energy values given in Table 1 and trying all allowed J values for a transition to the ground level (with J=15/2), i.e. J = 13/2, 15/2 or 17/2. For this task, the computer program ELEMENTS was used (Windholz & Guthöhrlein 2003; Windholz 2016). When a line was found in the FT spectra, a 2 cm^{-1} wide section containing the line was extracted from the full spectrum.

In total, 13 lines were analysed, as listed in Table 2. This table also contains the six lines from Table 1, which are observed in our spectra. Level energies and J quantum numbers of the combining levels are given according to the NIST Atomic Spectra Database (Kramida et al. 2024). The SNR from our FT spectrum, measured with Ar as buffer gas is listed in the seventh column.

As the number of investigated lines is small, we show all observed hfs patterns in Figures 1-6.

For the determination of the level energy of the levels under investigation, only one transition is used in each case, and this is the transition to the ground state having $E = 0$ per definition. The ground state does not contribute to the uncertainty and therefore the uncertainty in determining the level energy of the upper levels results only from the wavenumber of the transition between the two levels. This uncertainty is estimated to be 0.01 cm^{-1}, which is composed of 0.005 cm^{-1} reading accuracy when determining the centre of gravity of the line and 0.005 cm^{-1} accuracy of the calibration. For the other lines the difference $\Delta\sigma = \sigma - (E_u - E_l)$ between the experimental wavenumber σ and the calculated difference between the level energies of the upper and lower levels E_u and E_l, respectively, is listed in the eighth column.

In order to determine the J-values, the J-values of the combining levels as well as the hyperfine structure (hfs) of the lines were taken into account. The possibilities for the J values of the investigated levels are restricted by the transition rules for electric dipole radiation and limited to $\Delta J = \pm 1$. This results in three possible J values for the levels under investigation when using a transition to the ground state. If other lines were available for a level under investigation, the J-choice may have been further restricted. The hfs was fitted for all possible J values and checked to see which J fit best. For the investigation of the hfs, the FITTER program (Zeiser et al. 2022) was used. This program iteratively fits a calculated hfs line profile to the experimental intensity distribution using a least-square method. For all lines, the hfs constants A and B of the respective other level are known from the literature. These values were fixed during the fitting procedure. Additionally, the hfs line profile parameters were fixed, and intensity ratios of the individual hfs components were constrained using theoretical intensity ra-

Table 2. Ho I lines measured by means of Fourier transform spectroscopy and analysed in order to determine hyperfine structure constants, sorted by levels of even parity; E_e, J_e, E_o, J_o: Energy and J-value for levels of even and odd parity, respectively.

E_e (cm^{-1})	J_e	E_o (cm^{-1})	J_o	λ_{air} (nm)	σ (cm^{-1})	SNR	$\Delta\sigma$ (cm^{-1})	A_e (MHz)	B_e (MHz)	com.
27 931.68	13/2	0.00	15/2	357.914	27 931.67	710	0.00	657 (2)	-500 (50)	
		5 419.70	13/2	444.084	22 511.94	2	0.03	only simulated		a
28 000.44	13/2	0.00	15/2	357.035	28 000.44	190	0.00	544 (1)	690 (10)	
28 229.74	13/2	0.00	15/2	354.135	28 229.74	210	0.00	992 (4)	1580 (390)	b
		5 419.70	13/2	438.281	22 810.00	17	0.04	993 (12)	2060 (850)	
		18 572.28	15/2	1 035.188	9 657.44	4	0.02	only simulated		c
		19 276.94	15/2	1 116.649	8 952.91	3	-0.11	only simulated		d
28 967.07	13/2	0.00	15/2	345.121	28 967.07	190	0.00	801 (12)	850 (510)	
		5 419.70	13/2	424.557	23 547.34	14	0.03	only simulated		e
31 231.24	13/2	0.00	15/2	320.099	31 231.24	4	0.00	only simulated		f
		5 419.70	13/2	387.314	25 811.51	24	0.03	596 (3)	1430 (150)	
		8 605.16	11/2	441.844	22 626.07	32	0.01	601 (4)	1270 (340)	
31 374.23	17/2	0.00	15/2	318.641	31 374.23	22	0.00	792 (4)	670 (500)	g

a) very weak, simulation fits reasonably well (in the noise), b) blend, fit with two transitions, c) unresolved, weak, but structure fits well, d) very weak, good resolved, structure fits, e) fits well, f) very weak and g) unresolved

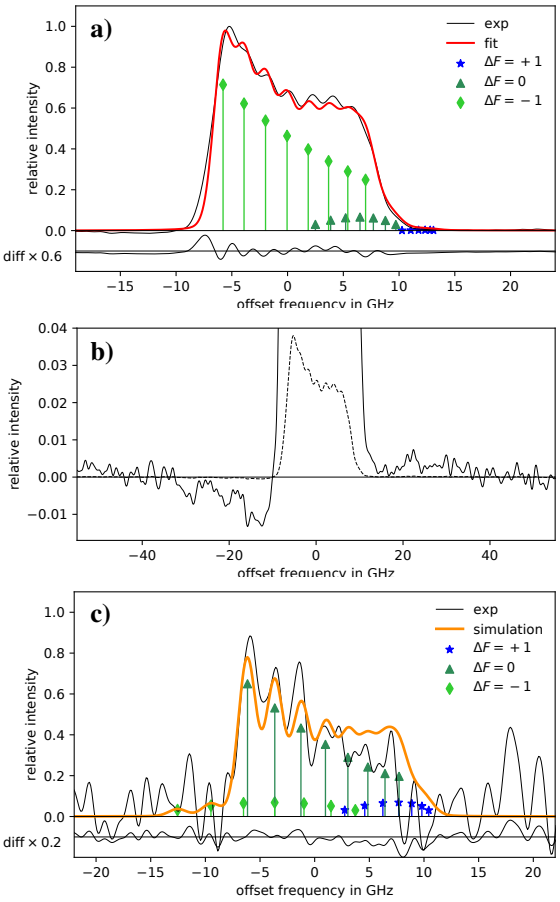

Figure 1. Lines including the even-parity energy level E = 27 931.68 cm^{-1}, J = 13/2; a) fit of FT-line at σ = 27 931.68 cm^{-1}; b) section of the experimental curve of figure (a) with the y-axis zoomed in to illustrate the asymmetry; c) simulation of FT-line at σ = 22 511.94 cm^{-1}.

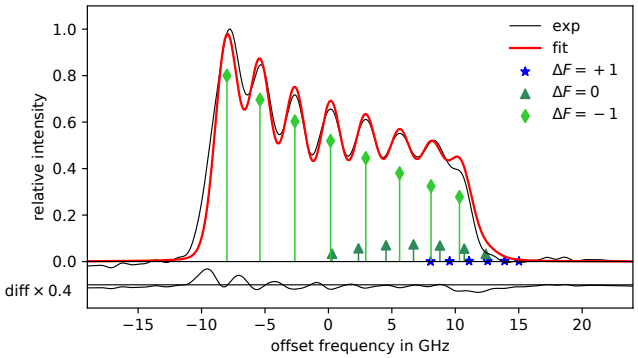

Figure 2. Line including the even-parity energy level E = 28 000.44 cm^{-1}, J = 13/2; fit of FT-line at σ = 28 000.44 cm^{-1}.

tios. In previous work (Özdalgiç et al. 2019c) we have already gained a lot of experience in fitting lines from these FT spectra. We used the same profile function as Özdalgiç et al. (2019c) – a Voigt profile – which fits the single hfs components more accurately than Gaussian or Lorentzian profiles. In this reference the full width at half maximum (FWHM) of the Voigt profile is investigated and as a result the FWHM for the Lorentzian and the Gaussian parts are given as a function of the line wavenumber. These results were used to fix the FWHM during the hfs fitting in the current study.

In all cases, the appropriate J-value for fitting the hfs could be determined with certainty. Of course the hfs parameters and J-values of the upper investigated level must fit to all transitions involving this level.

Our spectra exhibit a slight asymmetry in the spectral lines, which is already discussed in detail in Özdalgiç et al. (2019c). To illustrate this, a section of the experimental curve from Figure 1a is shown in Figure 1b, in which the x- and y-axes are scaled differently. To aid understanding, the curve from

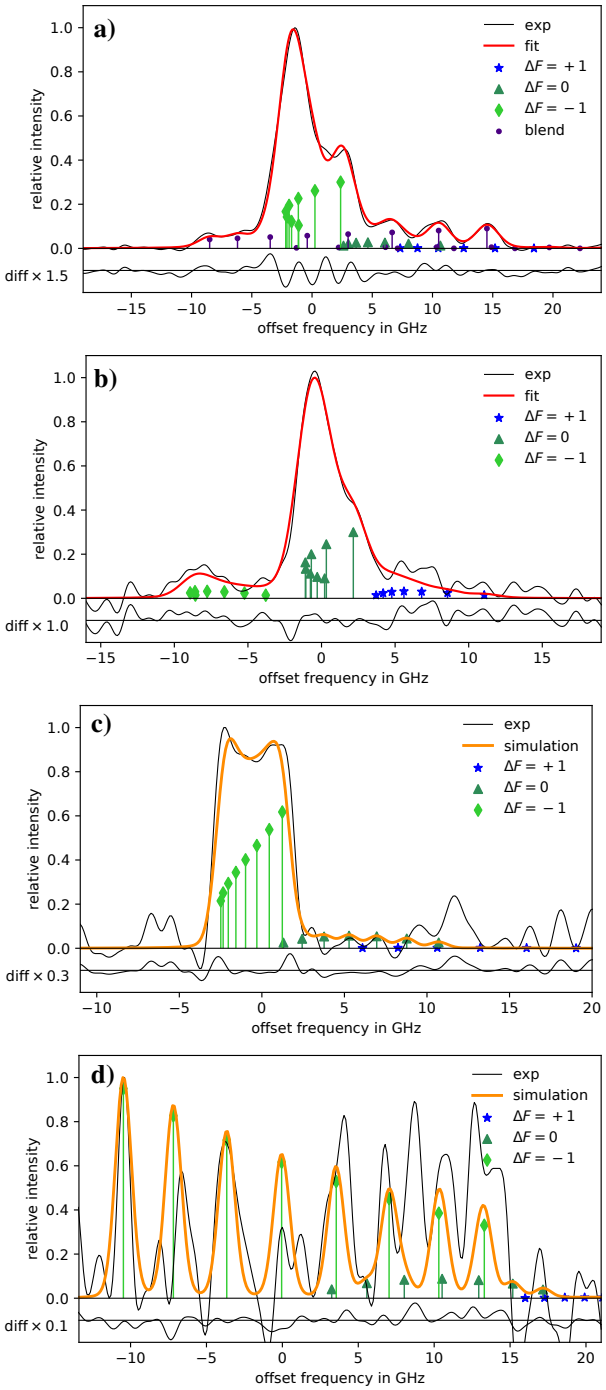

Figure 3. Lines including the even-parity energy level E = 28 229.74 cm^{-1}, J = 13/2; a) fit of FT-line at σ = 28 229.74 cm^{-1}, fitted together with another blending known line (transition at λ = 354.134 nm from E = 37 971.48 cm^{-1}, odd, J=17/2 to E=9 741.50 cm^{-1}, even, J=19/2); b) fit of FT-line at σ = 22 810.00 cm^{-1} ; c) simulation of FT-line at σ = 9 657.44 cm^{-1} ; d) simulation of FT-line at σ = 8 952.91 cm^{-1}.

Figure 1a is reproduced with new scaling. The asymmetry is especially significant for strong lines, leading to notable differences between the fitted and experimental curves, particularly for narrowly split lines. Nevertheless, the J value can be clearly

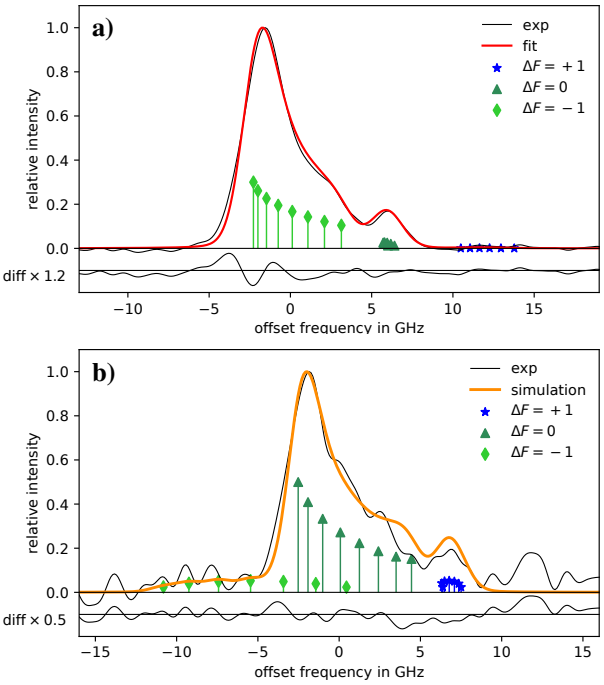

Figure 4. Lines including the even-parity energy level E = 28967.07 cm^{-1}, J = 13/2; a) fit of FT-line at σ = 28967.07 cm^{-1}; b) simulation of FT-line at σ = 23547.34 cm^{-1}.

determined and the A and B factors can also be reliably determined within the specified limits.

Two of the six levels yielded excellent results with more than two lines. For one level we could investigate three and for another one four transitions. For two other levels, exactly two lines were analysed, one of which was only fitted in each case; the other line is only simulated. Even so, the results can also be considered to be reliable here. For the remaining two levels, only one line was identified with no second line to confirm their existence. However, if the levels do exist, then the assignment of the J value is fairly clear.

4. CONCLUSION

We analysed 13 lines from FT spectra in order to investigate the six levels of atomic Ho, previously noted in the literature with only approximate energy values and without a J-value. We were able to determine the J values, provide more precise information on the energy value and specify hfs constants for all six levels. Hfs constants of all six levels could be determined and are published here for the first time.

Five of the six levels have a J-value of 13/2, all of which lie between 27 900 and 31 250 cm^{-1}, increasing the number of even levels with this J-value in this energy range considerably. In the theoretical investigation of the fine- and hyperfine structure of the even-parity configurations of Holmium done by Stefanska et al. (2018a), there are theoretical predictions which can now be filled with our experimental equivalence. An exact

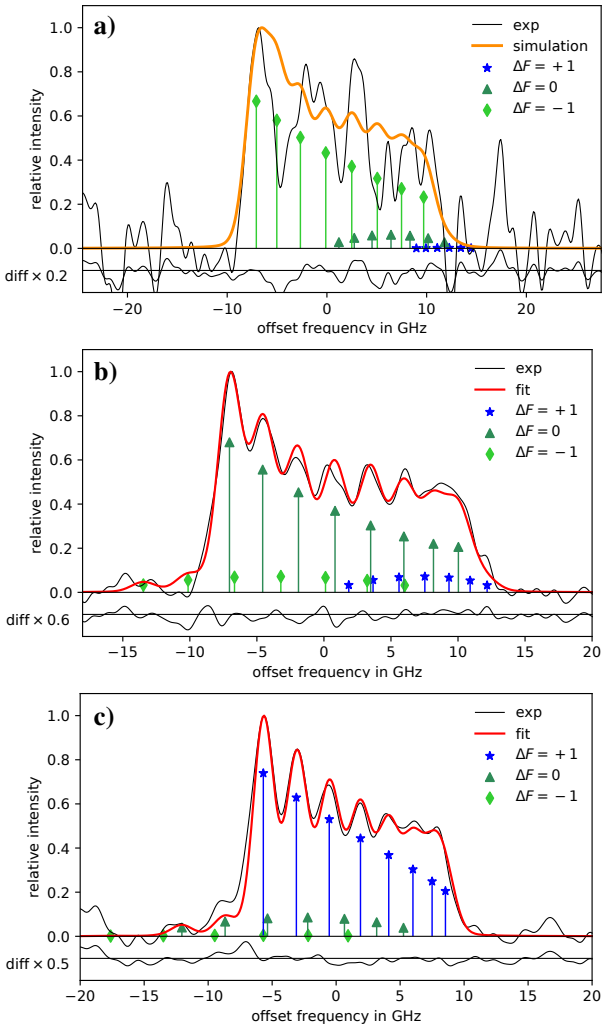

Figure 5. Lines including the even-parity energy level E = 31231.24 cm^{-1}, J = 13/2; a) simulation of FT-line at σ = 31231.24 cm^{-1}; b) fit of FT-line at σ = 25811.51 cm^{-1}; c) fit of FT-line at σ = 22626.07 cm^{-1}.

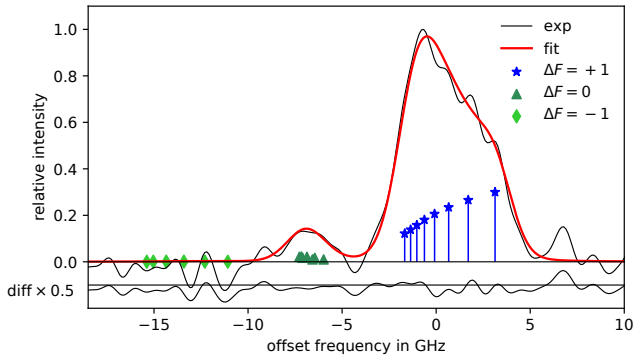

Figure 6. Line including the even-parity energy level E = 31374.23 cm^{-1}, J = 17/2; fit of FT-line at σ = 31374.23 cm^{-1}.

allocation of the experimental levels to the theoretical energies still needs to be clarified. It would be interesting to carry out the semi-empirical analysis of the even-parity configurations again, including the levels that we have newly provided with J-values and hfs constants.

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LIST OF AUTHOR ORCIDS

S. Kröger https://orcid.org/0000-0003-4991-9176
Gö. Başar https://orcid.org/0000-0002-2428-8163
I. K. Öztürk https://orcid.org/0000-0002-3664-3388
S. K. Barka https://orcid.org/0000-0001-5789-1738
L. Windholz https://orcid.org/0000-0001-6078-6154
R. Ferber https://orcid.org/0000-0002-6313-5768

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