



UNIVERSITY OF LEEDS

This is a repository copy of *Lidar soundings of the mesospheric nickel layer using Ni(³F) and Ni(³D) transitions*.

White Rose Research Online URL for this paper:
<http://eprints.whiterose.ac.uk/140655/>

Version: Supplemental Material

Article:

Gerding, M, Daly, S orcid.org/0000-0001-7957-4514 and Plane, J orcid.org/0000-0003-3648-6893 (2019) Lidar soundings of the mesospheric nickel layer using Ni(³F) and Ni(³D) transitions. *Geophysical Research Letters*, 46 (1). pp. 408-415. ISSN 0094-8276

<https://doi.org/10.1029/2018GL080701>

(c) 2018. American Geophysical Union. All Rights Reserved. This is an author produced version of a paper published in *Geophysical Research Letters*. Uploaded in accordance with the publisher's self-archiving policy.

Reuse

Items deposited in White Rose Research Online are protected by copyright, with all rights reserved unless indicated otherwise. They may be downloaded and/or printed for private study, or other acts as permitted by national copyright laws. The publisher or other rights holders may allow further reproduction and re-use of the full text version. This is indicated by the licence information on the White Rose Research Online record for the item.

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.



eprints@whiterose.ac.uk
<https://eprints.whiterose.ac.uk/>

Supporting Information for “Lidar soundings of the mesospheric nickel layer using Ni(³F) and Ni(³D) transitions”

M. Gerding¹, S. Daly², J. M. C. Plane²

¹Leibniz-Institute of Atmospheric Physics at University Rostock, Kühlungsborn, Germany.

²School of Chemistry, University of Leeds, Leeds LS2 9JT, U.K.

Contents

1. Figure S1: Energy level diagram for Ni
2. Text S1: The relative populations of Ni(³F) and Ni(³D)

Introduction

In this Supporting Information we provide an energy level diagram (Figure S1) with all relevant transitions for pumping either the Ni(³F) ground state or the low-lying excited Ni(³D) state. Additionally we describe the calculations of the relative thermal populations of Ni(³F) and Ni(³D) which are needed for the computation of Ni densities from the lidar backscatter signal (Text S1).

Figure S1: Energy level diagram for Ni

In Figure S1 we present the energy level diagram for Ni based on the spectroscopic data published by Kramida et al. [2018]. Only the most relevant transitions are shown for clarity, and weaker transitions are omitted. The two transitions used for excitation are marked blue. All wavelengths are given in air. The line thickness roughly represents the strength of the emission, with Einstein coefficients denoted in the Figure. Note that Ni has five isotopes with masses between 57.9 and 63.9 amu, but line separation is within the bandwidth of the lidar.

Corresponding author: M. Gerding, gerding@iap-kborn.de

Corresponding author: J. M. C. Plane, j.m.c.plane@leeds.ac.uk

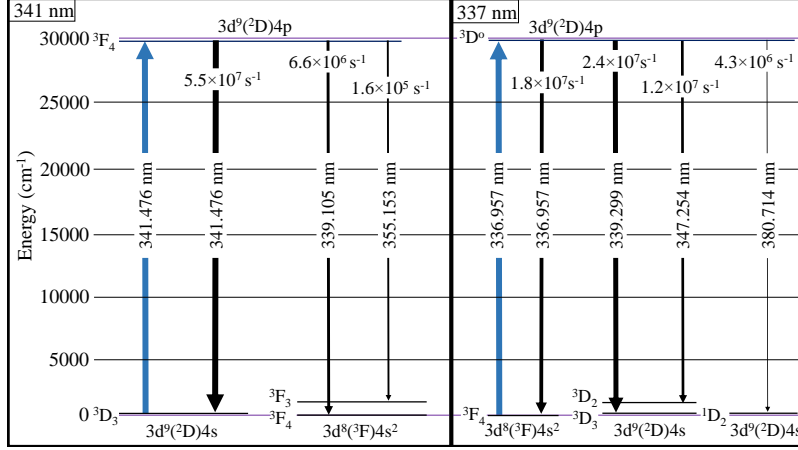


Figure 1. Energy level diagram for Ni with the most important transitions [Kramida *et al.*, 2018]. Wavelengths are given with respect to air. From the Einstein coefficients we get branching fractions (i.e. relative emission intensities) for pumping at 341 nm of 11% and 89% at 339 nm and 341 nm, respectively. For pumping at 337 nm the relative emission intensities are 31%, 41%, 20% and 7% at 337 nm, 339 nm, 347 nm and 381 nm, respectively.

Text S1: The relative populations of Ni(3F) and Ni(3D)

The ground state of Ni is a 3F_J state which has three spin-orbit multiplets with total angular momenta $J_i = 4, 3$ and 2 and energies $\epsilon_i = 0, 1332.2$ and 2216.5 cm^{-1} [Kramida *et al.*, 2018]. The degeneracy of the i th multiplet is given by $g_i = (2J_i + 1)$, and so are 9, 7 and 5 for these multiplets, respectively.

The first excited state of Ni is the 3D_J state with three spin-orbit multiplets given by $J_i = 3, 2$ and 1 , and with $\epsilon_i = 204.8, 879.8$ and 1713.0 cm^{-1} above the 3F_4 ground state; the degeneracies of these multiplets are 7, 5 and 3, respectively.

The electronic partition function for Ni is then given by $Q_{elec} = \sum_{i=1}^6 g_i e^{-\epsilon_i/kT}$, where k is the Boltzmann constant and T is temperature. Note that the contribution from higher electronic states is negligible. The thermal population of each state is then $g_i e^{-\epsilon_i/kT}/Q_{elec}$. Between 100 and 240 K, the relative population of the Ni(3D_3) state can be calculated from the expression $0.57 \exp(-265.8/T)$. The population varies from 3.9% to 18.5% over this temperature range.

References

Kramida, A., Ralchenko, Yu., Reader, J. and NIST ASD Team (2018). NIST Atomic Spectra Database (version 5.5.6), [Online]. Available: <https://physics.nist.gov/asd>. National Institute of Standards and Technology, Gaithersburg, MD.