

Calibrated lanthanide atomic data for kilonova radiative transfer: Atomic structure and opacities

Andreas Flörs^{1,*}, Ricardo Ferreira da Silva^{2,3}, José Pires Marques^{2,3},
Jorge Miguel Sampaio^{2,3} and Gabriel Martínez-Pinedo^{1,4,5}

¹*GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, D-64291 Darmstadt, Germany*

²*Laboratório de Instrumentação e Física Experimental de Partículas (LIP),
Avenida Professor Gama Pinto 2, 1649-003 Lisboa, Portugal*

³*Faculdade de Ciências da Universidade de Lisboa, Rua Ernesto de Vasconcelos,
Edifício C8, 1749-016, Lisboa, Portugal*

⁴*Institut für Kernphysik (Theoriezentrum), Fachbereich Physik, Technische Universität Darmstadt,
Schlossgartenstraße 2, D-64289 Darmstadt, Germany*

⁵*Helmholtz Forschungsakademie Hessen für FAIR (HFHF),
GSI Helmholtzzentrum für Schwerionenforschung,
Planckstraße 1, D-64291 Darmstadt, Germany*



(Received 10 July 2025; accepted 23 February 2026; published 23 March 2026)

The early spectra of the kilonova AT2017gfo following the binary neutron star merger GW170817 exhibit numerous features shaped by r-process nucleosynthesis products. Although a few species were tentatively detected, no third-peak elements were unambiguously identified, as the amount of atomic data required for radiative transfer modeling is immense. Although comprehensive atomic data, including atomic opacities, is now available for many elements, wavelength-calibrated data remain limited to a few selected ions. To examine the atomic opacities of all singly and doubly ionized lanthanides, from La ($Z = 57$) to Yb ($Z = 70$), we perform atomic structure calculations using the FAC code. Our calculations incorporate an innovative optimization of the local central potential and the number of configurations considered, alongside a calibration technique aimed at enhancing agreement between theoretical and experimental atomic energy levels. We assess the accuracy of the computed data, including energy levels and electric dipole (E1) transition strengths, as well as their impact on kilonova opacities. We find that strong transitions [$\log(gf) > -1$] are in good agreement with both experiments and semiempirical calculations. For ions with substantial experimental data, the computed opacities exhibit good agreement with prior calculations. By calibrating low-lying energy levels with experimental data, we have identified 66 722 transitions with experimentally calibrated wavelength information, rendering future lanthanide line identifications through radiative transfer modeling feasible. In total, our calculations encompass 28 ions, yielding 146 849 energy levels below the ionization threshold and 29 337 507 transitions among these levels.

DOI: [10.1103/jxqw-7ynk](https://doi.org/10.1103/jxqw-7ynk)

I. INTRODUCTION

The discovery of the kilonova (KN) AT2017gfo [1–5], associated with the gravitational wave event GW170817 [6,7], marked a major milestone in astrophysics. This multimessenger observation provided direct evidence that binary neutron star mergers are a site of rapid neutron-capture (r-process) nucleosynthesis [8–14] and that the electromagnetic emission

from such events is powered by the radioactive decay of freshly synthesized heavy elements [15–17].

The kilonova light curve undergoes rapid temporal evolution. For AT2017gfo, this manifested as a spectral transition from blue optical emission at early times to redder, near-infrared wavelengths at later epochs [18–21]. This spectral evolution is driven by the opacity of the ejected material, which depends sensitively on the atomic structure of the r-process elements. In particular, lanthanides with their partially filled $4f$ electron shells strongly influence the opacity due to their complex spectra and large number of low-energy transitions [21–24]. These transitions lead to strong line blanketing in the optical and near-infrared bands, reducing optical flux and shifting emission toward longer wavelengths [21,23,24].

*Contact author: a.flors@gsi.de

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International license](https://creativecommons.org/licenses/by/4.0/). Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

While the distinction between “blue” and “red” KNe is often linked to the presence or absence of lanthanides in the ejecta, recent multidimensional radiative transfer simulations have shown that this dichotomy may oversimplify the complex interplay between ejecta composition, geometry, and viewing angle [25–28]. Nonetheless, lanthanide-rich ejecta remain a critical factor in shaping KN spectra and must be accurately treated in radiative transfer models [18,21,29].

Even the simplest KN radiative transfer models, assuming local thermodynamic equilibrium (LTE), spherical symmetry, and steady-state conditions, require accurate and complete atomic data to model opacities [24]. For LTE calculations, knowledge of energy levels and transition probabilities is sufficient, but the computation of these quantities for lanthanides is highly nontrivial. Their complex atomic structure, driven by a large number of electrons, strong electron-electron correlations, partially filled $4f$ orbitals, and relativistic effects, limits both the accuracy and completeness of theoretical predictions.

Prior to the observational breakthrough provided by AT2017gfo, the opacity of r-process ejecta had already been the subject of theoretical investigation through atomic structure calculations [18,19,30–32]. Nonetheless, the detection of AT2017gfo significantly accelerated efforts to compute atomic data for lanthanides and other second or third r-process peak elements. These initiatives have spanned a range of ionization states: some groups (e.g., [33–39]) have focused on highly charged ions (fifth to tenth ionization stages) that dominate the early-time (< 1 day) KN emission, while others have concentrated on low-charge species (neutral through fourth ionization), which are most relevant for interpreting light curves and spectra at later epochs, such as those observed in AT2017gfo. These studies can be further categorized into those targeting individual elements [40–45] and those aiming to cover a broader set of elements or ionization stages (e.g., [21,24,46–51]). A substantial portion of this work has concentrated on lanthanide ions, owing to their characteristically high line opacities, which play a dominant role in shaping KN spectra. Motivated by similar considerations, actinide ions have also been investigated, albeit to a lesser extent and in a smaller number of studies [44,49,52].

To support these efforts, a variety of atomic structure codes have been employed, including AUTOSTRUCTURE [53], FAC [54], GRASP [55], HULLAC [56], HFR [57], LASER [58], and MCDGME [59]. These codes adopt differing approaches to strike a balance between computational efficiency and the level of physical accuracy required to model the complex electron configurations of heavy, open-shell ions. Some studies have targeted individual ions in detail to assess and improve the accuracy of computed atomic data, while others have aimed to produce extensive datasets covering many species, thereby enabling comprehensive radiative transfer simulations of KNe.

Despite these advances, KN models remain subject to considerable uncertainties, primarily due to the limitations of the available atomic data. Accurate modeling of heavy element spectra requires sophisticated configuration interaction (CI) methods that include relativistic effects. However, the validation of such theoretical predictions is constrained by the scarcity of experimental data, especially for low-ionization lanthanide species. Experimental benchmarks, such as measured energy levels or transition wavelengths, are limited, and given the vast number of relevant ions, this shortfall is unlikely to be fully addressed in the near future. As a result, theoretical results must be carefully validated through cross-comparison with available experimental data, spectral features observed in stellar atmospheres, and consistency checks against previous theoretical calculations.

One of the principal goals of KN modeling is the secure identification of spectral signatures corresponding to second- and third-peak r-process elements, which are synthesized in the aftermath of neutron star mergers. These identifications are essential for understanding the detailed nucleosynthetic pathways and for constraining the elemental yields produced in such extreme environments. For instance, tentative detections of lanthanide elements in KN spectra have already been reported (see [60]), demonstrating the feasibility of using KN observations to probe heavy element formation. However, to move beyond tentative identification toward systematic abundance measurements, models require highly reliable atomic data, particularly accurate opacities that govern radiative transfer in the ejecta.

The calculation of these opacities hinges on both the completeness and accuracy of the atomic structure data, namely, energy levels, oscillator strengths, and transition wavelengths. While reasonably complete atomic datasets exist for many first- and second-peak r-process elements, these datasets often rely on theoretical structure calculations which, despite being state of the art, can suffer from substantial wavelength inaccuracies. Recent work (e.g., [26,44,61,62]) has highlighted that even small errors in predicted wavelengths can significantly impair the ability to match synthetic spectral features with observed lines. In extreme cases, discrepancies exceeding 50% between theoretical and experimental wavelengths have been found, rendering confident line identifications effectively impossible.

To mitigate this issue, theoretical energy levels can be corrected, or calibrated, using experimental spectroscopic data. Such calibrations serve to anchor theoretical predictions in empirically verified energy structures, thereby improving the fidelity of predicted wavelengths. In previous work, we developed a calibration scheme that grouped levels by their parity and total angular momentum, applying a uniform shift within each group to align the theoretical level structure with available experimental energies [44]. This method enhanced the agreement between calculated

and experimental transition wavelengths, but the resulting accuracy—while improved—was still insufficient to enable unambiguous line identifications in most cases.

A fundamental challenge lies in the absence of a general, automated method for associating theoretical energy levels with experimental ones. The quantum mechanical labeling of levels (e.g., in terms of configuration, term symbols, and mixing coefficients) is often ambiguous or incomplete, particularly in complex open-shell systems typical of lanthanides and actinides. As a result, identifications between calculated and measured levels must be done manually, requiring careful inspection of level energies, their LS term contributions, and quantum numbers. Reliable wavelength predictions are central to the interpretation of astrophysical observations and to our understanding of the cosmic origin of the heavy elements.

The objective of the present study is to generalize and extend our previous atomic structure calculations for Nd II and Nd III to encompass all 28 singly and doubly ionized lanthanide species. For each ion for which experimental spectroscopic data are available, we apply a level calibration procedure to align the computed energy levels with measured values. In Sec. II, the general theory of atomic structure, the FAC code, and our calibration procedure are reviewed. In Sec. III, we present the results of our atomic structure calculations for all singly and doubly ionized lanthanides. For each ion, we also discuss the accuracy of the calculated energy levels compared to available experimental data. In Sec. IV, we focus on the permitted E1 transitions between our calculated and calibrated energy levels. We compare oscillator strengths to both experimental data used in stellar spectroscopy as well as other theoretical works. From the oscillator strengths, we derive opacities for LTE conditions, which will be compared to the literature. Finally, in Sec. V, we summarize our findings and conclude with an outlook.

II. METHODS

A. Atomic structure calculations

For our computations, we employ the Flexible Atomic Code (FAC) [54], an open-source package for relativistic atomic structure. FAC operates by diagonalizing the Dirac-Coulomb Hamiltonian

$$H_{\text{DC}} = \sum_{i=1}^N (c\alpha_i \cdot \mathbf{p}_i + (\beta_i - 1)c^2 + V_i) + \sum_{i<j}^N \frac{1}{r_{ij}}, \quad (1)$$

where α_i and β_i represent the 4×4 Dirac matrices and V_i is the potential from the nuclear charge. The screened hydrogenic approximation accounts for vacuum polarization and self-energy corrections. The Breit interaction, included in the zero-energy approximation for the exchanged photon, accounts for recoil and retardation effects.

The FAC code performs relativistic CI calculations. In this approach, an atomic state function (ASF), Ψ , is expressed as a superposition of N_{CSF} configuration state functions (CSFs), Φ_i , that share the same total angular momentum J and parity P :

$$\Psi(nJM_J P) = \sum_{i=1}^{N_{\text{CSF}}} c_i^n \Phi_i(\gamma_i JM_J P), \quad (2)$$

where c_i are the expansion coefficients and γ_i refers to the additional quantum numbers that uniquely characterize each CSF.

The entire calculation is performed within a jj -coupling scheme, and the output is presented accordingly.

The ASFs and the corresponding eigenvalues are obtained by diagonalization of the Hamiltonian in Eq. (1) in the basis of N_{CSF} configuration state functions. For a specific collection of configurations, these eigenvalues provide the optimal energy estimations. Typically, including more configurations enhances the precision of the wave functions, albeit with a significant increase in both computational time and memory demand. In this study, the quantity of configurations is chosen based on the ion's complexity. For ions with a half-filled f shell, we include fewer than ten configurations, while ions at the extremes of the lanthanide series may involve hundreds. The influence of additional configurations on the precision of the computed energies was examined by Flörs *et al.* [44] for neodymium and uranium ions.

A significant benefit over the multiconfiguration Dirac-Fock method as implemented in codes such as GRASP [55] or MCDPFGME [59] is the inherent orthogonality of all electron orbitals, as they are all subjected to the same potential. Consequently, the eigenvalues and mixing coefficients are computed only once, which dramatically lowers the numerical complexity of the task.

In FAC, this shared potential is constructed using fictitious mean configurations (FMCs), i.e. averaged electronic configurations designed to represent the collective occupancy pattern of many closely related levels. The FMC is obtained through a self-consistent Dirac-Fock-Slater iteration, yielding a stable set of one-electron radial orbitals computed from the Dirac equation, albeit without optimization for any specific configuration. This approach is highly computationally efficient, since orthogonality is enforced by construction; however, the use of averaged potentials can compromise accuracy for systems with strong configuration interaction.

Our approach constructs FMCs to account for the number of active electrons, distributed across various configurations. By altering the fractional occupation numbers, the weight of each configuration in the mean configuration construction can be adjusted. Consistent with earlier work on neodymium, the number of configurations is chosen such that further additions produce only minimal changes to the wave functions and, consequently, to the resulting level

TABLE I. Configurations included in the FAC calculations for lanthanide ions. The presented configurations are sorted by energy based on the lowest level of each configuration. The FMC weights used for the radial optimization of the potential are given for each ion.

Ion	FMC weights	No. ^a	Configurations
La II	$4f^{1.62}5d^{0.38}$	111	$5d^2, 5d^1 6s^1, 6s^2, 4f^1 6s^1, 4f^1 5d^1, 5d^1 6p^1, 6s^1 6p^1, 4f^1 6p^1, 5d^1 7s^1, 5d^1 6d^1, 4f^2, 6s^1 7s^1,$ $4f^1 7s^1, 5d^1 7p^1, 6p^2, 4f^1 6d^1, 4f^1 5f^1, 4f^1 7p^1, 5d^1 5f^1, 5d^1 7d^1, 6s^1 6d^1, 5d^1 8s^1, 5d^1$ $8d^1, 4f^1 6f^1, 5d^1 5g^1, 6s^1 7p^1, 5d^1 8p^1, 5d^1 6f^1, 4f^1 8s^1, 4f^1 8p^1, 6s^1 8s^1, 4f^1 7d^1, 5f^1 6s^1,$ $4f^1 5g^1, 5d^1 9s^1, 6s^1 7d^1, 5d^1 9d^1, 4f^1 8d^1, 5d^1 9p^1, 6s^1 8p^1, 5g^1 6s^1, 6s^1 9s^1, 6s^1 6f^1, 6s^1$ $8d^1, 6p^1 7s^1, 6p^1 7p^1, 6s^1 9p^1, 6p^1 6d^1, 6s^1 9d^1, 5f^1 6p^1, 6p^1 8p^1, 6p^1 8s^1, 6p^1 7d^1, 6p^1$ $6f^1, 5g^1 6p^1, 6p^1 8d^1, 7s^2, 6d^2, 6d^1 7s^1, 7s^1 7p^1, 6d^1 7p^1, 5f^1 7s^1, 5f^1 6d^1, 7p^2, 7s^1 8s^1,$ $5f^1 7p^1, 6d^1 7d^1, 6d^1 8s^1, 7s^1 7d^1, 5f^2, 6d^1 8p^1, 7s^1 8p^1, 5g^1 6d^1, 5g^1 7s^1, 6f^1 7s^1, 6d^1 8d^1,$ $6d^1 6f^1, 7s^1 8d^1, 7p^1 8p^1, 7p^1 8s^1, 5f^1 8s^1, 7p^1 7d^1, 5f^1 7d^1, 5f^1 6f^1, 5f^1 8p^1, 6f^1 7p^1,$ $5g^1 7p^1, 5f^1 5g^1, 8s^2, 7p^1 8d^1, 7d^2, 5f^1 8d^1, 7d^1 8s^1, 8p^2, 8s^1 8p^1, 5g^1 7d^1, 5g^1 8s^1, 5g^2, 7d^1$ $8p^1, 6f^2, 6f^1 7d^1, 7d^1 8d^1, 6f^1 8s^1, 5g^1 8p^1, 6f^1 8p^1, 5g^1 6f^1, 8s^1 8d^1, 5g^1 8d^1, 8p^1 8d^1,$ $6f^1 8d^1, 8d^2$
La III	$4f^{1.00}$	23	$5d^1, 4f^1, 6s^1, 6p^1, 7s^1, 6d^1, 5f^1, 7p^1, 8s^1, 7d^1, 5g^1, 6f^1, 8p^1, 9s^1, 8d^1, 6g^1, 7f^1, 9p^1, 10s^1,$ $9d^1, 7g^1, 8f^1, 8g^1$
Ce II	$4f^{1.86}5d^{0.96}6s^{0.10}6p^{0.08}$	277	$4f^1 5d^2, 4f^1 5d^1 6s^1, 4f^2 6s^1, 4f^2 5d^1, 4f^1 6s^2, 4f^1 5d^1 6p^1, 4f^2 6p^1, 4f^1 6s^1 6p^1, 5d^3, 5d^2$ $6s^1, 5d^1 8s^2, 5d^1 7s^2, 5d^1 6s^2, 4f^1 5d^1 7s^1, 4f^2 7s^1, 4f^1 5d^1 6d^1, 4f^2 6d^1, 4f^1 5d^1 7p^1, 4f^2$ $7p^1, 4f^2 5f^1, 4f^1 5d^1 5f^1, 4f^1 6s^1 7s^1, 4f^1 6p^2, 4f^1 5d^1 8s^1, 4f^2 8s^1, 4f^1 5d^1 7d^1, 4f^1 6s^1$ $6d^1, 4f^1 5d^1 8p^1, 4f^2 7d^1, 4f^2 8p^1, 4f^1 5d^1 6f^1, 4f^2 6f^1, 4f^1 5d^1 5g^1, 4f^2 5g^1, 4f^1 6s^1 7p^1,$ $4f^1 5d^1 8d^1, 4f^2 8d^1, 4f^1 5f^1 6s^1, 4f^1 5d^1 9s^1, 5d^2 6p^1, 4f^1 5d^1 9p^1, 4f^1 6s^1 8s^1, 4f^1 6s^1$ $7d^1, 4f^1 5d^1 9d^1, 4f^1 6s^1 8p^1, 4f^1 6s^1 6f^1, 4f^1 5g^1 6s^1, 4f^1 6s^1 8d^1, 4f^1 6p^1 7s^1, 4f^1 6s^1$ $9s^1, 4f^1 6s^1 9p^1, 4f^1 6p^1 6d^1, 5d^1 6s^1 6p^1, 4f^1 6s^1 9d^1, 4f^1 6p^1 7p^1, 4f^3, 4f^1 5f^1 6p^1, 5d^2$ $7s^1, 4f^1 6p^1 8s^1, 5d^2 6d^1, 4f^1 6p^1 7d^1, 4f^1 6p^1 8p^1, 4f^1 6p^1 6f^1, 4f^1 5g^1 6p^1, 5d^2 7p^1, 4f^1$ $6p^1 8d^1, 5d^2 5f^1, 5d^2 8s^1, 4f^1 7s^2, 5d^2 7d^1, 4f^1 6d^1 7s^1, 5d^2 8p^1, 4f^1 6d^2, 5d^1 6s^1 7s^1, 5d^2$ $6f^1, 5d^2 5g^1, 6p^1 6s^2, 5d^1 6p^2, 4f^1 7s^1 7p^1, 5d^1 6s^1 6d^1, 5d^2 8d^1, 4f^1 6d^1 7p^1, 4f^1 5f^1 7s^1,$ $4f^1 5f^1 6d^1, 5d^1 6s^1 7p^1, 5d^1 5f^1 6s^1, 4f^1 7p^2, 4f^1 5f^1 7p^1, 4f^1 7s^1 8s^1, 4f^1 5f^2, 4f^1 6d^1$ $8s^1, 4f^1 7s^1 7d^1, 5d^1 6s^1 8s^1, 4f^1 6d^1 7d^1, 6s^1 6p^2, 4f^1 7s^1 8p^1, 5d^1 6s^1 7d^1, 4f^1 6d^1 8p^1,$ $4f^1 6f^1 7s^1, 4f^1 5g^1 7s^1, 5d^1 6s^1 8p^1, 4f^1 6d^1 6f^1, 4f^1 5g^1 6d^1, 5d^1 6s^1 6f^1, 5d^1 5g^1 6s^1,$ $4f^1 7s^1 8d^1, 4f^1 7p^1 8s^1, 4f^1 5f^1 8s^1, 4f^1 6d^1 8d^1, 5d^1 6s^1 8d^1, 4f^1 5f^1 7d^1, 4f^1 7p^1 7d^1,$ $4f^1 5f^1 8p^1, 4f^1 7p^1 8p^1, 4f^1 5f^1 5g^1, 5d^1 6p^1 6d^1, 4f^1 5g^1 7p^1, 4f^1 5f^1 6f^1, 4f^1 6f^1 7p^1,$ $6d^1 6s^2, 6s^2 7s^1, 4f^1 5f^1 8d^1, 4f^1 7p^1 8d^1, 5d^1 6p^1 7s^1, 5d^1 6s^1 9s^1, 5d^1 6s^1 9p^1, 4f^1 8s^2,$ $4f^1 7d^1 8s^1, 6s^2 7p^1, 4f^1 7d^2, 4f^1 8s^1 8p^1, 5d^1 6s^1 9d^1, 4f^1 7d^1 8p^1, 4f^1 6f^1 8s^1, 5d^1 6p^1$ $7p^1, 4f^1 5g^1 8s^1, 4f^1 6f^1 7d^1, 4f^1 5g^1 7d^1, 5f^1 6s^2, 4f^1 6f^1 8p^1, 4f^1 5g^1 6f^1, 4f^1 5g^1 8p^1,$ $5d^1 5f^1 6p^1, 4f^1 8p^2, 4f^1 5g^2, 4f^1 6f^2, 4f^1 8s^1 8d^1, 6s^2 8s^1, 4f^1 7d^1 8d^1, 6s^2 7d^1, 4f^1 8d^2,$ $5d^1 6p^1 8s^1, 6s^2 8p^1, 4f^1 5g^1 8d^1, 6s^1 6p^1 7s^1, 4f^1 8p^1 8d^1, 5d^1 6p^1 7d^1, 4f^1 6f^1 8d^1, 6f^1$ $6s^2, 5g^1 6s^2, 5d^1 6p^1 8p^1, 5d^1 6p^1 6f^1, 6s^2 8d^1, 5d^1 5g^1 6p^1, 6s^1 6p^1 6d^1, 5d^1 6p^1 8d^1, 6s^1$ $6p^1 7p^1, 5d^1 6d^1 7s^1, 5d^1 6d^2, 5f^1 6s^1 6p^1, 5d^1 6d^1 7p^1, 6s^1 6p^1 8s^1, 5d^1 5f^1 6d^1, 6s^1 6p^1$ $7d^1, 6s^1 6p^1 8p^1, 6s^1 6p^1 6f^1, 5d^1 7s^1 7p^1, 5g^1 6s^1 6p^1, 6s^1 6p^1 8d^1, 5d^1 6d^1 8s^1, 5d^1 5f^1$ $7s^1, 5d^1 6d^1 7d^1, 5d^1 6d^1 8p^1, 5d^1 5g^1 6d^1, 5d^1 6d^1 6f^1, 5d^1 7p^2, 5d^1 7s^1 8s^1, 5d^1 7s^1 7d^1,$ $5d^1 6d^1 8d^1, 5d^1 5f^1 7p^1, 5d^1 7s^1 8p^1, 6s^1 7s^2, 5d^1 5f^2, 6s^1 6d^1 7s^1, 5d^1 6f^1 7s^1, 5d^1 5g^1$ $7s^1, 5d^1 7s^1 8d^1, 6s^1 7s^1 7p^1, 5d^1 7p^1 8s^1, 5d^1 5f^1 8s^1, 5d^1 7p^1 7d^1, 5d^1 5f^1 7d^1, 6s^1 6d^2,$ $5f^1 6s^1 7s^1, 5d^1 5f^1 8p^1, 5d^1 7p^1 8p^1, 5d^1 6f^1 7p^1, 5d^1 5g^1 7p^1, 5d^1 5f^1 5g^1, 5d^1 5f^1 6f^1,$ $6s^1 6d^1 7p^1, 5f^1 6s^1 6d^1, 5d^1 7p^1 8d^1, 5d^1 5f^1 8d^1, 6s^1 7s^1 8s^1, 6s^1 7s^1 7d^1, 5d^1 7d^1 8s^1,$ $6s^1 7p^2, 6s^1 7s^1 8p^1, 5f^1 6s^1 7p^1, 5d^1 7d^2, 5g^1 6s^1 7s^1, 6s^1 6f^1 7s^1, 5d^1 8s^1 8p^1, 6s^1 6d^1$ $8s^1, 5d^1 7d^1 8p^1, 5d^1 6f^1 8s^1, 5d^1 5g^1 8s^1, 5d^1 6f^1 7d^1, 5f^2 6s^1, 6s^1 6d^1 7d^1, 5d^1 5g^1 7d^1,$ $6s^1 7s^1 8d^1, 5d^1 5g^1 8p^1, 5d^1 8p^2, 6s^1 6d^1 8p^1, 5d^1 5g^1 6f^1, 5d^1 5g^2, 6s^1 6d^1 6f^1, 5d^1 6f^2,$ $5d^1 8s^1 8d^1, 5d^1 6f^1 8p^1, 5d^1 7d^1 8d^1, 5g^1 6s^1 6d^1, 6s^1 7p^1 8s^1, 6s^1 7p^1 7d^1, 5f^1 6s^1 8s^1,$ $6s^1 6d^1 8d^1, 5d^1 5g^1 8d^1, 5f^1 6s^1 7d^1, 5d^1 8p^1 8d^1, 5f^1 5g^1 6s^1, 5d^1 6f^1 8d^1, 6s^1 7p^1 8p^1,$ $5f^1 6s^1 8p^1, 6s^1 6f^1 7p^1, 5g^1 6s^1 7p^1, 5f^1 6s^1 6f^1, 5d^1 8d^2, 6s^1 7p^1 8d^1, 5f^1 6s^1 8d^1, 6s^1$ $8s^2, 6s^1 7d^1 8s^1, 6s^1 7d^2, 6s^1 8s^1 8p^1, 6s^1 7d^1 8p^1, 5g^1 6s^1 8s^1, 6s^1 6f^1 8s^1, 6s^1 6f^1 7d^1, 5g^1$ $6s^1 7d^1, 5g^1 6s^1 8p^1, 6s^1 8p^2, 5g^1 6s^1 6f^1, 6s^1 6f^2, 5g^2 6s^1, 6s^1 6f^1 8p^1, 6s^1 8s^1 8d^1, 6s^1$ $7d^1 8d^1, 5g^1 6s^1 8d^1, 6s^1 8p^1 8d^1, 6s^1 6f^1 8d^1, 6s^1 8d^2$

(Table continued)

TABLE I. (Continued)

Ion	FMC weights	No. ^a	Configurations
Ce III	$5p^{5.6}4f^{2.40}$	111	$4f^2, 4f^1 5d^1, 4f^1 6s^1, 5d^2, 4f^1 6p^1, 5d^1 6s^1, 4f^1 6d^1, 4f^1 7s^1, 5d^1 6p^1, 4f^1 5f^1, 4f^1 7p^1, 4f^1 8s^1, 6s^2, 4f^1 7d^1, 4f^1 6f^1, 4f^1 8p^1, 4f^1 5g^1, 4f^1 8d^1, 4f^1 9s^1, 4f^1 9p^1, 5d^1 6d^1, 4f^1 9d^1, 6s^1 6p^1, 5d^1 7s^1, 5d^1 7p^1, 5d^1 5f^1, 6p^2, 5d^1 8s^1, 5d^1 7d^1, 5d^1 5g^1, 5d^1 8p^1, 5d^1 6f^1, 6s^1 7s^1, 6s^1 6d^1, 5d^1 8d^1, 5f^1 6s^1, 6s^1 7p^1, 5d^1 9s^1, 5d^1 9p^1, 5d^1 9d^1, 6s^1 8s^1, 6s^1 7d^1, 6p^1 6d^1, 5g^1 6s^1, 6p^1 7s^1, 6s^1 8p^1, 6s^1 6f^1, 6s^1 8d^1, 5f^1 6p^1, 6p^1 7p^1, 6p^1 8s^1, 6p^1 7d^1, 6p^1 8p^1, 6p^1 6f^1, 5g^1 6p^1, 6p^1 8d^1, 6d^2, 7s^2, 6d^1 7s^1, 5f^1 6d^1, 5f^1 7s^1, 6d^1 7p^1, 7s^1 7p^1, 5f^2, 5f^1 7p^1, 7p^2, 6d^1 7d^1, 6d^1 8s^1, 7s^1 8s^1, 7s^1 7d^1, 5g^1 6d^1, 6d^1 6f^1, 6d^1 8p^1, 6f^1 7s^1, 5g^1 7s^1, 7s^1 8p^1, 5f^1 7d^1, 5f^1 8p^1, 5f^1 8s^1, 5f^1 5g^1, 6d^1 8d^1, 5f^1 6f^1, 7p^1 7d^1, 7p^1 8s^1, 7s^1 8d^1, 6f^1 7p^1, 7p^1 8p^1, 5g^1 7p^1, 5f^1 8d^1, 7p^1 8d^1, 7d^2, 8s^2, 7d^1 8s^1, 5g^1 7d^1, 6f^1 7d^1, 5g^1 8s^1, 6f^1 8s^1, 5g^2, 8s^1 8p^1, 7d^1 8p^1, 5g^1 6f^1, 6f^1 8p^1, 5g^1 8p^1, 8p^2, 6f^2, 7d^1 8d^1, 8s^1 8d^1, 5g^1 8d^1, 6f^1 8d^1, 8p^1 8d^1, 8d^2$
Pr II	$4f^{2.98}5d^{0.52}6s^{0.50}$	27	$4f^3 6s^1, 4f^3 5d^1, 4f^2 5d^2, 4f^2 5d^1 6s^1, 4f^2 6s^2, 4f^3 6p^1, 4f^2 5d^1 6p^1, 4f^3 7s^1, 4f^2 6s^1 6p^1, 4f^3 6d^1, 4f^3 7p^1, 4f^3 5f^1, 4f^3 5g^1, 4f^3 6f^1, 4f^2 6s^1 7s^1, 4f^2 6p^2, 4f^2 6s^1 6d^1, 4f^2 6s^1 7p^1, 4f^2 5f^1 6s^1, 4f^4, 4f^1 5d^2 6s^1, 4f^2 6s^1 6f^1, 4f^2 5g^1 6s^1, 4f^1 5d^1 6s^2, 4f^1 5d^1 6s^1 6p^1, 4f^1 6p^1 6s^2, 4f^1 6s^1 6p^2$
Pr III	$4f^{3.00}$	17	$4f^3, 4f^2 5d^1, 4f^2 6s^1, 4f^2 6p^1, 4f^1 5d^2, 4f^1 5d^1 6s^1, 4f^2 7s^1, 4f^2 6d^1, 4f^2 5f^1, 4f^2 7p^1, 4f^2 6f^1, 4f^2 8s^1, 4f^2 5g^1, 4f^1 5d^1 6p^1, 4f^1 6s^2, 4f^1 6s^1 6p^1, 4f^1 6p^2$
Nd II	$4f^{4.00}6s^{0.35}5d^{0.65}$	30	$4f^4 6s^1, 4f^4 5d^1, 4f^3 5d^2, 4f^3 5d^1 6s^1, 4f^4 6p^1, 4f^3 6s^2, 4f^3 5d^1 6p^1, 4f^4 7s^1, 4f^3 6s^1 6p^1, 4f^4 6d^1, 4f^4 7p^1, 4f^4 5f^1, 4f^4 8s^1, 4f^4 7d^1, 4f^4 8p^1, 4f^4 5g^1, 4f^4 6f^1, 4f^4 8d^1, 4f^4 6g^1, 4f^4 7f^1, 4f^3 5d^1 6d^1, 4f^4 7g^1, 4f^4 8f^1, 4f^4 8g^1, 4f^3 6p^2, 4f^3 5d^1 5f^1, 4f^3 6s^1 7s^1, 4f^3 6s^1 6d^1, 4f^3 5d^1 6f^1, 4f^3 5d^1 5g^1$
Nd III	$4f^{4.00}$	30	$4f^4, 4f^3 5d^1, 4f^3 6s^1, 4f^3 6p^1, 4f^3 7s^1, 4f^3 6d^1, 4f^2 5d^2, 4f^3 5f^1, 4f^3 7p^1, 4f^3 8s^1, 4f^3 7d^1, 4f^3 6f^1, 4f^3 8p^1, 4f^3 5g^1, 4f^2 5d^1 6s^1, 4f^3 8d^1, 4f^3 7f^1, 4f^3 6g^1, 4f^3 8f^1, 4f^3 7g^1, 4f^3 8g^1, 4f^2 5d^1 6p^1, 4f^2 6s^2, 4f^2 6s^1 6p^1, 4f^2 5d^1 6d^1, 4f^2 5d^1 5f^1, 4f^2 6p^2, 4f^2 5d^1 5g^1, 4f^2 5d^1 6f^1, 4f^2 5d^1 6g^1$
Pm II	$4f^{4.91}6s^{1.09}$	11	$4f^5 6s^1, 4f^5 5d^1, 4f^4 5d^1 6s^1, 4f^5 6p^1, 4f^4 6s^2, 4f^4 6s^1 6p^1, 4f^4 6s^1 6d^1, 4f^4 5f^1 6s^1, 4f^4 6s^1 7d^1, 4f^4 6s^1 6f^1, 4f^4 5g^1 6s^1$
Pm III	$4f^{5.00}$	21	$4f^5, 4f^4 5d^1, 4f^4 6s^1, 4f^4 6p^1, 4f^4 7s^1, 4f^4 6d^1, 4f^3 5d^2, 4f^4 7p^1, 4f^4 8s^1, 4f^3 5d^1 6s^1, 4f^4 7d^1, 4f^4 8p^1, 4f^4 8d^1, 4f^3 5d^1 6p^1, 4f^3, 4f^3 6s^1 6p^1, 4f^3 5d^1 6d^1, 4f^3 6p^2, 4f^3 6s^1 6d^1, 4f^3 6p^1 6d^1, 4f^3 6d^2$
Sm II	$4f^{5.65}5d^{0.87}6s^{0.43}6p^{0.05}$	7	$4f^6 6s^1, 4f^6 5d^1, 4f^5 5d^1 6s^1, 4f^6 6p^1, 4f^5 6s^2, 4f^5 6s^1 6p^1, 4f^7$
Sm III	$4f^{5.84}5d^{0.11}6s^{0.05}$	34	$4f^6, 4f^5 5d^1, 4f^5 6s^1, 4f^5 6p^1, 4f^5 7s^1, 4f^5 6d^1, 4f^5 7p^1, 4f^5 5f^1, 4f^4 5d^2, 4f^5 8s^1, 4f^5 7d^1, 4f^5 5g^1, 4f^5 8p^1, 4f^5 6f^1, 4f^5 8d^1, 4f^4 5d^1 6s^1, 4f^4 5d^1 6p^1, 4f^4 6s^2, 4f^4 6s^1 6p^1, 4f^4 5d^1 7s^1, 4f^4 5d^1 7p^1, 4f^4 6p^2, 4f^4 5d^1 7d^1, 4f^4 6s^1 7s^1, 4f^4 6s^1 7p^1, 4f^4 6s^1 7d^1, 4f^4 6p^1 7s^1, 4f^4 6p^1 7p^1, 4f^4 6p^1 7d^1, 4f^4 7s^2, 4f^4 7s^1 7p^1, 4f^4 7p^2, 4f^4 7s^1 7d^1, 4f^4 7p^1 7d^1, 4f^4 7d^2$
Eu II	$4f^{6.81}5d^{0.18}6s^{1.01}$	10	$4f^7 6s^1, 4f^7 5d^1, 4f^6 5d^2, 4f^6 5d^1 6s^1, 4f^7 6p^1, 4f^7 7s^1, 4f^6 5d^1 6p^1, 4f^7 6d^1, 4f^8, 4f^7 8s^1$
Eu III	$4f^{6.72}5d^{0.18}6s^{0.09}6p^{0.01}$	13	$4f^7, 4f^6 5d^1, 4f^6 6s^1, 4f^6 6p^1, 4f^6 7s^1, 4f^6 6d^1, 4f^6 7p^1, 4f^6 8s^1, 4f^6 7d^1, 4f^6 8p^1, 4f^5 5d^1 6s^1, 4f^5 5d^1 6p^1, 4f^5 6s^1 6p^1$
Gd II	$4f^{7.94}5d^{0.26}6p^{0.80}$	8	$4f^7 5d^1 6s^1, 4f^7 6s^2, 4f^7 5d^2, 4f^8 6s^1, 4f^8 5d^1, 4f^7 6s^1 6p^1, 4f^7 5d^1 6p^1, 4f^8 6p^1$
Gd III	$4f^{7.85}6s^{0.15}$	10	$4f^7 5d^1, 4f^8, 4f^7 6s^1, 4f^7 6p^1, 4f^7 7s^1, 4f^7 6d^1, 4f^7 7p^1, 4f^7 5f^1, 4f^7 7d^1, 4f^7 6f^1$
Tb II	$4f^{8.89}6s^{0.05}6p^{1.06}$	8	$4f^9 6s^1, 4f^8 5d^1 6s^1, 4f^8 5d^2, 4f^8 6s^2, 4f^9 5d^1, 4f^9 6p^1, 4f^8 6s^1 6p^1, 4f^8 5d^1 6p^1$
Tb III	$4f^{8.79}6s^{0.21}$	9	$4f^9, 4f^8 5d^1, 4f^8 6s^1, 4f^8 6p^1, 4f^8 7s^1, 4f^8 6d^1, 4f^8 5f^1, 4f^8 8p^1, 4f^8 6f^1$
Dy II	$4f^{9.5}6s^{0.55}5p^{0.55}5d^{0.40}$	10	$4f^{10} 6s^1, 4f^9 5d^1 6s^1, 4f^9 6s^2, 4f^{10} 5d^1, 4f^9 5d^2, 4f^{10} 6p^1, 4f^9 6s^1 6p^1, 4f^9 5d^1 6p^1, 4f^9 6p^2, 4f^{11}$

(Table continued)

TABLE I. (*Continued*)

Ion	FMC weights	No. ^a	Configurations
Dy III	$4f^{9.73}5d^{0.27}$	9	$4f^{10}, 4f^9 5d^1, 4f^9 6s^1, 4f^9 6p^1, 4f^8 5d^2, 4f^8 5d^1 6s^1, 4f^8 5d^1 6p^1, 4f^8 6s^1 6p^1, 4f^8 6p^2$
Ho II	$4f^{10.92}6s^{1.08}$	15	$4f^{11} 6s^1, 4f^{11} 5d^1, 4f^{11} 6p^1, 4f^{10} 6s^2, 4f^{10} 5d^1 6s^1, 4f^{10} 5d^2, 4f^{10} 6s^1 6p^1, 4f^{10} 5d^1 6p^1, 4f^{10} 6p^2, 4f^{12}, 4f^9 5d^2 6s^1, 4f^9 5d^1 6s^2, 4f^9 5d^1 6s^1 6p^1, 4f^9 6p^1 6s^2, 4f^9 6s^1 6p^2$
Ho III	$4f^{10.74}6s^{0.26}$	15	$4f^{11}, 4f^{10} 5d^1, 4f^{10} 6s^1, 4f^{10} 6p^1, 4f^{10} 7s^1, 4f^{10} 6d^1, 4f^{10} 7p^1, 4f^{10} 5f^1, 4f^{10} 8s^1, 4f^{10} 7d^1, 4f^{10} 8p^1, 4f^{10} 9s^1, 4f^{10} 8d^1, 4f^{10} 9p^1, 4f^9 5d^1 6d^1$
Er II	$4f^{11.72}5d^{0.42}6s^{0.86}$	19	$4f^{12} 6s^1, 4f^{11} 6s^2, 4f^{11} 5d^1 6s^1, 4f^{12} 5d^1, 4f^{11} 5d^2, 4f^{12} 6p^1, 4f^{11} 6s^1 6p^1, 4f^{11} 5d^1 6p^1, 4f^{12} 7s^1, 4f^{12} 7p^1, 4f^{11} 6s^1 7s^1, 4f^{11} 5d^1 7s^1, 4f^{11} 5d^1 6d^1, 4f^{11} 5d^1 7p^1, 4f^{11} 6s^1 6d^1, 4f^{11} 6s^1 7p^1, 4f^{11} 7s^2, 4f^{13}, 4f^{11} 6d^2, 4f^{11} 7p^2$
Er III	$4f^{11.73}5d^{0.27}$	15	$4f^{12}, 4f^{11} 5d^1, 4f^{11} 6s^1, 4f^{11} 6p^1, 4f^{11} 7s^1, 4f^{11} 6d^1, 4f^{11} 7p^1, 4f^{11} 5f^1, 4f^{11} 8s^1, 4f^{11} 7d^1, 4f^{11} 8p^1, 4f^{11} 6f^1, 4f^{10} 5d^2, 4f^{11} 9s^1, 4f^{11} 8d^1, 4f^{11} 9p^1, 4f^{11} 6g^1, 4f^{10} 5d^1 6s^1, 4f^{10} 6s^2, 4f^{10} 5d^1 6p^1, 4f^{10} 6s^1 6p^1, 4f^{10} 5d^1 6d^1, 4f^{10} 5d^1 7s^1, 4f^{10} 5d^1 7p^1, 4f^{10} 6s^1 7s^1, 4f^{10} 6s^1 6d^1, 4f^{10} 5d^1 8s^1, 4f^{10} 5d^1 8p^1, 4f^{10} 6s^1 7p^1, 4f^{10} 6s^1 8s^1, 4f^{10} 6s^1 8p^1$
Tm II	$4f^{12.75}6p^{0.60}6s^{0.65}$	25	$4f^{13} 6s^1, 4f^{12} 6s^2, 4f^{12} 5d^1 6s^1, 4f^{13} 5d^1, 4f^{13} 6p^1, 4f^{12} 5d^2, 4f^{12} 6s^1 6p^1, 4f^{12} 5d^1 6p^1, 4f^{13} 7s^1, 4f^{13} 7p^1, 4f^{13} 6d^1, 4f^{13} 8s^1, 4f^{13} 8p^1, 4f^{12} 6s^1 7s^1, 4f^{12} 6p^2, 4f^{12} 6s^1 6d^1, 4f^{12} 6s^1 7p^1, 4f^{12} 6s^1 8s^1, 4f^{12} 6s^1 8p^1, 4f^{14}, 4f^{11} 5d^2 6s^1, 4f^{11} 5d^1 6s^2, 4f^{11} 5d^1 6s^1 6p^1, 4f^{11} 6p^1 6s^2, 4f^{11} 6s^1 6p^2$
Tm III	$4f^{12.70}6p^{0.30}$	15	$4f^{13}, 4f^{12} 5d^1, 4f^{12} 6s^1, 4f^{12} 6p^1, 4f^{12} 7s^1, 4f^{12} 6d^1, 4f^{12} 7p^1, 4f^{12} 8s^1, 4f^{12} 8p^1, 4f^{11} 5d^2, 4f^{11} 5d^1 6s^1, 4f^{11} 6s^2, 4f^{11} 5d^1 6p^1, 4f^{11} 6s^1 6p^1, 4f^{11} 6p^2$
Yb II	$4f^{13.60}6s^{1.40}$	40	$4f^{14} 6s^1, 4f^{13} 6s^2, 4f^{14} 5d^1, 4f^{13} 5d^1 6s^1, 4f^{14} 6p^1, 4f^{13} 5d^2, 4f^{13} 6s^1 6p^1, 4f^{14} 7s^1, 4f^{13} 5d^1 6p^1, 4f^{14} 6d^1, 4f^{14} 7p^1, 4f^{14} 5f^1, 4f^{14} 8s^1, 4f^{12} 5d^2 6s^1, 4f^{14} 8p^1, 4f^{14} 9s^1, 4f^{14} 6f^1, 4f^{13} 6s^1 7s^1, 4f^{14} 8d^1, 4f^{14} 7f^1, 4f^{14} 10s^1, 4f^{14} 9d^1, 4f^{14} 8f^1, 4f^{13} 6s^1 6d^1, 4f^{13} 6s^1 7p^1, 4f^{13} 6p^2, 4f^{14} 10d^1, 4f^{14} 9f^1, 4f^{14} 11d^1, 4f^{14} 10f^1, 4f^{14} 11f^1, 4f^{14} 12f^1, 4f^{14} 13f^1, 4f^{14} 14f^1, 4f^{13} 6s^1 8p^1, 4f^{13} 6s^1 8s^1, 4f^{12} 5d^1 6s^2, 4f^{12} 5d^1 6s^1 6p^1, 4f^{12} 6p^1 6s^2, 4f^{12} 6s^1 6p^2$
Yb III	$4f^{13.65}5d^{0.35}$	43	$4f^{14}, 4f^{13} 5d^1, 4f^{13} 6s^1, 4f^{13} 6p^1, 4f^{13} 7s^1, 4f^{13} 6d^1, 4f^{13} 7p^1, 4f^{13} 8s^1, 4f^{13} 8p^1, 4f^{12} 5d^2, 4f^{12} 5d^1 6s^1, 4f^{12} 6s^2, 4f^{12} 5d^1 6p^1, 4f^{12} 6s^1 6p^1, 4f^{12} 5d^1 7s^1, 4f^{12} 5d^1 6d^1, 4f^{12} 5d^1 7p^1, 4f^{12} 6p^2, 4f^{12} 6s^1 7s^1, 4f^{12} 5d^1 8s^1, 4f^{12} 6s^1 6d^1, 4f^{12} 5d^1 8p^1, 4f^{12} 6s^1 7p^1, 4f^{12} 6s^1 8s^1, 4f^{12} 6s^1 8p^1, 4f^{12} 6p^1 7s^1, 4f^{12} 6p^1 6d^1, 4f^{12} 6p^1 7p^1, 4f^{12} 6p^1 8s^1, 4f^{12} 6p^1 8p^1, 4f^{12} 7s^2, 4f^{12} 6d^1 7s^1, 4f^{12} 6d^2, 4f^{12} 7s^1 7p^1, 4f^{12} 6d^1 7p^1, 4f^{12} 7p^2, 4f^{12} 7s^1 8s^1, 4f^{12} 6d^1 8s^1, 4f^{12} 7s^1 8p^1, 4f^{12} 6d^1 8p^1, 4f^{12} 7p^1 8s^1, 4f^{12} 7p^1 8p^1, 4f^{12} 8s^2, 4f^{12} 8s^1 8p^1, 4f^{12} 8p^2$

^aNumber of included configurations.

energies [44]. Due to computational constraints, we could not extend the number of configurations beyond 4–10 for ions with a half-filled f subshell. We show all included configurations in Table I. For further details on the FAC calculations and the local central potential employed by FAC see Refs. [44,63].

B. Determination of FMC weights

To enhance the accuracy of our calculations, we implemented a systematic optimization of the FMC used to determine the optimal potential (for details see [63]). The optimization procedure employs a sequential model-based optimization algorithm, which is particularly effective for high-dimensional optimization problems. The algorithm constructs a Gaussian surrogate model to

approximate the objective function, balancing exploration of the parameter space with exploitation of known low-error regions.

The optimization process begins with an initial dataset derived from energetically ordered configurations. Subsequent points are determined through Latin hypercube sampling. The algorithm utilizes multiple acquisition functions simultaneously—lower confidence bounds, expected improvement, and probability of improvement—combined through a Gaussian processes-hedge strategy [64]. This approach probabilistically selects the best candidate for the next iteration using a softmax function applied to the computed acquisition functions.

To evaluate the performance of each iteration, we employ a weighted root mean square deviation between calculated values and reference data. The loss function ($\mathcal{L}$)

incorporates a Boltzmann factor at $T = 5000$ K accounting for the excitation energy of reference levels, promoting convergence to physically meaningful values:

$$\mathcal{L} = \sqrt{\frac{1}{N} \sum_{i=1}^N e^{-E_i^{\text{ref}}/kT} (\Delta E_i)^2}, \quad (3)$$

where ΔE_i represents the difference between the calculated and reference energy levels E_i^{ref} , N is the number of levels considered, and T is the excitation temperature. The squared differences are weighted by a Boltzmann factor, thereby assigning greater importance to low-lying energy levels, which are more significantly populated under thermodynamic conditions relevant to the plasma.

To avoid unphysical solutions, constraints are applied to the parameter space. In particular, the f subshell is restricted between $n_e - 2$ and $n_e + 2$ (where n_e is the number of electrons in the $n = 4$ and $n = 5$ f subshells in the ground configuration). Similarly, the $n = 6$ and $n = 7$ p subshells are limited between 0 and 1. These constraints ensure that the optimization explores physically meaningful configurations while allowing sufficient flexibility to improve the accuracy of the calculations.

C. Calibration to experimental data

The use of mean configurations in atomic structure calculations can inadvertently introduce significant discrepancies between theoretical and experimental energy levels, as demonstrated in several recent studies [44,61,62]. Shingles *et al.* [26] emphasized that transition wavelengths, determined by energy differences between levels connected by selection rules, can differ from experimental values by factors of several orders of magnitude, even for relatively simple elements such as strontium, which is generally considered more tractable than the lanthanides or actinides. Their results also demonstrated that synthetic spectra generated using uncalibrated *ab initio* atomic data for Sr, Y, and Zr differ markedly from those based on experimental data. Owing to the complex interplay between atomic transitions, plasma conditions, and the radiation field in radiative transfer simulations, these discrepancies propagated beyond the specific ions in question, influencing the emergent spectrum produced by all species included in the model. As a result, the reliable identification of r-process material in observed spectra depends critically on the precision of transition wavelength accuracy that is difficult to attain through *ab initio* calculations alone.

To address this, we apply a calibration to final energy levels and corresponding transition wavelengths, based on available low-lying experimental energy levels. This calibration procedure leaves the underlying orbitals and ASF compositions unchanged and instead modifies the transition energies and derived quantities, such as partition functions, through corrected excitation energies.

The calibration is performed by matching computed levels with experimental energy levels from the National Institute of Standards and Technology (NIST) Atomic Spectra Database (ASD) [65] and, where applicable, theoretical data from Database on Rare Earths at Mons University (DREAM) [66]. For Nd III and Dy III, these repositories do not provide sufficiently detailed data and we therefore instead adopt the data from [67,68], respectively. The calibration procedure is not applicable to ions for which experimental data beyond the ground state are unavailable. In atomic spectroscopy, LS coupling is typically used to classify energy levels, whereas theoretical calculations may employ jj - or LS -coupling schemes. The FAC code adopts jj coupling by default. To facilitate consistent labeling, we utilize the JJ2LSJ code [69], which transforms the jj -coupled CSFs produced by FAC into the LS -coupling scheme and assigns LS term labels to all calculated energy levels. This transformation is not bijective; multiple ASFs may share the same dominant LS label, particularly at higher excitation energies, where level mixing increases. We consider an LS label to be reliable when the squared leading LS composition exceeds 0.7.

The computed energy levels are initially grouped by orbital angular momentum L and parity, providing a natural basis for the analysis of their LS term composition. For each level, the leading LS term contributions are determined using JJ2LSJ, which transforms the jj -coupled wave functions into an approximate LS -coupled representation. This yields a squared leading contribution C^2 that quantifies the fraction of the level associated with a specific LS term. Experimental identification of levels is performed by comparing computed levels with available experimental data, using level spacing and configuration and LS term labels as criteria. Low-lying levels near the ground state are typically sparse, which facilitates matching. Identification is generally only feasible for levels with a squared leading LS contribution $C^2 > 0.7$, ensuring that the computed level is predominantly associated with a single LS term.

This identification procedure is performed iteratively, such that once a level is matched to experimental data, it is removed from the pool of unidentified levels. This reduces ambiguity in subsequent identification steps. Typically, only a small number of levels, ranging from a few tens up to roughly 200, can be identified in this manner, primarily limited by the availability of experimental energies and the extremely high level density above approximately 30000 cm^{-1} in our calculations. Experimentally identified levels in our dataset are referred to as “xmatch” levels. At present, no automated calibration procedure exists that simultaneously accounts for level spacing, dominant electron configurations, and quantum numbers with sufficient reliability. As a result, all calibrations were performed manually.

Levels that cannot be directly identified with experimental data are calibrated in bulk based on the statistical

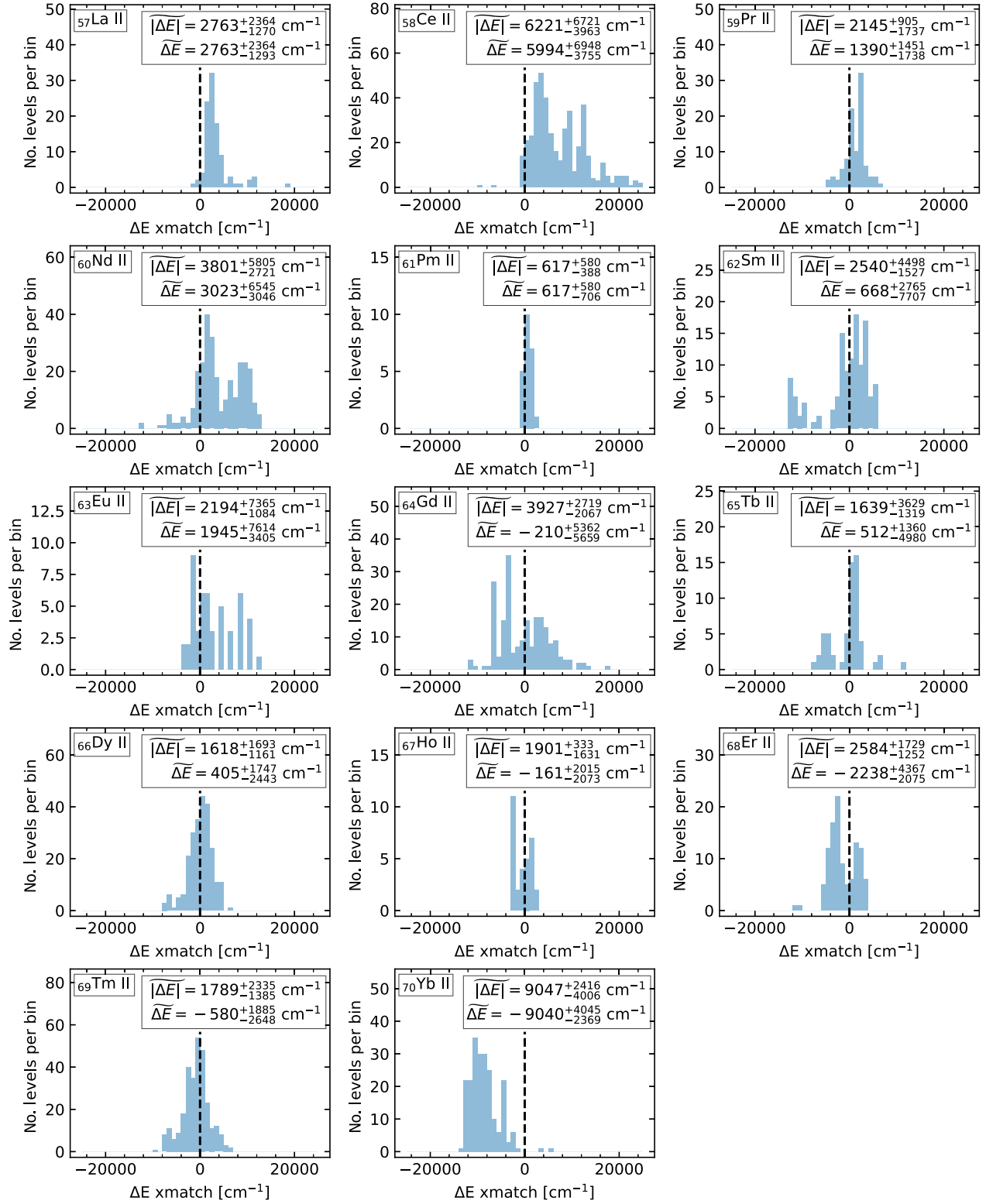


FIG. 1. Deviations between theoretical and experimental energy levels for singly ionized lanthanide ions for all xmatch levels (see Sec. II C). The figure shows the individual level energy deviations, together with the median absolute correction ($|\Delta E|$), the median correction (ΔE), and their respective 68% confidence interval.

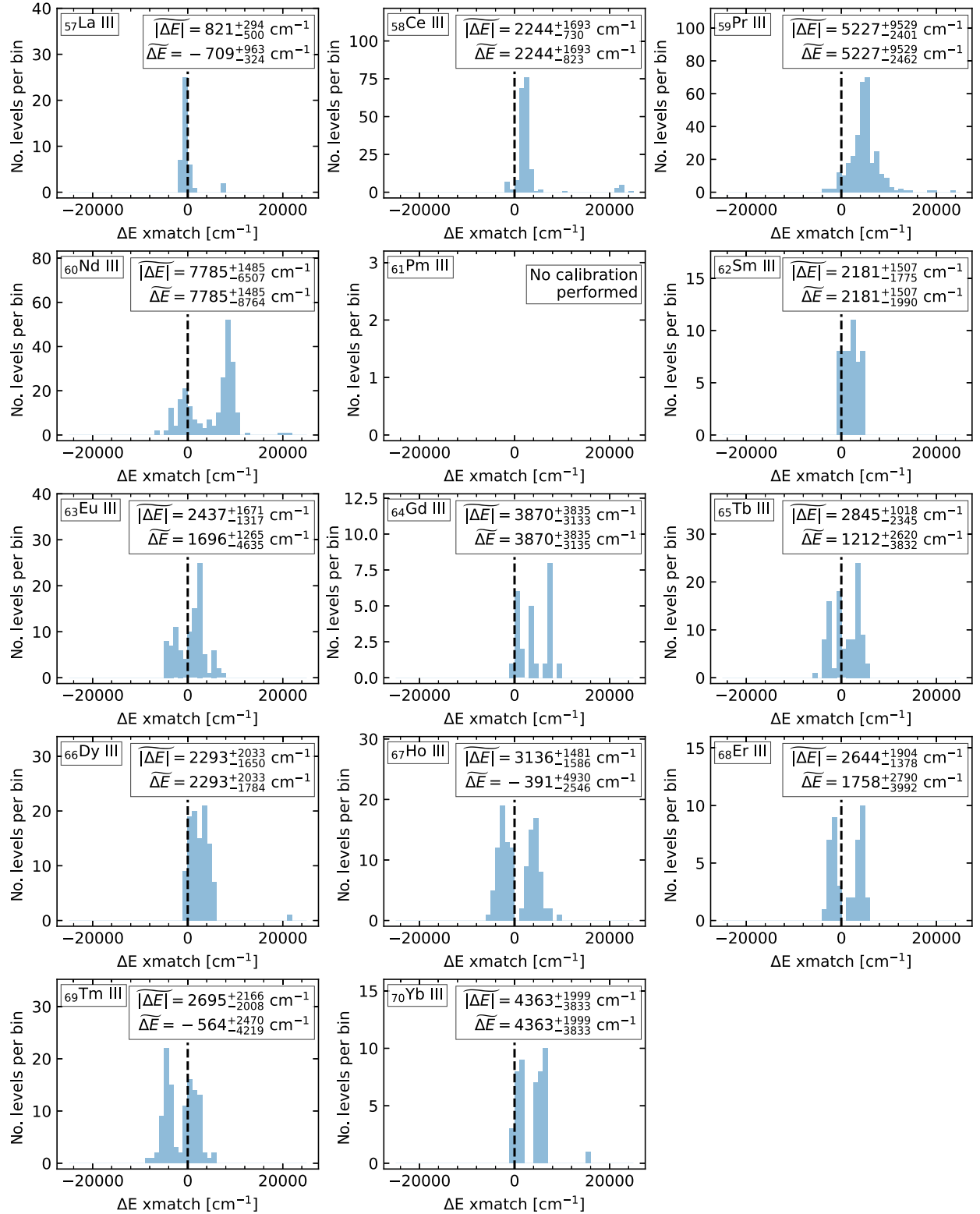


FIG. 2. Deviations between theoretical and experimental energy levels for doubly ionized lanthanide ions for all x_{match} levels (see Sec. II C). The figure shows the individual level energy deviations, together with the median absolute correction ($|\Delta E|$), the median correction (ΔE), and their respective 68% confidence interval. No calibration was performed for ^{61}Pm due to the absence of experimental data. For ^{60}Nd , calibration results are presented using experimental values from Ding *et al.* [67].

properties of the experimentally matched (*xmatch*) levels. Mean energy corrections are computed separately for each electronic configuration and for each $J - \pi$ group. For the configuration-based calibration, the mean energy shift ΔE_{conf} is determined from the set of experimentally identified (*xmatch*) levels belonging to the same configuration, defined as the average difference between computed and experimental energies within that configuration. Similarly, the J -parity-based correction $\Delta E_{\pi/J}$ is computed as the mean energy shift of all experimentally identified levels sharing the same total angular momentum J and parity. These two correction schemes exploit the fact that electronic configuration provides a meaningful classification when configuration mixing is weak, whereas J and parity remain robust quantum numbers even in the presence of strong configuration mixing. The correction scheme depends on the squared leading LS term contribution, C^2 , and is divided into three regimes.

- (1) *Configuration-secure levels* ($C^2 > 0.7$). Levels with a dominant leading contribution are considered securely associated with a specific configuration. Their energies are corrected using the mean energy shift of all experimentally identified levels of the same configuration, ΔE_{conf} .
- (2) *Configuration-inconclusive levels* ($C^2 < 0.5$). Levels with weak leading contributions are subject to strong configuration mixing and cannot be reliably assigned to a specific configuration. These levels are corrected using the mean energy shift of all experimentally identified levels within the same $J - \pi$ group, $\Delta E_{\pi/J}$, since J and parity remain good quantum numbers even under strong mixing.
- (3) *Intermediate levels* ($0.5 \leq C^2 \leq 0.7$). For levels with intermediate leading contributions, a linear interpolation between configuration-based and $J - \pi$ -based corrections is applied:

$$\Delta E(C) = \frac{0.7 - C^2}{0.2} \Delta E_{\pi/J} + \frac{C^2 - 0.5}{0.2} \Delta E_{\text{conf}}, \quad (4)$$

where C^2 is the squared leading LS contribution and ΔE_{conf} and $\Delta E_{\pi/J}$ are the mean corrections for a given configuration and for a total angular momentum or parity group, respectively. For example, a level with $C^2 = 0.6$ receives a correction that is equally weighted between the configuration-based and J/π -based calibrations. This approach ensures a smooth transition between the two regimes, avoiding discontinuities in the calibrated energies.

All levels are corrected either by direct identification (*xmatch*) or by falling into one of the three regimes discussed above. We apply the determined energy level corrections using the `CorrectEnergy` method, which applies calibration-derived energy offsets directly to the `FAC` level structure. We do not modify our derived wave functions in

any way. `FAC` recomputes all transition probabilities using the existing wave functions but the updated, calibrated energies. The published atomic data include metadata describing the energy calibration status for each transition, indicating whether both, one, or neither of the upper and lower levels were matched to experimental values or whether a bulk calibration (regimes 1–3) was applied. The details of the correction methodology are retained to inform radiative transfer modeling and to facilitate uncertainty estimates on spectral features.

An overview of the magnitude of energy corrections applied to singly and doubly ionized lanthanide species is provided in Figs. 1 and 2, respectively. Each figure displays the median correction along with the corresponding 34% intervals above and below the median. It is important to note that the majority of the energy correction distributions exhibit significant departures from Gaussianity, usually in the form of extended tails to higher energies.

III. ATOMIC STRUCTURE CALCULATIONS

In this work, we present atomic structure calculations performed with the `FAC` code for all singly and doubly ionized lanthanide elements, focusing on level energies and electric dipole (E1) transitions. Magnetic dipole (M1) and electric quadrupole (E2) transitions are beyond the scope of this study and will be addressed in future work. The computed results are systematically compared against available experimental and semiempirical datasets to evaluate their accuracy. Specifically, we benchmark our level energies and E1 transitions against five data sources: the NIST ASD [65], the DREAM database [66], and recent experimental measurements reported by Ferrara, Giarrusso, and Leone [70], Den Hartog, Voith, and Roederer [71], and Voith, Den Hartog, and Roederer [72]. While the NIST ASD is the standard reference for atomic structure data due to its stringent inclusion criteria, its coverage of lanthanide ions is limited, with only 705 validated transitions reported across 11 singly and doubly ionized species.

The DREAM database provides a much larger collection of spectroscopic parameters for lanthanides in low ionization stages, derived using the pseudorelativistic Hartree-Fock approach implemented in the `HFR` code. It includes 60 160 E1 transitions for singly and doubly ionized lanthanides, although the data are concentrated among a few well-characterized ions. Several ions in our sample either lack representation entirely or have only a limited number of transitions available in DREAM.

We obtained the correct ground-state configuration for all ions except Gd II. An overview of experimental and calculated ground states for all ions in this study is given in Table II.

For each lanthanide ion, we derived a median calibration correction from the absolute differences between the calculated and experimental energy levels. Applying these corrections brings the adjusted level energies into close

TABLE II. Overview of the ground-state configurations in our FAC atomic structure calculations and from experiments. Checkmarks in the NIST columns indicate that the calculated ground-state configuration matches the one reported on the NIST ASD.

Element	Singly ionized		Doubly ionized	
	FAC	NIST	FAC	NIST
La	$5d^2$	✓	$5d^1$	✓
Ce	$4f^1 5d^2$	✓	$4f^2$	✓
Pr	$4f^3 6s^1$	✓	$4f^3$	✓
Nd	$4f^4 6s^1$	✓	$4f^4$	✓
Pm	$4f^5 6s^1$	✓	$4f^5$	✓
Sm	$4f^6 6s^1$	✓	$4f^6$	✓
Eu	$4f^7 6s^1$	✓	$4f^7$	✓
Gd	$4f^7 5d^2$	$4f^7 5d^1 6s^1$	$4f^7 5d^1$	✓
Tb	$4f^9 6s^1$	✓	$4f^9$	✓
Dy	$4f^{10} 6s^1$	✓	$4f^8 6s^2$	✓
Ho	$4f^{11} 6s^1$	✓	$4f^{11} 6s^1$	✓
Er	$4f^{12} 6s^1$	✓	$4f^{12}$	✓
Tm	$4f^{13} 6s^1$	✓	$4f^{13}$	✓
Yb	$4f^{14} 6s^1$	✓	$4f^{14}$	✓

agreement with the available spectroscopic data. The resulting absolute calibration values for all ions discussed in the following subsections are shown in Figs. 1 and 2.

A. Atomic datasets

1. Lanthanum ($Z=57$)

La III and, to a lesser extent, La II exhibit the most straightforward spectra among the lanthanides. Initial experimental investigations of La II were carried out in early studies [73,74], with the latter providing comprehensive energy level assignments. Zeeman spectroscopy was later employed to refine the g factors of previously identified levels [75]. More recently, updated energy levels were measured via Fourier transform spectroscopy [76].

After a first analysis of the La III spectrum [77,78] and subsequent refinements [74,79,80], a major reevaluation was carried out in 1967, utilizing a sliding spark source to record lines from 2100 to 11 000 Å [81].

In total, 115 and 41 energy levels arising from 13 and 23 configurations have been reported for La II and La III, respectively. The compilation by Martin [82] revised nearly all known La II levels and associated configurations. For La III, energy levels reconstructed from DREAM transitions are in close agreement with values in the NIST database.

Given the comparatively simple electronic structure of lanthanum ions, analogous to cesium and barium, with one or two valence electrons, we constructed atomic models comprising 111 configurations (including single and double excitations up to $8s$, $8p$, $8d$, $6f$) for La II and 23 configurations with single excitations up to $10s$, $9p$, $9d$, $8f$, $8g$ for La III (see Table I).

We successfully identified all levels of La III and 108 out of 115 levels of La II. The wide spacing of energy levels simplified level identification and reduced the dependence on detailed experimental cross-matching. Most level identifications were made using LS term assignments. The computed level structures are shown in Figs. 17 and 18.

2. Cerium ($Z=58$)

The classification of the Ce II spectrum was initiated in early work [83,84], which identified approximately 300 levels along with their associated g factors and configurations. Further measurements were carried out in the 1970s, leading to the cataloging of 192 odd- and 288 even-parity levels originating from five and seven configurations, respectively [85].

The spectrum of Ce III was initially investigated in early studies [86,87], which reported energy levels corresponding to seven configurations. A definitive identification of the ground-state configuration $4f^2$ was achieved only later [80], along with an almost complete set of Ce III levels for 14 of the 17 experimentally confirmed configurations. Subsequent measurements completed the level structure [88].

Both Ce II and Ce III are experimentally well characterized up to $50\,000\text{ cm}^{-1}$. The NIST ASD [65] includes 480 levels from 12 Ce II configurations and 214 levels from 17 Ce III configurations, each accompanied by configuration information. Additional Ce III levels are available in the DREAM database [66]. However, due to the lack of configuration assignments and the high level density near $50\,000\text{ cm}^{-1}$, these levels are not suitable for calibration purposes.

Our atomic structure models include 111 and 282 configurations for Ce II and Ce III, respectively, with single and double excitations from the ground state up to $8s$, $8p$, $8d$, $6f$, $5g$. All configurations used are listed in Table I. The resulting energy levels, separated by parity, are shown in Figs. 19 and 20.

For Ce II, odd-parity levels match experimental data closely, but even-parity levels exhibit a systematic offset of approximately 8000 cm^{-1} . Attempts to optimize the central potential to reduce this discrepancy while maintaining agreement for the odd levels were unsuccessful. In Ce III, the even-parity levels show better agreement, while the odd levels are subject to deviations both at low and high excitation. Nonetheless, the offset in Ce III odd-parity levels is less severe than that seen in Ce II even-parity levels. We successfully identified 441 Ce II and 209 Ce III levels.

3. Praseodymium ($Z=59$)

Praseodymium is among the most extensively studied lanthanides. Early determinations of Pr II energy levels appeared in foundational work [89] and were subsequently expanded using Fourier transform spectroscopy [90,91]. These efforts were followed by remeasurements of

39 levels [92] and further additions obtained through laser-induced fluorescence techniques [93–95].

For Pr III, a total of 234 odd and 167 even levels have been identified [96,97], with supplementary data available from subsequent studies [98–100].

Experimental energy levels for Pr II and Pr III were compiled by Martin, Zalubas, and Hagan [82] and are included in the NIST ASD [65]. We make use of 111 Pr II and 400 Pr III levels with identified electronic configurations (see Table III). For comparative purposes, we also include levels reconstructed from transitions in the DREAM database [66], although these lack configuration details and are therefore excluded from calibration.

Our atomic structure models are built from 27 and 17 configurations for Pr II and Pr III, respectively, including all configurations listed in the NIST ASD. We also include single and double excitations up to $7s$, $7p$, $7d$, $5f$, $5g$

yielding additional levels below the ionization potential, which are important for opacity.

The resulting theoretical energy levels for both parity classes are shown in Figs. 21 and 22. The agreement between our uncalibrated results and experimental data is generally good. We successfully identified 97 Pr II and 370 Pr III levels.

4. Neodymium ($Z=60$)

The interpretation of the Nd II spectrum began with a comprehensive reference volume [82], which incorporated foundational measurements of 20 low-lying even levels and 57 upper odd levels [101]. Subsequent extensive experimental data were primarily derived from doctoral theses [102,103] and were further supplemented by spectroscopic analyses [104,105], leading to the identification of approximately

TABLE III. Summary of available energy levels and transitions from the NIST and DREAM databases for singly and doubly ionized lanthanides. Also shown are the number of configurations, levels, transitions, and calibrated transitions below the ionization energy for each ion in the calibrated FAC dataset.

Ion	NIST			DREAM		Ferrara + 24	FAC calibrated below E_{ion}			
	No. config	No. levels	No. lines	No. levels	No. lines	No. lines	No. config	No. levels	No. lines	No. lines calib.
La II	14	115	84	...	...	...	44	472	17 743	1239
La III	23	41	0	40	131	...	23	41	219	219
Ce II	12	480	283	501	15 989	...	42	2829	408 639	14 592
Ce III	17	214	255	214	2935	...	23	303	7212	3787
Pr II	9	192	0	58	144	157	18	3689	571 453	881
Pr III	10	400	0	539	18 331	...	15	1105	63 935	9436
Nd II	8	744	0	61	106	681	27	9994	3 336 077	5434
Nd III ^a	2	29	0	30	52	...	21	4580	667 955	3675
Pm II	3	171	0	...	...	...	7	4990	913 018	0
Pm III	1	1	0	...	...	...	14	5526	797 829	0
Sm II	6	376	7	71	162	585	6	6145	1 111 875	1106
Sm III	2	43	0	39	81	...	16	11 869	2 558 907	119
Eu II	10	141	13	...	...	45	10	6781	888 646	224
Eu III	4	105	0	106	893	...	11	8470	1 308 810	893
Gd II	8	314	0	...	...	...	8	12 394	3 070 318	2909
Gd III	5	25	0	19	44	...	10	6298	814 002	85
Tb II	8	140	8	...	...	...	8	16 092	5 245 495	445
Tb III	4	111	0	106	913	...	9	8385	1 335 501	928
Dy II	9	563	17	...	...	275	9	12 493	3 580 925	4617
Dy III ^b	1	1	0	107	1304	...	6	3958	355 148	1246
Ho II	4	43	4	...	...	...	9	5192	646 913	106
Ho III	4	121	0	122	1325	...	14	4658	462 551	1162
Er II	8	360	11	17	19	359	16	5072	838 067	983
Er III	4	48	0	115	1308	...	18	2837	195 156	216
Tm II	9	361	13	297	7881	...	17	1517	114 318	7307
Tm III	4	120	0	120	1479	...	11	650	16 361	1200
Yb II	29	340	10	269	6792	...	34	348	8849	3711
Yb III	6	47	0	53	271	...	14	161	1585	202
Total								146 849	29 337 507	66 722

^aWe used data from [67] for the calibration of Nd III instead of data from DREAM and NIST ASD.

^bA total of 106 experimental energy levels from four configurations of Spector, Sugar, and Wyart [68] are used for the calibration of Dy III instead of data from the NIST ASD.

500 odd and nearly 200 even levels. Although updates and corrections to these datasets have been incorporated into the NIST energy database, the most recent revision from 2002 remains unpublished [106].

For Nd III, the earlier compilation [82] includes only 29 spectroscopic levels, based on unpublished work [107] that drew on experimental investigations using grating spectroscopy of spark discharges [108,109]. These levels correspond to the even-parity ground configuration $4f^4$ and the odd-parity excited configuration $4f^35d^1$. An additional 11 levels from the same excited configuration were later identified [110] and supported by stellar spectroscopy [111]. More recently, a significantly extended set of 144 experimentally determined levels has been published [67], covering the $4f^4$, $4f^35d^1$, $4f^36s^1$, and $4f^36p^1$ configurations, based on emission spectra from Penning and hollow cathode discharge lamps.

In this work, we include a comprehensive dataset comprising 744 Nd II levels, most accompanied by detailed electronic structure and LS term information. For Nd III, we incorporate the new experimental dataset from Ding *et al.* [67], resulting in a total of 264 identified energy levels.

The FAC calculations presented here follow an established methodology [44], employing a set of 30 electronic configurations (Table I) that includes single-electron excitations up to a principal quantum number of $n = 8$ and

double excitations up to $n = 6$. This configuration set has been demonstrated to achieve opacity convergence, as the inclusion of additional configurations neither increases the overall opacity nor improves the accuracy of energy levels most relevant for opacity calculations.

Using the newly published Nd III experimental data as a calibration basis, we identify 26 of the 29 (NIST) and 30 (DREAM) known levels within our calculations. The majority correspond to odd-parity states, with only five even-parity levels belonging to the $4f^45I$ multiplet identified. The scarcity of high-lying even-parity experimental levels introduces systematic uncertainties in our models, potentially resulting in deviations of several electron volts for these states.

Including the dataset of Ding *et al.* [67] increases the number of identified Nd III levels to 231, enhancing the identification by an order of magnitude. Figure 3 compares FAC calculations calibrated with NIST and DREAM data and those incorporating the new dataset. The updated calibration modifies energies by approximately 0.5 eV near 20 000 cm^{-1} and up to 2 eV for even-parity levels above 60 000 cm^{-1} . These changes affect both experimentally identified and unobserved levels (see Sec. II C). Given the sensitivity of opacity calculations to level energy accuracies, the impact of these data on opacity is discussed in Sec. IV B. The publicly released dataset

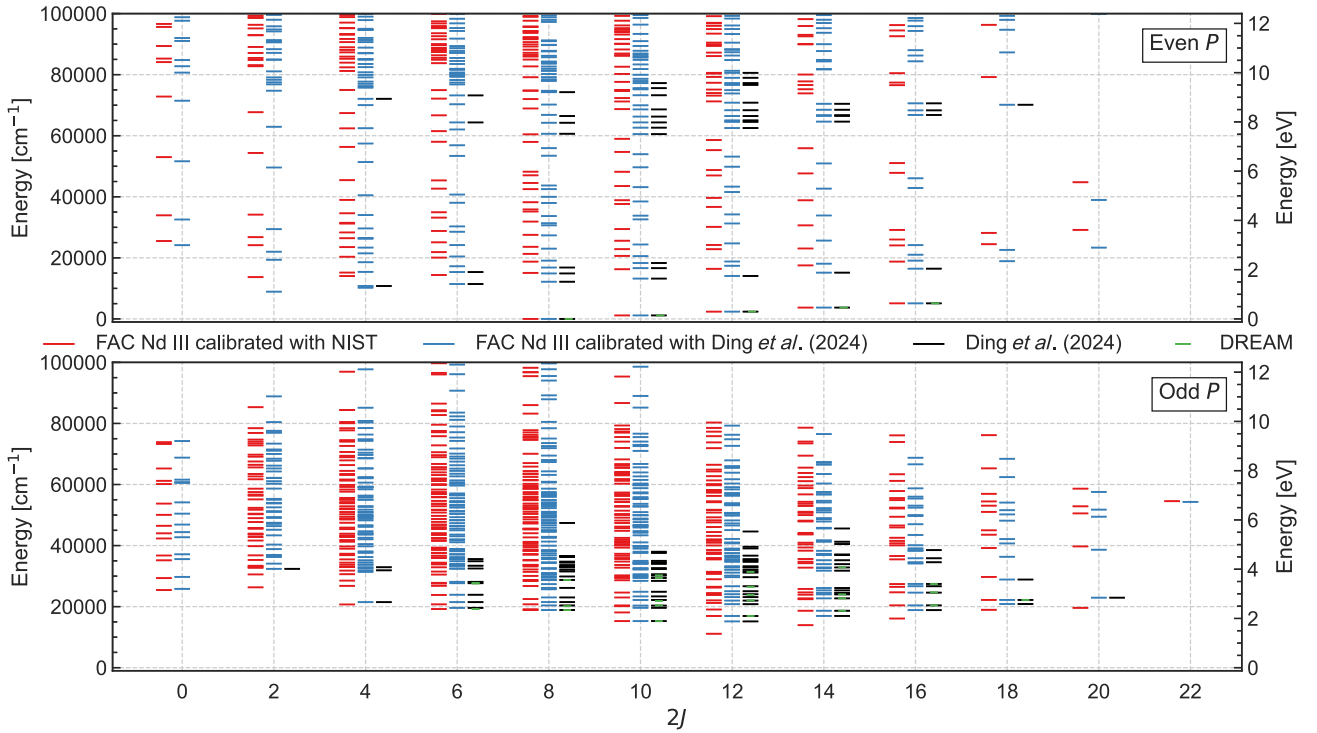


FIG. 3. Comparison of the energy levels for Nd III for even (top) and odd (bottom) parity using the FAC code. Red horizontal lines indicate the calculation, which was calibrated on experimental NIST and DREAM data, while blue lines indicate the level energies calibrated on the extensive dataset from Ding *et al.* (black horizontal bars [67]). Identification of higher-lying states, for which the agreement with measurements is generally worse, leads to an increase in the applied correction (see Fig. 2).

corresponds to the calibration that includes the Ding *et al.* [67] measurements.

We apply a calibration correction of 3801 cm^{-1} to Nd II and 7785 cm^{-1} to Nd III. The latter is a substantial increase relative to the correction based on NIST and DREAM alone (3376 cm^{-1}), reflecting the poorer agreement at higher excitation energies absent in earlier data.

5. Promethium ($Z=61$)

The analysis of promethium spectra presents distinct experimental challenges due to the absence of stable isotopes. Initial observations of Pm II identified levels within the $4f^5 6s^1$ ground configuration [112], followed by an extended classification of transitions [113]. These early efforts were later summarized in a comprehensive compilation Martin, Zalubas, and Hagan [82]. Subsequent work identified five additional energy levels associated with the $4f^5 5d^1$ configuration [114].

Experimental data for Pm III remain extremely limited. An initial study confirmed only the ground level [115], with further spectroscopic investigations hindered by the radioactive nature of promethium, which complicates the preparation of stable and sufficiently pure samples.

Our FAC atomic structure models include seven electronic configurations for Pm II and 14 for Pm III, as listed in Table I. All experimentally verified configurations are included, along with single and double excitations up to $7s$, $7p$, $7d$, $6f$ for both ionization stages.

The computed energy levels are shown in Figs. 25 and 26. For Pm II, we identify 23 experimental levels, allowing the application of a calibration correction of 617 cm^{-1} . These correspond exclusively to odd-parity levels from the ground-state multiplet. No even-parity levels could be confidently matched due to the relatively high excitation energies of known experimental levels ($20\,000$ – $30\,000\text{ cm}^{-1}$) and the absence of spectroscopic term designations. The even-parity region in our FAC calculations is highly congested, precluding unambiguous identification.

For Pm III, the absence of experimental reference levels beyond the ground state precludes meaningful calibration. Nevertheless, our calculations correctly recover the ground-state configurations $4f^5 6s^1$ for Pm II and $4f^5$ for Pm III, in agreement with the NIST ASD [65].

6. Samarium ($Z=62$)

The spectrum of Sm II was initially explored in early work that reported 40 even-parity and over 200 odd-parity levels [116]. This dataset was later expanded through analysis of Zeeman splitting, leading to the identification of more than 70 even and 300 odd levels [117].

For Sm III, only 43 energy levels are currently available, derived primarily from spark emission spectroscopy [118]. A small number of additional $4f^6 5D$ levels have been determined in solid-state environments; however, these values may

differ significantly from those of free ions, with discrepancies reaching several hundred cm^{-1} (e.g., [82,118]).

We use the dataset compiled by Martin, Zalubas, and Hagan [82] and hosted by the NIST ASD, which lists 376 and 43 levels for Sm II and Sm III, respectively. While all Sm III levels include configuration assignments, only 127 of the Sm II levels have associated data. Additionally, the experimental data for even-parity states of Sm III are sparse, with just eight levels identified across seven distinct J/π groups. DREAM-derived levels are also included but duplicate those found in NIST ASD.

Our FAC atomic structure models comprise seven configurations for Sm II and 35 for Sm III, including all experimentally confirmed configurations. We also include single and double excitations up to $6s$, $6p$, $5d$, $4f$ for the singly ionized ion and $8s$, $8p$, $7d$, $6f$ for the doubly ionized species (see Table I).

With the exception of even-parity levels in Sm II, our calculated level structure agrees well with the experimental datasets (see Figs. 27 and 28). In many cases, the deviation from experimental levels is less than 3000 cm^{-1} . However, the even-parity levels of Sm II exhibit a systematic offset of approximately $12\,000\text{ cm}^{-1}$. We identify 122 levels in Sm II.

7. Europium ($Z=63$)

The earliest investigations of the Eu II spectrum identified nine levels associated with the $4f^7 6s^1$, $4f^1 5d^1$, $4f^7 6p^1$ configurations [119]. This was followed by a more comprehensive study based on spark spectra and Zeeman measurements, which assigned LS terms to 156 levels from 1861 observed transitions [120]. Subsequent measurements provided isotope shifts and identified 13 additional levels [121]. Some of the term assignments in the earlier compilation [120] remain tentative and are therefore excluded from the reference set adopted in this work.

The Eu III spectrum was first examined in detail through the identification of 105 energy levels [122]. A more recent reanalysis of previously unidentified lines led to the addition of 39 levels, with energies spanning from $34\,816$ to $86\,209\text{ cm}^{-1}$ [123].

A revised compilation by Martin, Zalubas, and Hagan [82] includes 141 Eu II levels from ten configurations and 105 Eu III levels from four configurations. Many identified levels lie above $30\,000\text{ cm}^{-1}$, where dense level spacing complicates assignment. Nevertheless, a sufficient number of low-lying Eu III and odd-parity Eu II levels are experimentally constrained.

Our atomic structure model for Eu II includes all ten confirmed configurations and incorporates single and double excitations up to $8s$, $6p$, $6d$, $4f$. For Eu III, we consider the $4f^7$, $4f^6 6s^1$, $4f^6 6p^1$, and $4f^7 5d^1$ configurations. The identified levels in our calculations match well with experimental data.

The large upper bound in the correction for Eu II (see Fig. 1) arises from significant offsets in levels involving the $4f^6 5d^2$, $4f^6 5d^1 6s^1$, and $4f^7 6p^1$ configurations.

8. Gadolinium ($Z=64$)

The spectrum of Gd II was initially examined using Zeeman pattern analysis, leading to the identification of nine odd and 11 even levels [124]. From over 2600 arc spectral lines, 137 energy levels were subsequently derived [125], followed by the identification of an additional 178 levels through spark spectroscopy [126]. High-energy states above $35\,000\text{ cm}^{-1}$ were later added to the dataset [127]. A comprehensive compilation includes 164 odd and 150 even levels [82], with configuration assignments provided in related spectroscopic analyses [128].

The Gd III spectrum was investigated using spark discharge spectroscopy in a series of early studies [129–131], although line blending among different ionization stages posed substantial challenges. A reevaluation of these data, including previously unpublished results, yielded 25 confirmed energy levels [82].

In our FAC atomic structure model, gadolinium is treated with a minimal configuration set to ensure a manageable CI space due to its complex electronic structure. This results in 46 733 and 23 053 computed energy levels for Gd II and Gd III, respectively. For calibration, we use 239 Gd II and 25 Gd III experimental levels with assigned configurations.

Despite the limited CI expansion, the agreement for Gd II is satisfactory. Our calculations recover a ground-state configuration of $4f^7 5d^1 6s^1$, which differs from the experimental ground state $4f^7 5d^2$ by less than 2500 cm^{-1} (see Table II). This discrepancy arises from the difficulty in balancing configuration mixing.

9. Terbium ($Z=65$)

The Tb II spectrum was initially characterized through hyperfine structure measurements and optical Zeeman spectroscopy, revealing transitions associated with two configurations [132]. Due to its midshell electronic structure, terbium displays a dense level spectrum with numerous overlapping lines, generally of low to moderate intensity. The observed transitions were categorized into two systems: system A, involving odd-parity lower levels (primarily from the $4f^9 6s^1$ configuration), and system B, involving even-parity lower levels. At the time of the initial study, the ground-state configuration had not been definitively assigned to either system, and only relative energies were provided. Additional levels were later identified using similar experimental techniques [133], with further revisions and compilations included in subsequent analyses [134]. Despite these efforts, the experimental characterization of Tb II remains incomplete, with only a limited number of low-lying states firmly established.

The Tb III spectrum was examined using hollow-cathode discharge spectroscopy [135]. From over 2500 observed

lines, a curated set of 485 lines was used to reconstruct 111 energy levels, which are considered complete up to approximately $20\,000\text{ cm}^{-1}$.

Our atomic structure models include all experimentally confirmed configurations (Table I). Due to the complexity of terbium's mid-lanthanide electronic structure, configuration interaction expansion is limited. Despite this, our FAC calculations yield 40 502 and 17 440 levels for Tb II and Tb III, respectively.

Despite the high level density above $20\,000\text{ cm}^{-1}$, we identify 60 experimental levels in Tb II and 103 in Tb III.

10. Dysprosium ($Z=66$)

Early analyses of the Dy II spectrum identified several recurring energy differences [136], with further patterns revealed through the identification of six constant differences between spectral lines [137]. Additional structural insights were provided through Zeeman-effect studies that attributed specific transitions to the $4f^{10} 6s^1$ configuration [138]. Substantial progress in understanding the structure of Dy II was made through absorption spectra obtained from oxyacetylene flames [139]. Zeeman structure analyses of 129 transitions further contributed to the dataset [140], alongside the documentation of over 22 000 optical and near-infrared lines [141]. Building upon this extensive line list, additional levels were identified through new Zeeman measurements [142–144], resulting in most of the currently known 563 energy levels. More recently, 24 previously unreported levels were revealed using Fourier transform spectroscopy [145].

Spectroscopic data for Dy III remain considerably limited. Initial investigations identified several energy levels, though a comprehensive analysis was not achieved [146]. Additional levels were later documented through semi-empirical calculations [68].

Our FAC model incorporates ten electronic configurations for Dy II and nine for Dy III (see Table I). These include all experimentally verified configurations, with additional single and double excitations from the ground state ensuring comprehensive coverage of relevant atomic transitions. We identified 341 experimental levels for Dy II within our calculations, with calibration corrections of 1618 cm^{-1} . For Dy III we use level information from Spector, Sugar, and Wyart [68], as the NIST ASD only contains information on the ground state. We identified a total of 106 experimental levels for Dy III.

11. Holmium ($Z=67$)

Initial spectroscopic investigations of singly ionized holmium focused on the splitting between the two lowest levels of the $4f^{11} 6s^1$ configuration, along with two excited levels, determined through hyperfine structure analysis [147]. This work was later expanded through the analysis of 547 spectral lines, leading to the identification of eight additional excited levels [148]. Further structural insights

into the $4f^{11}6p^1$ electronic configuration were obtained using 13 known energy levels, resulting in the discovery of four previously unreported levels [149]. A more extensive study employed ultraviolet Fourier transform spectroscopy to analyze 303 spectral lines and determine energy levels and hyperfine constants for 100 states, including 41 not documented in earlier datasets [150].

The Ho III spectrum was initially analyzed through the identification of 42 energy levels, which included the $4f^{11}$ ground configuration as well as levels associated with three additional known configurations [151,152]. The assignment of these levels was supported in part by theoretical predictions [153]. Additional levels were later reported in unpublished work [154], and a more comprehensive analysis identified 80 of the currently known 120 levels [155]. Most of the newly characterized levels were attributed to the $4f^{10}5d^1$ configuration, with further additions to the $4f^{11}$ configuration including the 4F term.

Our FAC atomic structure model includes 15 electronic configurations for Ho II and 15 for Ho III, which encompass all experimentally confirmed configurations plus SD excitations as detailed in Table I. We successfully identified 42 levels for Ho II and 119 levels for Ho III.

12. Erbium ($Z=68$)

The spectroscopic analysis of Er II began with the identification of eight low-lying levels belonging to the $4f^{12}6s^1$ configuration, based on Zeeman measurements and wavelength data [156–158]. These levels were subsequently reanalyzed and grouped into four J_1j terms according to their energy separations [159]. Theoretical calculations employing electrostatic parameters provided further insight into the $4f^{12}6s^1$ configuration [160], while additional spectroscopic data expanded the known set of low-lying levels [161–163]. Infrared spectral observations later led to the identification of four levels within the $4f^{12}5d^1$ configuration [164]. A more recent and comprehensive reassessment of the Er II spectrum combined theoretical modeling with new experimental measurements to assign 130 even-parity levels to the $4f^{12} \{6s^1, 5d^1\}$ and $4f^{11} \{6s^16p^1, 5d^16p^1\}$ configurations and 230 odd-parity levels to the $4f^{12}6p^1$ and $4f^{11} \{5d^16s^1, 5d^2, 6s^2\}$ configurations [165].

Initial investigations of the Er III spectrum were based on early spectroscopic studies [153,166]. A more comprehensive analysis was subsequently carried out using spark discharge spectra [167]. The set of known energy levels was later reevaluated and expanded from 45 to 115 through the application of semiempirical parametric methods [100,168–170].

In our calculations, we utilized 19 configurations for Er II and 31 for Er III, as detailed in Table I. We identified 153 experimental levels for Er II and 46 levels for Er III.

13. Thulium ($Z=69$)

Early spectroscopic investigations of Tm II identified four levels of the ground state using Zeeman effect measurements [137]. Additional levels were observed through absorption spectroscopy in fuel-rich oxyacetylene flames [139] and further expanded using spectra obtained from electrodeless discharge tubes [171,172]. Level assignments to the $4f^{13}6p^1$ and $4f^{12} \{5d^16s^1, 6s^2, 6s^16p^1\}$ configurations were introduced in subsequent analyses [173] and continued in later spectroscopic studies [174,175]. More recently, new odd- and even-parity levels were presented, along with revised JJ values for several states using the Racah-Slater method [176]. The three lowest terms of the spectrum were also computed using the configuration interaction with perturbation theory method [177].

For Tm III, spectroscopic data were initially compiled and subsequently expanded in successive works [178,179], with additional theoretical analysis contributing further refinements [180].

We obtained 361 levels of nine configurations for Tm II and 120 levels from four configurations for Tm III. Adopting level energies from the DREAM database [66] yields fewer levels in the case of Tm II, whereas for Tm III all levels from the NIST ASD [65] are reconstructed.

Our FAC atomic structure model incorporates 25 configurations for Tm II and 15 for Tm III, including all experimentally confirmed configurations as detailed in Table I and correctly replicating the experimental ground levels. We identified 289 experimental levels for Tm II from nine configurations and 114 levels for Tm III from four configurations.

14. Ytterbium ($Z=70$)

A comprehensive spectroscopic analysis of Yb II documented 315 levels spanning even- and odd-parity configurations, with level assignments informed by Zeeman pattern analysis [181]. Subsequent work assigned six additional levels to the $4f^{13}5d^2$ configuration [182]. The emission spectrum was later reexamined, accompanied by theoretical investigations of configurations such as $4f^{13}5d6p^1$, $4f^{13}5d^2$, and others not included in the NIST database [183].

The Yb III spectrum was previously analyzed in foundational studies [184,185], with one additional level of the $4f^{13}5d^1$ configuration added in later work [186]. Owing to the relative simplicity of its electronic structure, the spectrum of Yb III is comparatively well understood.

Our FAC computations include 40 configurations for Yb II and 15 for Yb III, as detailed in Table I. We successfully identified 216 experimental levels from 29 configurations for Yb II and 46 levels from six configurations for Yb III. Both experimental ground-state levels are correctly reproduced in our calculations.

B. Results of the atomic structure calculations

The results of our FAC computations pertaining to singly and doubly ionized lanthanides are encapsulated in Table III. Leveraging experimental data for the calibration procedure, we have identified 66 722 E1 transitions with precise wavelengths (where both upper and lower levels are identified and calibrated) within our computed data. For only a single ion (Pm III), among the 28 ions investigated in this study, we were unable to identify any levels beyond the ground state; consequently, we cannot provide precise wavelengths for this ion. In summary, we identified 29 337 507 transitions below the ionization threshold, stemming from 146 849 energy levels. The total calculated transitions with precise wavelengths are significantly fewer than those experimentally confirmed for certain ions, notably Ce II, Pr III, Dy III, Er III, and Yb II. In these cases, crucial information for identifying their upper and lower energy levels among the experimentally measured energy levels is absent. DREAM solely offers energies and angular momentum for the levels pertinent to the transition. Unless these levels are also available in the NIST ASD and details on the electronic configuration and/or the principal contribution to the spectroscopic term are available, we cannot use the upper and lower levels from DREAM transitions in our calibration procedure. Furthermore, due to significant mixing between configurations at energies beyond $\sim 30\,000\text{ cm}^{-1}$, the identification of experimental levels within our calculations is infeasible in numerous instances.

We emphasize that the number of transitions with accurate wavelengths in our data, despite being lower than those available in the DREAM database, is still extremely important for future line identification in KNe. Experimentally confirmed transitions alone cannot be used in radiative transfer simulations, as the bulk of the opacity comes from lines without experimental information, requiring theoretical atomic structure calculations to fill the gaps.

We show a comparison of all our calculated energy levels with published theoretical calculations using the HULLAC (V1 [24]; V2 [50]), HFR [51], and GRASP [47,48,187] codes in Figs. 4 and 5 for singly and doubly ionized ions, respectively.

For the first ionization stage, our results exhibit excellent agreement with the aforementioned published atomic structure datasets. Variations in the density of levels primarily stem from the calibration procedure applied to low-lying energy levels. The inclusion of additional electronic configurations beyond those considered in earlier studies [47,48,50] often results in a marked increase in the density of energy levels near the ionization threshold. This enhancement arises directly from the broader range of configuration state functions incorporated in the present FAC calculations.

For Sm II, computational limitations prevented the inclusion of as many configurations as those employed in previous studies [47,50], leading to an underestimation of the level density above 7 eV for this ion. In addition to

bound levels, our models also include a substantial number of autoionizing states above the ionization potential. As illustrated in Fig. 4, the overall distribution of energy levels tends to peak at excitation energies exceeding the ionization threshold.

For singly ionized species in the second half of the lanthanide series, moderate disagreement arises in comparisons with HFR calculations. This is particularly evident for energy levels close to the ground state, where our FAC levels have been calibrated against experimental data. In contrast, the HFR results predict a significantly higher density of low-lying levels, which is inconsistent with existing experimental constraints. This artificial overdensity of near-ground levels in HFR models contributes to an increase in predicted opacity, as discussed in Sec. IV B 1.

For doubly ionized lanthanides, we observe more pronounced discrepancies between our results and those from HFR and HULLAC. While HULLAC calculations tend to show a decline in level density approaching the ionization threshold, both our calibrated FAC results and the HFR data exhibit a marked increase. In our case, the number of autoionizing levels surpasses that of bound states by roughly an order of magnitude, an outcome directly attributable to the broader configuration state function space included in the FAC calculations.

A notable discrepancy emerges when comparing the present results with those reported in a recent study [51], whose HFR calculations exhibit a pronounced increase in the number of levels at intermediate excitation energies, beginning at approximately 15 eV (see Fig. 5). While this elevated level density is consistent with HULLAC and FAC trends in the first half of the lanthanide series, it far exceeds the values for the second half, surpassing our bound level counts by more than an order of magnitude. For many ions in the latter group, where our FAC level structure has been calibrated to experimental data and reproduces observed level densities, the HFR results are in clear disagreement with empirical evidence. The implications of these discrepancies for radiative transfer and opacity calculations are further explored in Sec. IV B 1.

IV. OPACITIES

A. Oscillator strengths

In this section, we present electric dipole (E1) transitions, along with corresponding oscillator strengths and radiative lifetimes, for all 28 singly and doubly ionized lanthanide ions considered in this study. The transitions were computed in the Babushkin (length) gauge, and all relevant quantities for radiative transfer applications are provided in machine-readable format in Table V in Appendix A. The level indices used in the transition data correspond to those listed in Table IV.

To complement the more general databases introduced in Sec. III, we also benchmark our results against transition

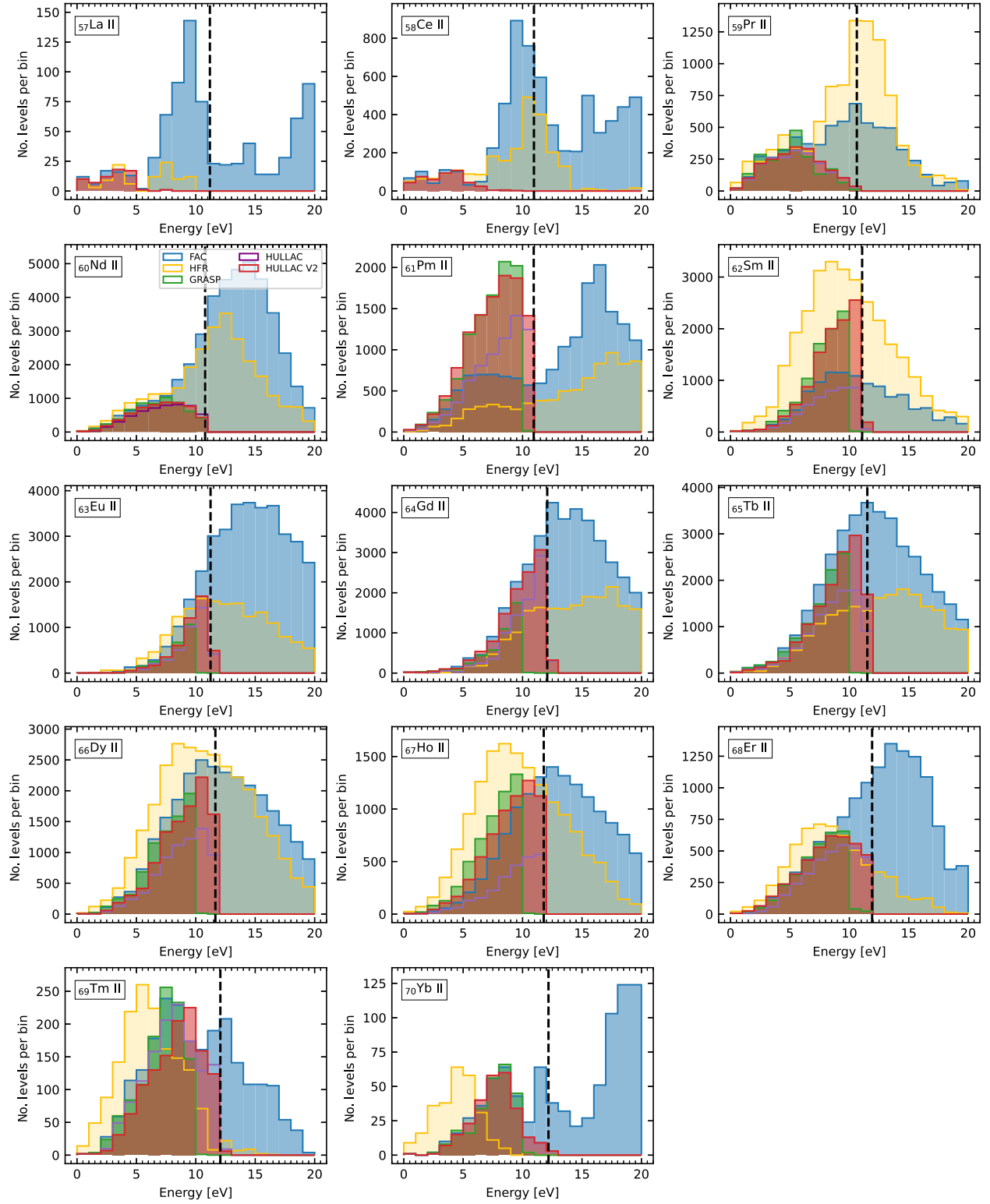


FIG. 4. Distributions of energy levels for singly ionized lanthanide ions. Different colors represent datasets computed with various atomic structure codes: FAC (this work; calibrated data) shown in blue, HULLAC shown in purple for version V1 [24] and red for version V2 [50], HFR in yellow [51], and GRASP in green [47,48,187]. Vertical dashed lines indicate the ionization thresholds of the respective ions.

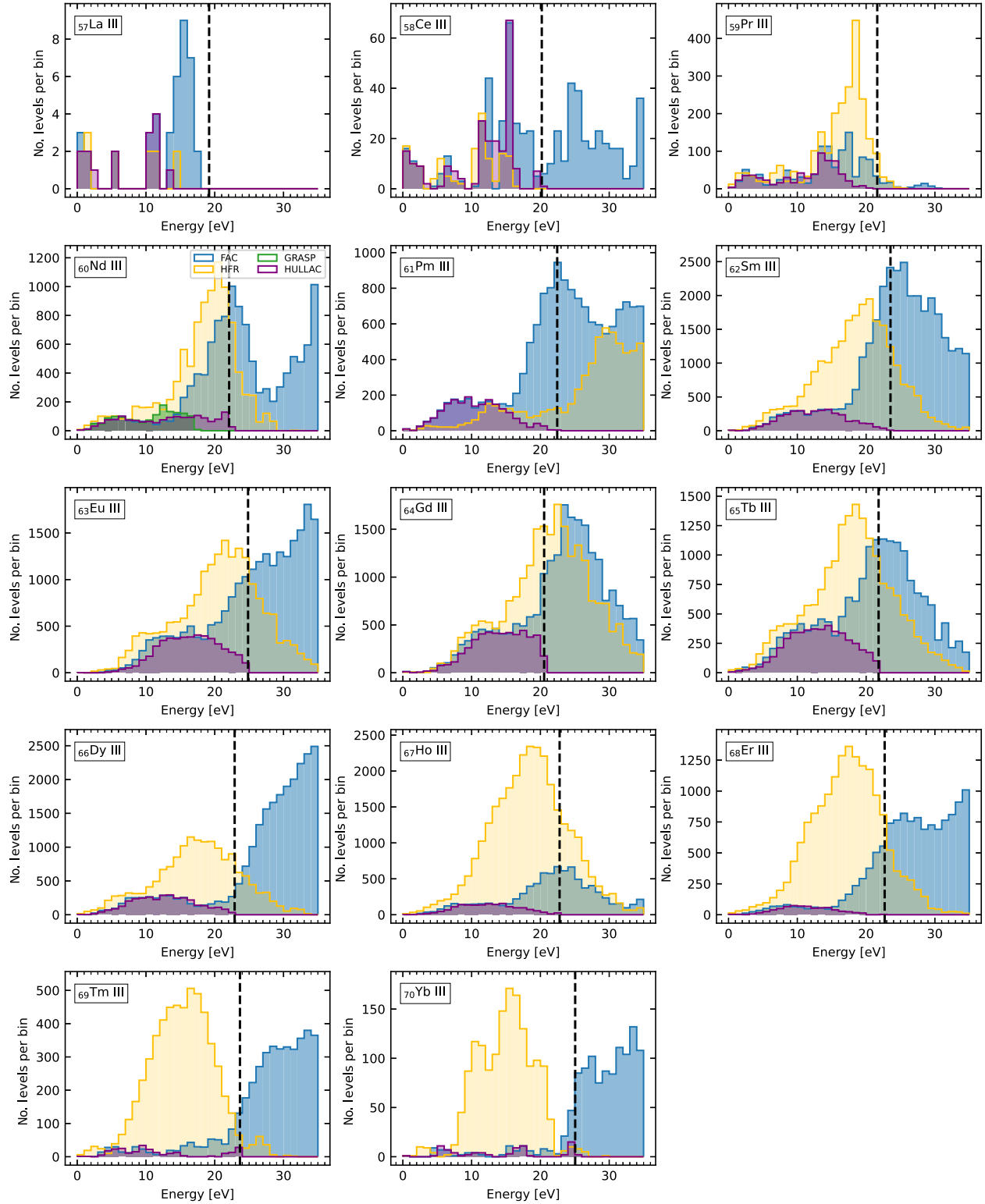


FIG. 5. Distributions of energy levels for doubly ionized lanthanide ions. Different colors represent datasets computed with various atomic structure codes: FAC (this work; calibrated data) shown in blue, HULLAC V1 shown in purple [24], HFR in yellow [51], and GRASP in green [187]. Vertical dashed lines indicate the ionization thresholds of the respective ions.

data obtained from high-resolution experiments reported in recent dedicated studies. Hollow cathode lamp spectroscopy was carried out using the Catania Astrophysical Observatory Spectropolarimeter [70]. In parallel, branching ratios were derived from emission spectra recorded with two different high-resolution spectrometers [71,72]. A detailed overview of the experimental levels and transitions used for comparison with our calculated dataset is provided in Table III.

Figure 6 compares transition data from the NIST Atomic Spectra Database and from recent measurements for six singly ionized lanthanide elements [70], alongside atomic structure calculations performed in this work using the FAC code. Similarly, Fig. 7 presents a comparison of our results for Gd II and Tm II with experimental data obtained in high-resolution spectroscopic studies [71,72]. In all cases, we include only those transitions for which both the upper and lower energy levels have been experimentally calibrated. Where available, theoretical oscillator strengths from the DREAM database are also included for comparison.

For strong transitions, defined here as those with $\log(gf) > -1$, we find that our FAC calculations are

generally consistent with experimental data, yielding a typical scatter of approximately 0.5 dex around the one-to-one relation $\log(gf)_{\text{FAC}} = \log(gf)_{\text{exp}}$. However, for weaker transitions with $\log(gf) < -1$, we observe a systematic discrepancy: the experimentally derived oscillator strengths are frequently higher than those predicted by our calculations. This behavior is partly expected, as experimental techniques are often limited to detecting transitions with at least moderate strength [typically down to $\log(gf) \sim -2$], inherently biasing the comparison against the full set of theoretically predicted weak lines. Nevertheless, one would anticipate a comparable number of transitions where experiments yield smaller oscillator strengths than theory, yet such cases appear underrepresented. Most weak transitions in our FAC dataset exhibit significantly suppressed $\log(gf)$ values relative to experimental findings.

This trend is not unique to our results. A similar pattern was noted in previous studies, such as Fig. 4 of [71], where experimental data were compared with GRASP calculations [48]. The fact that this discrepancy arises across different

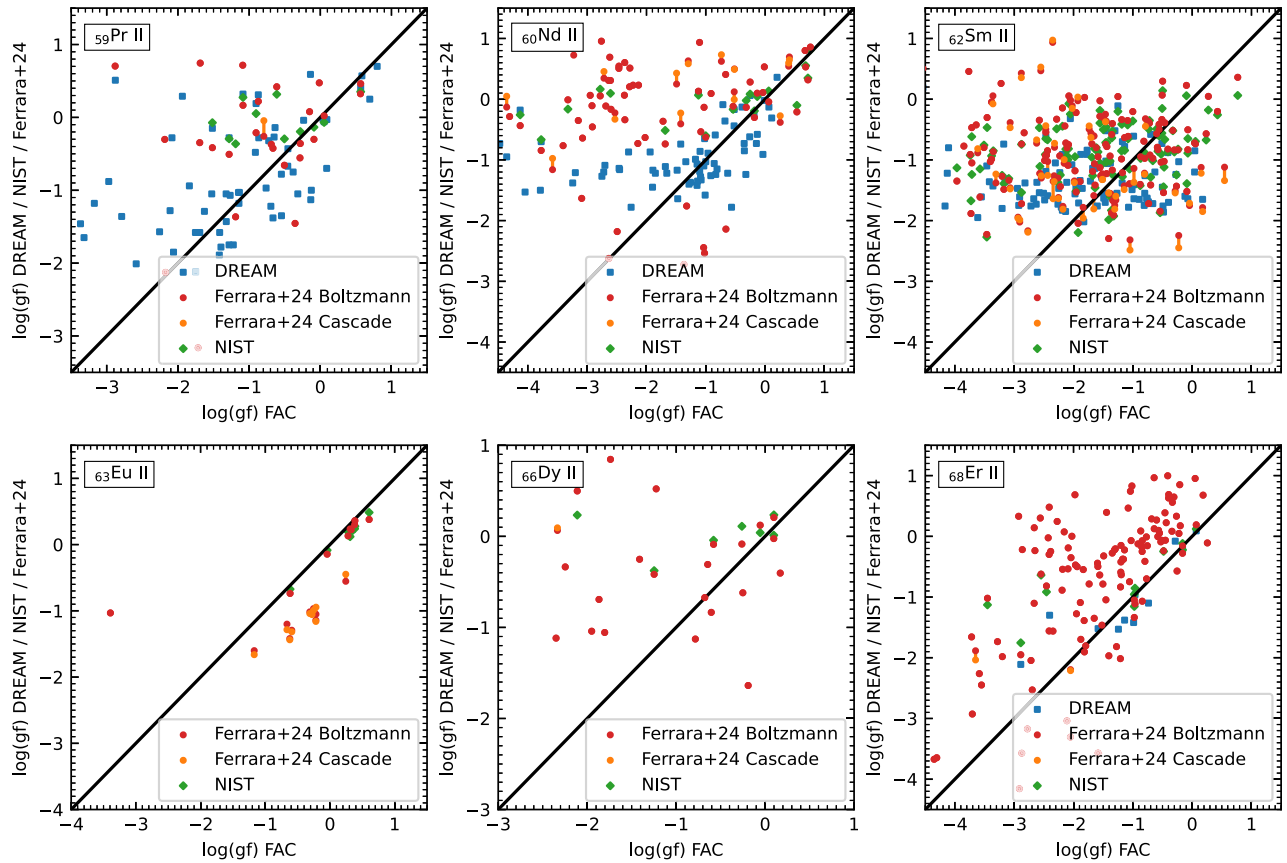


FIG. 6. Oscillator strengths derived from experimental measurements by Ferrara, Giarrusso, and Leone [70] and the NIST Atomic Spectra Database [65], as well as from theoretical calculations available in the DREAM database [66], are compared with those obtained in this work using the FAC code for transitions in which both upper and lower energy levels have been identified. In both the DREAM dataset and our FAC calculations, energy levels were calibrated to experimental values, and oscillator strengths were computed based on these calibrated energies.

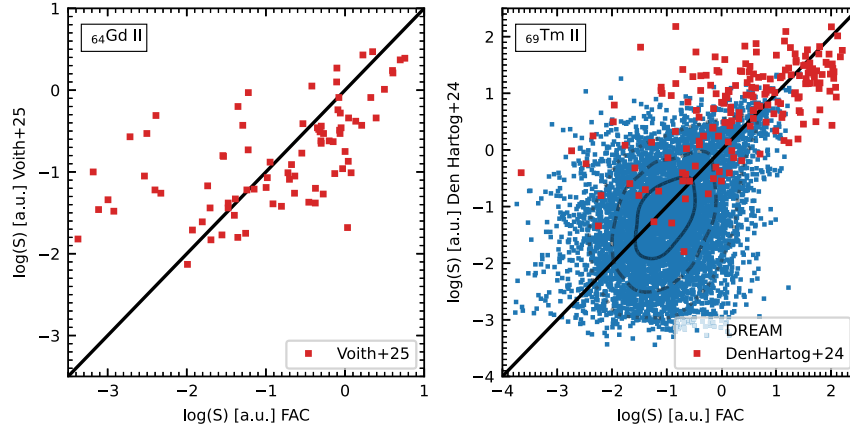


FIG. 7. Atomic line strengths S obtained from experimental measurements by Voith, Den Hartog, and Roederer [72] and Den Hartog, Voith, and Roederer [71], along with theoretical values derived from the DREAM database [66], are compared with results from our FAC calculations for transitions in which both the upper and lower energy levels have been identified. In both the DREAM dataset and our FAC computations, energy levels were calibrated to experimental data, and oscillator strengths were derived using these calibrated values. For visual clarity contour lines indicate regions containing 20%, 50% and 80% of all identified DREAM transitions.

atomic structure codes—*ab initio* GRASP and semiempirical FAC—as well as across three distinct experimental setups (used in Figs. 6 and 7) suggests that it is not attributable to a specific theoretical model or measurement technique. If such systematic underestimation of oscillator strengths by theoretical methods is widespread, the implications for KN opacity modeling and, particularly, mass estimations based on synthetic spectra could be significant.

In Figs. 8 and 9, we further compare our FAC oscillator strengths with calibrated theoretical data from the DREAM database, which are based on HFR calculations [66]. Although the large number of transitions (see Table III) naturally results in considerable scatter, especially among weak lines with $\log(gf) < -1$, we generally find good agreement between the two theoretical datasets for most ions. Notable exceptions include Nd II, for which a similar trend to the experimental comparisons is observed: weak lines are substantially weaker in our FAC calculations compared to the HFR results. In contrast, Sm II exhibits a flat distribution of oscillator strengths within the range $\log(gf) \sim [-2, 0]$, in line with experimental observations.

For the remaining ions, FAC and HFR oscillator strengths are generally distributed around the one-to-one correspondence in Figs. 8 and 9. It is worth noting that the degree of scatter correlates with the number of experimentally known levels: ions with many experimentally calibrated levels tend to exhibit larger scatter due to the increased complexity of higher-lying electronic configurations, whereas ions with only a few low-lying measured states, typically involving simpler near-ground configurations, show tighter agreement.

B. Bound-bound opacities

This study aims to deliver precise bound-bound opacities for conditions representative of kilonova ejecta, approximately a few days postmerger. The opacities presented here

have been calculated purely for demonstration rather than serving as direct inputs for radiative transfer simulations. All opacities shown in Figs. 11–15 were computed assuming a single-element plasma. In realistic ejecta, however, the ionization balance varies across different species, and the total electron density entering the single-element Saha equations is set collectively by all ionized elements. We offer a complete set of level energies and transitions for radiative transfer inputs instead of using precomputed opacities, which ionization balance approximations may significantly influence in monatomic plasmas.

In this work, we adopt the Sobolev formalism, which is widely used in transient radiative transfer. In the Sobolev optical depth

$$\tau_{i,k} = \frac{\pi e^2}{m_e c} f_k n_{i,k} \lambda_k t. \quad (5)$$

f_k is the oscillator strength of the line with transition wavelength λ_k and the corresponding lower level number density $n_{i,k}$, where the indices i and k indicate ionization states and level numbers, respectively. The number densities of the lower levels can be computed by assuming LTE holds, using the Saha ionization

$$\frac{n_i}{n_{i-1}} = \frac{Z_i(T) g_e}{Z_{i-1}(T) n_e} e^{-E_{\text{ion}}/k_B T} \quad (6)$$

and Boltzmann excitation equations

$$n_{i,k} = \frac{g_k}{Z_i(T)} e^{-E_k/k_B T} n_i, \quad (7)$$

where g_k is the multiplicity of the level ($2J_k + 1$), E_k is the level excitation energy, E_{ion} are the ionization energies, and

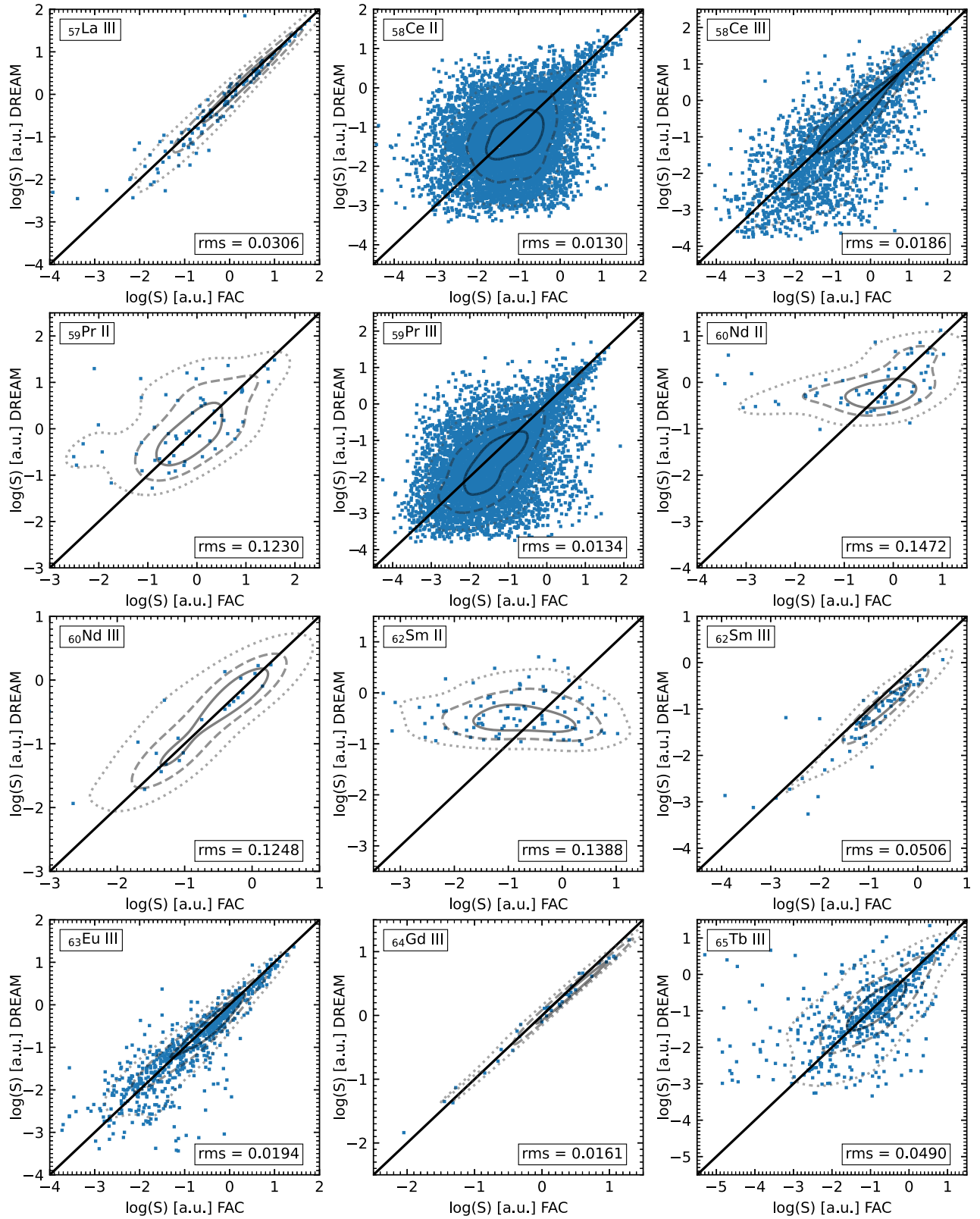


FIG. 8. The same as Fig. 6 but for ions for which only oscillator strengths from the DREAM database [66] are available. Shown are ions from $^{57}\text{La III}$ to $^{65}\text{Tb III}$.

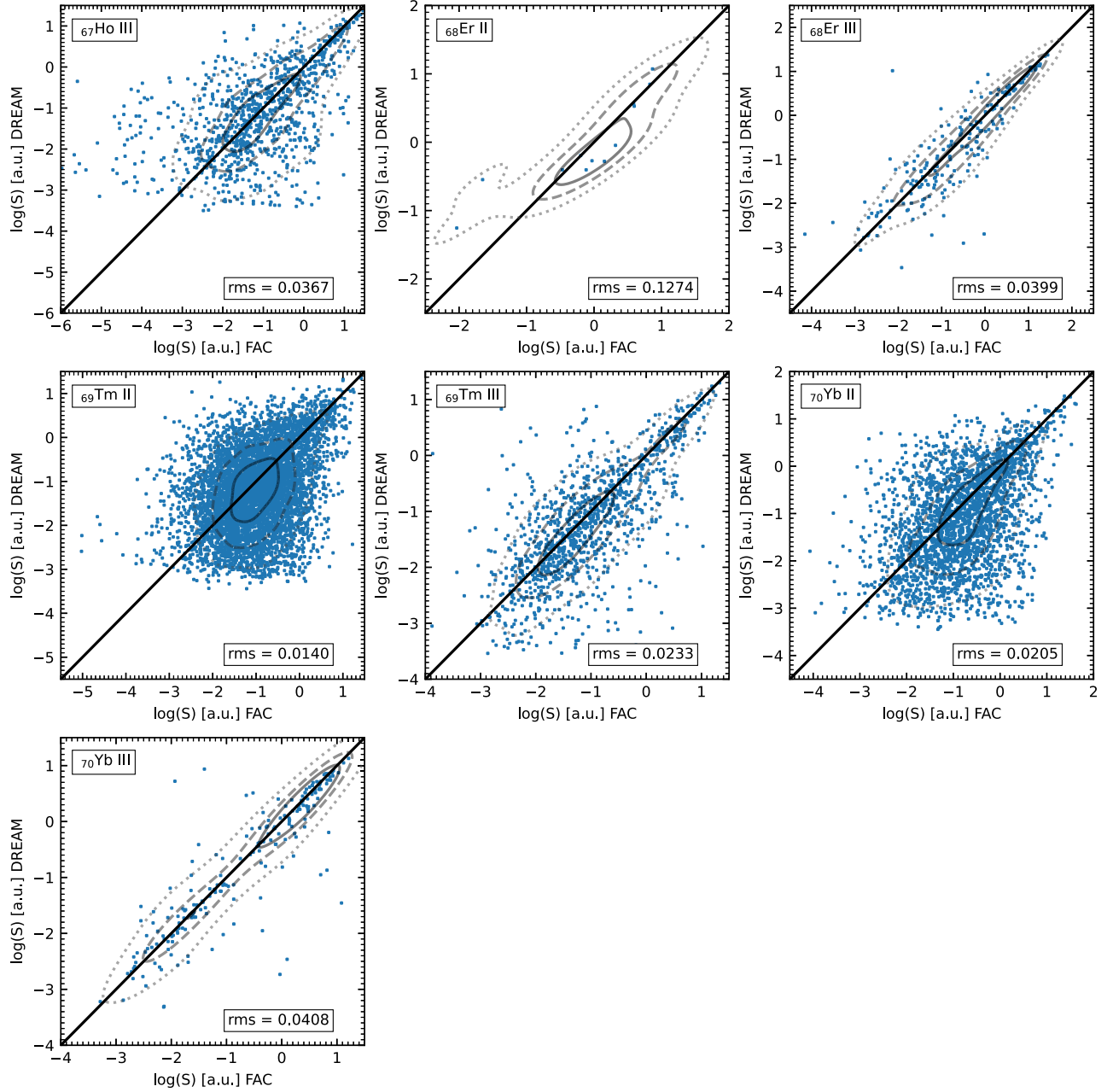


FIG. 9. The same as Fig. 6 but for ions for which only oscillator strengths from the DREAM database [66] are available. Shown are ions from $_{67}\text{Ho III}$ to $_{70}\text{Yb III}$.

$Z_i(T)$ are the partition functions:

$$Z_i(T) = \sum_k g_k e^{-E_k/k_B T}. \quad (8)$$

By applying the Sobolev optical depth, expansion opacities can be calculated (refer to [18,19,188]):

$$\kappa_{\text{exp}}(\lambda) = \frac{1}{c t \rho} \sum_{i,k} \frac{\lambda_k}{\Delta \lambda} (1 - e^{-\tau_{i,k}}), \quad (9)$$

where t indicates the time after the merger, ρ represents the ejecta density, $\Delta \lambda$ is the width of the bin, and λ_l is the wavelength of the transition.

The absolute scale of the opacity curves is unaffected by the choice of bin width, as demonstrated in prior studies [24,44]. In the limit of very narrow bin widths and weak transitions, the expansion opacity reduces to the line-binned form [46]. The combination of large velocity gradients typical of kilonova ejecta and the wavelength separation between prominent spectral lines fulfills the conditions required for the Sobolev approximation [24].

For a general discussion of the Sobolev approximation in the context of expanding atmospheres, see [189] and the treatment provided in the standard reference text [190].

In this work, we calculate all opacities presuming LTE conditions within the ejecta (see Refs. [191,192] for a discussion on non-LTE influences on kilonova opacities). We assume LTE is a suitable approximation in the initial days of the KN evolution. LTE opacities solely depend on the plasma state of the ejecta—temperature, density and time postmerger—as well as its composition [see Eqs. (5)–(8)].

We adopt $T = 5000$ K, $t = 1$ day postmerger, and $\rho = 10^{-13}$ g cm $^{-3}$, in line with prior research on KN opacities (see [21,24,44,187] among others). These values are based on simple blackbody fits to the observed 1.4-day spectrum of AT2017gfo and estimates of ejecta mass from light curve modeling. In LTE, temperatures do not differentiate between plasma and radiation.

We resolve the ionization balance using ionization energies from the NIST ASD [65]. In constructing the Saha equations, partition functions for all ion stages are ideally necessary, yet, given the physical conditions ($T < 10000$ K), only ions up to 3 times ionized are required. As calculated level energies for neutral and triply ionized species are not provided in this work, we source these values from the NIST ASD. While there are ample data for neutral species, triply ionized ions frequently lack excited states beyond the ground state. Thus, we caution that using our computed opacities near the transition to a triply ionized plasma might entail uncertainties in the ionization balance due to underestimated partition functions. For lanthanide ions, this transition is anticipated around 8000 K.

In the temperature range inferred from continuum fitting of AT2017gfo (2000–5000 K), only singly and doubly ionized species are expected to be significantly populated. For ions with available experimental data, uncertainties in partition functions are estimated to be below 5%. Overall, the impact of these uncertainties on the Saha equilibrium is comparatively modest when set against the larger variations in level energies and transition strengths observed across different atomic datasets for lanthanides. Although highly excited states often show the greatest discrepancies between atomic structure models, their contribution to the ionization balance is negligible due to suppression by the exponential factor in Eq. (8). Partition functions exert the strongest influence near the temperature regimes where the dominant ionization stage changes.

Figure 10 shows ion fractions for neutral through triply ionized species, based on our calibrated atomic data. Ionization transitions occur over relatively narrow temperature intervals, with most lanthanide species transitioning within ~ 400 K. An exception is the III $\leftrightarrow$ IV transition, which is expected to span a broader temperature range. Missing atomic levels can lead to underestimates in partition functions and shift the temperature at which

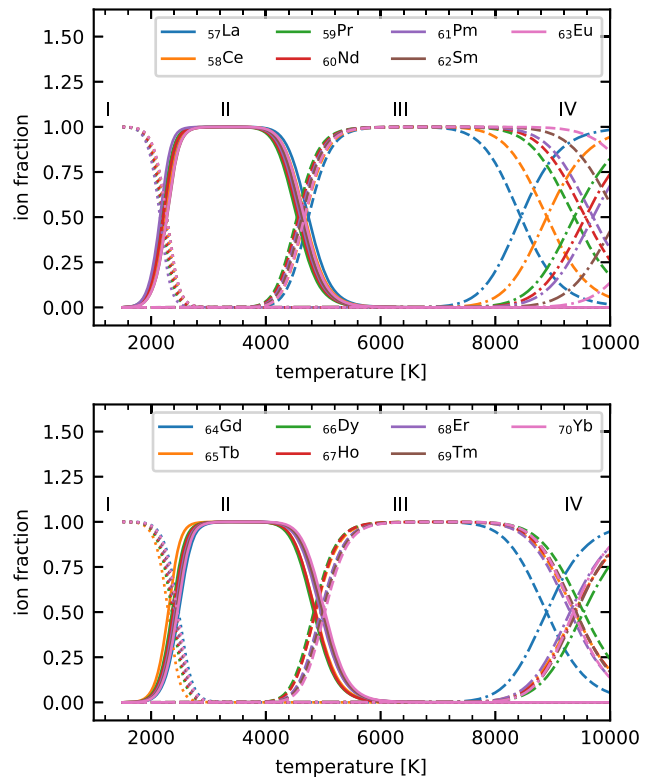


FIG. 10. Ion fractions of neutral to triply ionized lanthanides as a function of temperature. Data of the singly (II) and doubly (III) ionized species was computed with the FAC code. Data of the other two ionization stages (I and IV) were substituted from Kurucz’ GFALL. Top panel: ions from $_{57}\text{La}$ to $_{63}\text{Eu}$. Bottom panel: ions from $_{64}\text{Gd}$ to $_{70}\text{Yd}$.

ionization transitions occur, depending on the ratio between the partition functions of successive ionization stages. It is important to note that the present analysis is valid only within the range 2500–8500 K, where singly and doubly ionized species are dominant.

1. Lanthanide expansion opacity

Expansion opacities, computed using Eqs. (7)–(9), were evaluated for a gas with $T = 5000$ K and $\rho = 10^{-13}$ g cm $^{-3}$ at an epoch of $t = 1$ day. Under these conditions, lanthanides are partially ionized, with the dominant contributions to the opacity arising from singly and doubly ionized species, as shown in Fig. 10. Comparative opacity results based on both uncalibrated and calibrated atomic structures are shown in Figs. 11 and 12, alongside data from previous studies [24,47,48,50,51,187].

In the majority of cases, the calibrated opacities obtained in this work are higher than the original V1 HULLAC results reported in earlier work [24]. This increase is partly attributable to the inclusion of a more extensive set of CSFs, which leads to a denser atomic-level structure. At typical ejecta temperatures during the first week following a KN event (3000–10000 K), only a

limited number of low-lying energy levels are thermally populated due to Boltzmann suppression of higher-energy states. Consequently, the inclusion of additional atomic levels near the ionization threshold increases the number of available upper states for transitions originating from thermally populated low-lying levels. This leads to an enhanced absorption probability at short wavelengths (with $hc/\lambda \sim E_{\text{ion}}$), thereby increasing the overall opacity in the ultraviolet and optical regimes. In contrast, atomic models that omit these near-threshold configurations underestimate the number of such transitions and thus yield systematically lower opacities in this spectral region.

Although the inclusion of additional atomic states enhances the opacity at short wavelengths, the astrophysical impact of this increase remains limited. In KN ejecta, the emergent radiation at early times (e.g., $t = 1$ day post-merger) is predominantly emitted redward of ~ 3000 Å [193]. At shorter wavelengths, such as ~ 1000 Å—corresponding to photon energies near the ionization thresholds of singly ionized lanthanides (~ 10 eV)—the radiation field is intrinsically weak. Despite elevated opacities in this spectral region, the limited number of photons capable of interacting with these transitions means that their contribution to radiative transfer is minimal. Consequently, opacity enhancements blueward of ~ 3000 Å are unlikely to exert a significant influence on the overall radiation transport in kilonova models.

The updated HULLAC calculations exhibit substantially improved agreement with both the present FAC results and the GRASP-based datasets from earlier studies [47,48,50,187]. In contrast, atomic data reported in a recent HFR-based study yield significantly higher opacities for many lanthanide species [51]. This discrepancy is primarily attributable to elevated level densities at low and intermediate excitation energies, as illustrated in Figs. 4 and 5. In particular, for the latter half of the singly ionized series and for most doubly ionized species, the HFR-based level densities exceed those from FAC, HULLAC (V2), and GRASP by a considerable margin, resulting in opacity enhancements of up to a factor of 2.

Discrepancies in the red tail of the opacity between the FAC, V2 HULLAC, and GRASP calculations shown in Figs. 11 and 12 reflect differences in ground-state configurations, the density of low-lying levels, and the atomic structure methods employed. While previous efforts have focused on maximizing completeness in opacity datasets [24,50], the approach adopted in this work places additional emphasis on accurately reproducing low-lying energy levels, particularly those below $30\,000\text{ cm}^{-1}$. One notable exception is Gd II, where our calculated ground state differs from that reported in NIST ASD by approximately 2500 cm^{-1} . In general, a higher level density near the ground state correlates with increased opacity due to the larger number of accessible transitions. While the long-wavelength tail of the opacity remains relatively consistent across the FAC,

HULLAC, and GRASP results, differences of up to an order of magnitude in peak opacities are observed.

For ions lacking robust experimental constraints, expansion opacities are subject to larger uncertainties. This effect is especially pronounced for Pm III, where the HULLAC-based opacities reported in recent work exceed those obtained from the present FAC calculations by approximately a factor of 2 [50]. Such discrepancies are exacerbated at $T = 5000$ K, where doubly ionized species dominate for several elements, yet experimental data are sparse or entirely lacking.

2. Planck mean opacity

Both line-by-line and, more generally, wavelength-dependent radiative transfer calculations generally provide the highest accuracy for modeling emergent spectra. However, gray opacities remain a widely used simplification in KN light curve models where radiative diffusion is the dominant transport mechanism. The Planck mean opacity is defined by

$$\kappa_{\text{mean}} = \frac{\int_0^\infty B_\lambda(T) \kappa_{\text{exp}}(\lambda) d\lambda}{\int_0^\infty B_\lambda(T) d\lambda}, \quad (10)$$

where $B_\lambda(T)$ is the Planck function at temperature T and $\kappa_{\text{exp}}(\lambda)$ is the expansion opacity as introduced in Eq. (9). The use of Planck mean opacities assumes the radiation field closely resembles a blackbody spectrum, a condition typically met during the early phases of KN evolution (as inferred from blackbody fits in [3,193–195]). However, this assumption has been challenged in recent work, e.g., [26,196], which shows that in multidimensional, time-dependent simulations, such a blackbody radiation field may not be realized.

Assuming that the line-forming region can be approximated by a blackbody in the early epochs (up to approximately 5 days postmerger), Planck mean opacities remain a useful diagnostic for quantifying the bulk ejecta opacity. We compute Planck mean opacities at $T = 5000$ K for each lanthanide ion, based on the atomic structure datasets described in Sec. IV B 1, assuming an ejecta density of $\rho = 10^{-13}\text{ g cm}^{-3}$ and $t = 1$ day. These results are calculated for individual species, and extending them to mixed compositions would require solving the Saha equation with the appropriate abundances. The Planck mean opacity peaks for most lanthanides between 4000 and 5000 K.

Figure 13 summarizes the Planck mean opacities at $T = 5000$ K across the lanthanide series. Among all species, neodymium ($Z = 60$) exhibits the highest opacity. A double-peaked structure is evident, with minima corresponding to ions having either an empty, half-filled, or fully filled f shell. These configurations reduce the number of low-lying levels and consequently the number of accessible transitions. While the low opacity of closed-shell ions is expected, the reduced opacity for half-filled shells is somewhat counterintuitive. As the f subshell is filled,

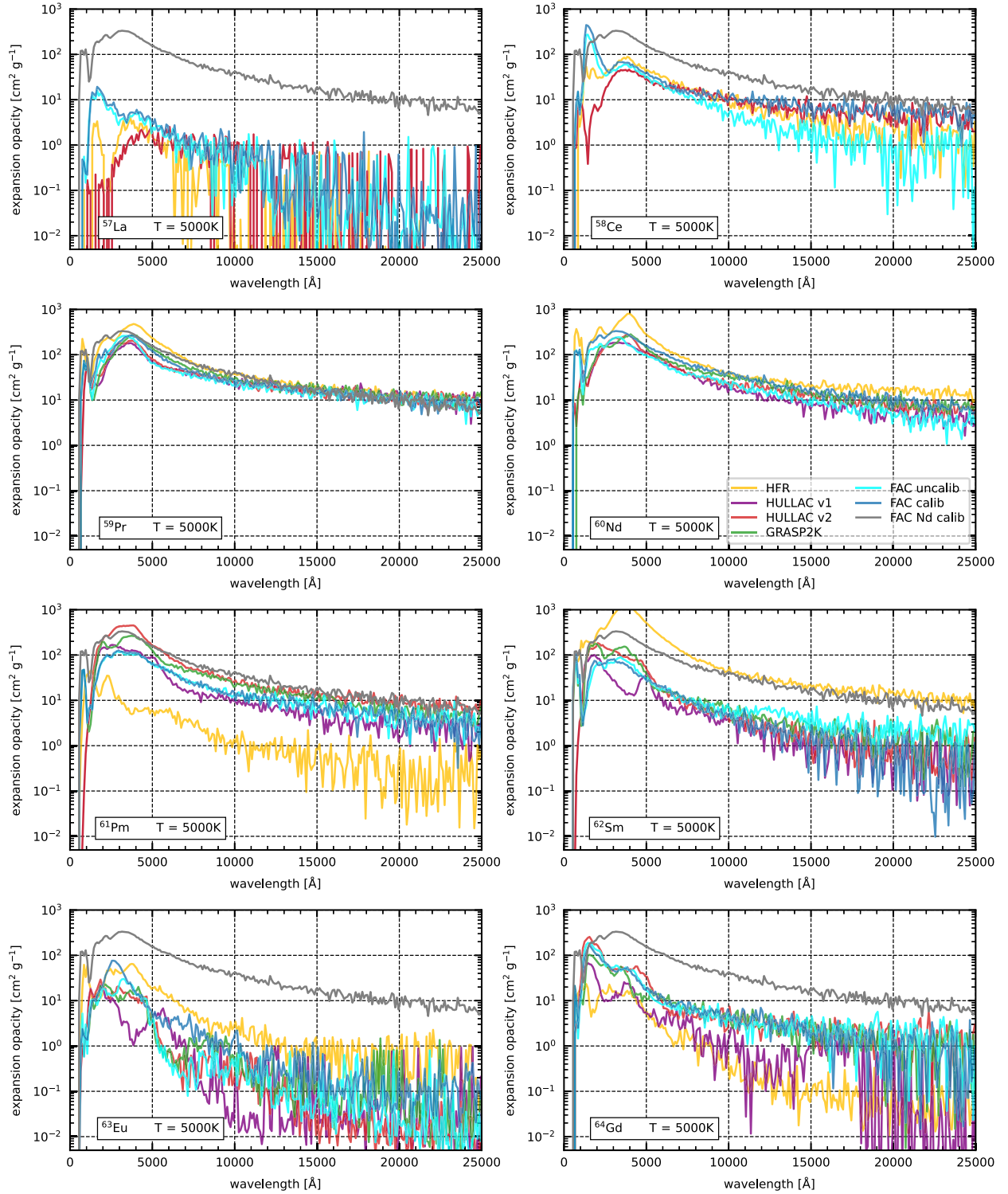


FIG. 11. Expansion opacity results for ions from $Z = 57$ (La) to $Z = 64$ (Gd) are presented at $T = 5000$ K, $\rho = 10^{-13}$ g cm $^{-3}$, and $t = 1$ day, using a bin width of 100 Å. The comparison includes uncalibrated (light blue) and calibrated (dark blue) FAC calculations, as well as HULLAC data from two versions: V1 (purple) [24] and V2 (red) [50]. Results from GRASP calculations (green) are also shown, based on datasets from previous studies [47,48,187]. For GRASP, missing data for doubly ionized species were substituted with calibrated FAC results. Finally, data from HFR (yellow) from [51] are also included. For ease of comparison across species, the expansion opacity of Nd derived from FAC calculations is included in gray in all panels.

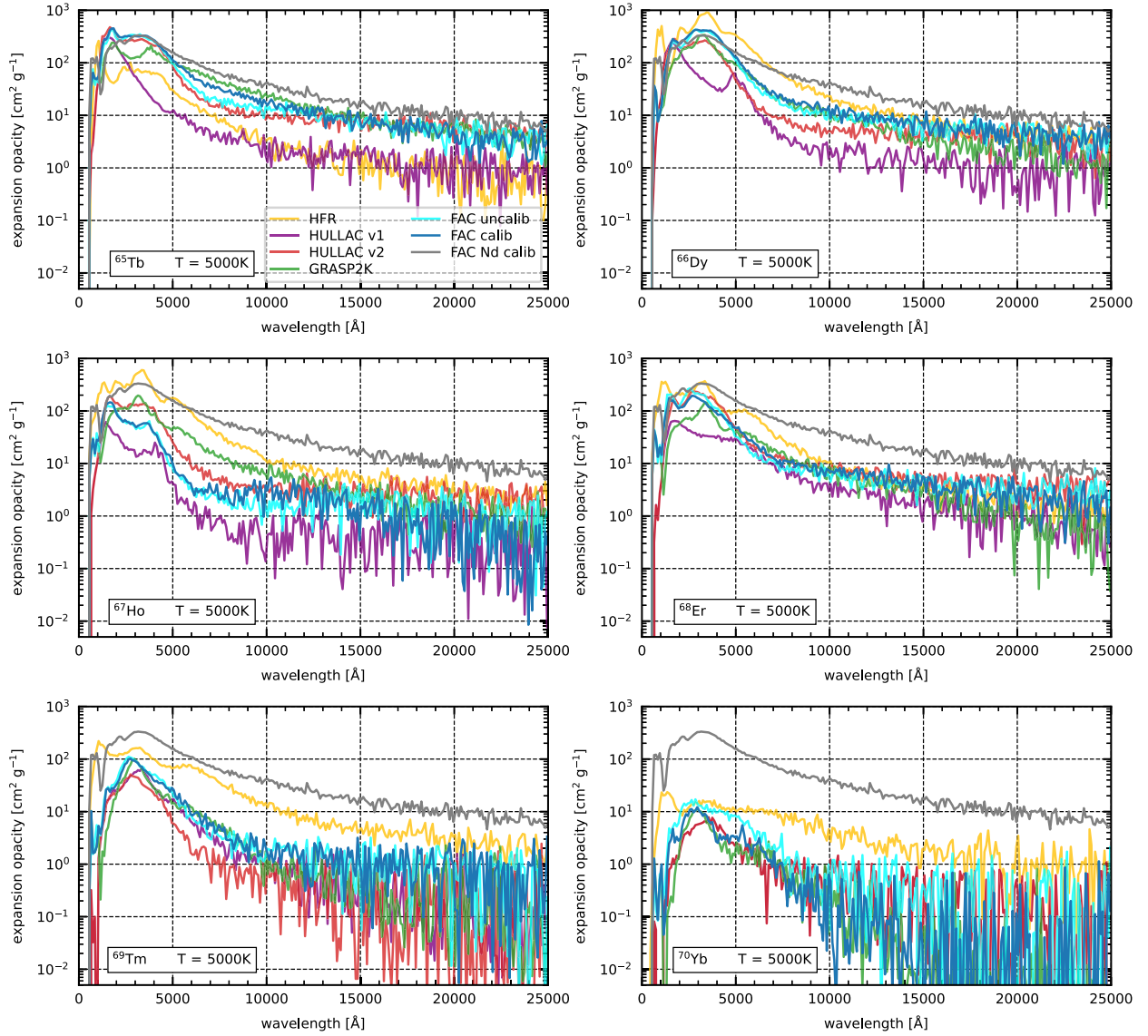


FIG. 12. Expansion opacity results for ions from $Z = 65$ (Tb) to $Z = 70$ (Yb) are presented at $T = 5000$ K, $\rho = 10^{-13}$ g cm $^{-3}$, and $t = 1$ day, using a bin width of 100 Å. The comparison includes uncalibrated (light blue) and (dark blue) FAC calculations, as well as HULLAC data from two versions: V1 (purple) [24] and V2 (red) [50]. Results from GRASP calculations (green) are also shown, based on datasets from previous studies [47,48,187]. For GRASP, missing data for doubly ionized species were substituted with calibrated FAC results. Finally, data from HFR (yellow) from [51] are also included. For ease of comparison across species, the expansion opacity of Nd derived from FAC calculations is included in gray in all panels.

the number of low-energy levels (below 20 000 cm $^{-1}$) tends to decrease [21,24,46], resulting in diminished opacity despite the high overall transition count.

The spread in Planck mean opacities among the lanthanides spans nearly 2 orders of magnitude. For instance, La II, Eu II, and Ho II show opacities around unity, whereas Pr II, Nd II, and Dy II range from 50 to 100 cm 2 g $^{-1}$. These calculations are based on single-species plasmas and do not reflect the exact contribution of each lanthanide to the total r-process opacity. Nevertheless, Fig. 13 provides a useful baseline for identifying opacity-dominant species under simplified conditions.

We observe good overall consistency between the various atomic structure codes, except for the HULLAC V1 and HFR datasets. Figure 14 quantifies the deviation of each dataset from the calibrated FAC results. Both HULLAC V2 and GRASP agree with FAC to within 20%. In contrast, HULLAC V1 underestimates opacity in the central lanthanides, while the HFR-based opacities for Pm II, Sm II, Gd II, Tb II, and Yb II exceed FAC values by factors of ~ 7 –10. These differences originate from the significantly enhanced density of low- and intermediate-lying levels in the doubly ionized HFR models.

Figures 15 and 16 display the temperature dependence of Planck mean opacities, calculated using both calibrated and

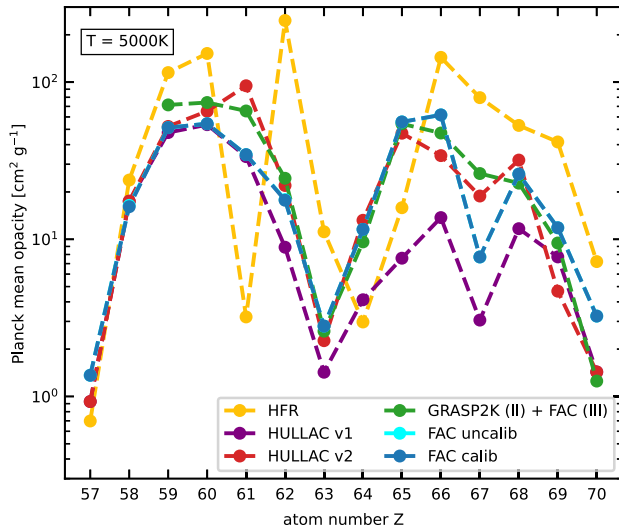


FIG. 13. Planck mean opacities are shown for monatomic lanthanide plasmas at $\rho = 10^{-13} \text{ g cm}^{-3}$, evaluated one day after merger at a temperature of 5000 K. The FAC results from this work are presented in cyan (uncalibrated) and blue (calibrated). For comparison, Planck mean opacities based on previously published datasets are also included, comprising HULLAC results from V1 (purple) and V2 (red) [24,50], HFR data (yellow) [51], and GRASP calculations (green) [47,48,187].

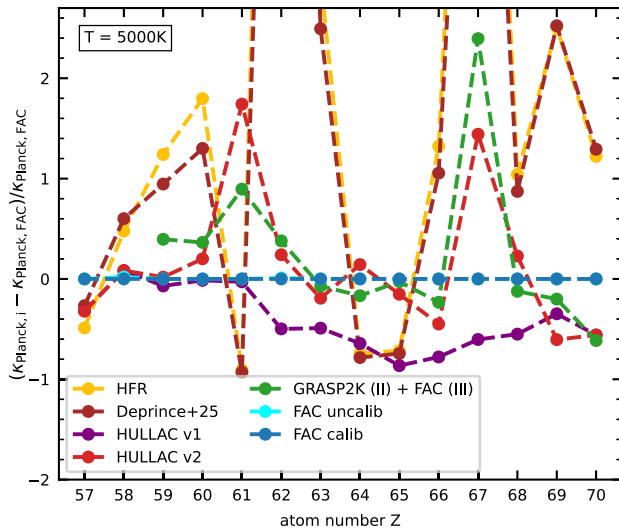


FIG. 14. Planck mean opacities are shown for monatomic lanthanide plasmas at $\rho = 10^{-13} \text{ g cm}^{-3}$, evaluated one day after merger at a temperature of 5000 K relative to the results of the calibrated FAC opacities. The FAC results from this work are presented in cyan (uncalibrated) and blue (calibrated). For comparison, Planck mean opacities based on previously published datasets are also included, comprising HULLAC results from V1 (purple) and V2 (red) [24,50], HFR data (yellow) [51], and GRASP calculations (green) [47,48,187].

uncalibrated data as well as previously published datasets. The decline of the Planck mean opacity at high temperatures results from the ionization shift from singly to doubly

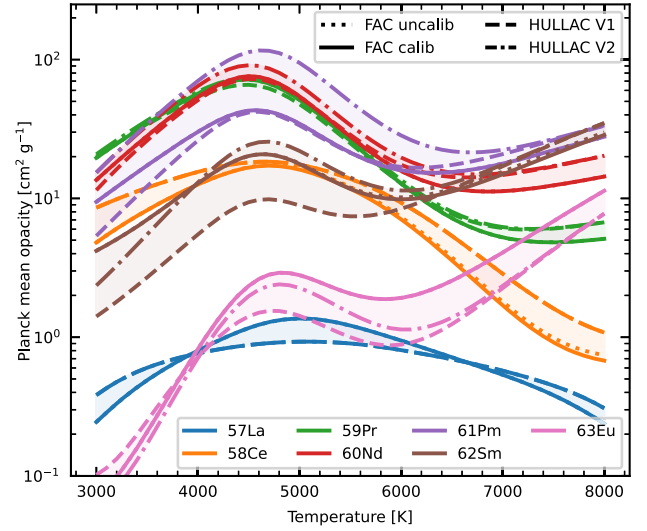


FIG. 15. Planck mean opacities are presented for monatomic lanthanide plasmas (La to Eu) at a density of $\rho = 10^{-13} \text{ g cm}^{-3}$ one day postmerger, as a function of plasma temperature. The results include both calibrated (solid lines) and uncalibrated (dotted lines) FAC calculations from this work. For comparison, published HULLAC datasets are also shown, with V1 represented by dashed lines [24] and V2 by dash-dotted lines [50].

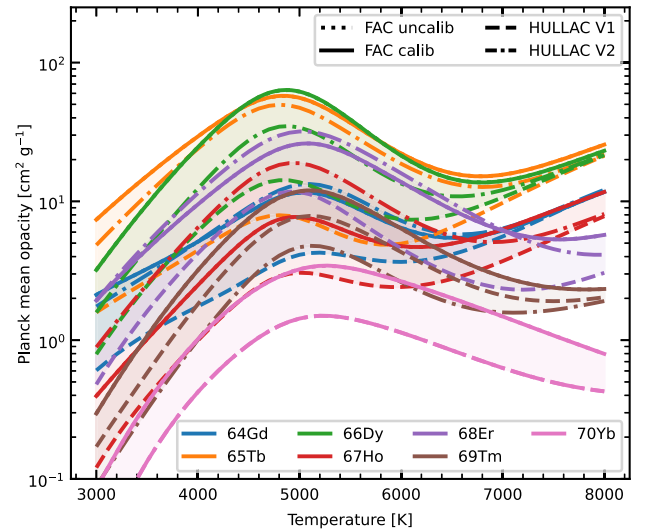


FIG. 16. Planck mean opacities are presented for monatomic lanthanide plasmas (Gd to Yb) at a density of $\rho = 10^{-13} \text{ g cm}^{-3}$ one day postmerger, as a function of plasma temperature. The results include both calibrated (solid lines) and uncalibrated (dotted lines) FAC calculations from this work. For comparison, published HULLAC datasets are also shown, with V1 represented by dashed lines [24] and V2 by dash-dotted lines [50].

ionized species near 4500 K, which generally yield lower opacities. At lower temperatures ($\lesssim 4000 \text{ K}$), the reduction in opacity is a result of the Planck spectrum overlapping with the falling tail of the expansion opacity curve, which scales as λ^{-1} [43]. Similarly, at high temperatures above $\sim 6500 \text{ K}$,

the convolution of the Planck spectrum and the expansion opacity yields an increased overlap, leading to a rise of the Planck mean opacity. As our calculations are restricted to up to doubly ionized species, we do not evaluate the Planck mean opacity above $T = 8000$ K, where contributions from triply ionized species become important (see Sec. IV B).

C. Effect of the fac calibration procedure on opacities

The primary effect of the calibration is a systematic shift and local redistribution of line positions in wavelength space, arising from coherent corrections to the calculated level energies. Importantly, the calibration procedure does not alter the underlying wave functions, transition probabilities (except for an energy dependence of the Einstein coefficients $A_{ji} \propto E^3 \times S$ or the oscillator strengths $f_{ij} \propto E \times S$) or the configuration space represented in the atomic model. As a result, the dominant line strengths and the statistical distribution of oscillator strengths are preserved, and the bulk opacity properties remain largely insensitive to the calibration. In this sense, the calibrated and uncalibrated datasets can be viewed as two representations of the same atomic structure, differing primarily in the absolute and relative placement of energy levels, rather than in the intrinsic atomic physics.

This effect is most pronounced in spectral regions where the opacity is dominated by transitions among low-lying and moderately excited states. In these regimes, the level density is relatively sparse, so individual or small groups of transitions can leave noticeable imprints on the opacity spectrum. Even modest systematic offsets in the uncalibrated level energies (e.g., Ce II even-parity levels or Sm II odd-parity levels; see Figs. 11 and 12) can therefore translate into visible opacity differences, particularly in the long-wavelength (“red”) tail. For most lanthanide ions, we observe good agreement between the calibrated and uncalibrated opacities at long wavelengths, with residual differences largely attributable to statistical fluctuations from the small number of transitions contributing to each wavelength bin in the expansion-opacity formalism. The calibration step aligns these low-lying level densities with experimental anchors, improving spectral fidelity in these sparsely populated regions.

By contrast, at shorter wavelengths and higher excitation energies, where the opacity arises from an extremely dense forest of transitions among strongly mixed excited configurations, the differences between calibrated and uncalibrated data are comparatively minor. In these regimes, the cumulative opacity is dominated by the statistical line density, rather than the precise placement of individual transitions. Small coherent shifts of many closely spaced lines tend to average out, resulting in only marginal changes to the overall opacity. Consequently, the calibration primarily enhances spectral fidelity and the placement of transition features, while leaving the high-energy opacity quasicontinuum essentially unchanged. Most lines in this

high-density regime are not fully calibrated to experimental data, as only the lower levels could be reliably identified due to the extreme level density.

It is also important to emphasise that the calibration does not introduce new physical processes or additional transitions. Instead, it refines the energetic alignment of an already complete line list. The uncalibrated FAC data represent the raw predictive output of our atomic structure model, while the calibrated data demonstrate improved consistency with experimental benchmarks. Overall, the comparison indicates that calibration acts as a refinement step, enhancing the physical plausibility of line placement without altering the main quantitative conclusions regarding opacities. For applications such as light-curve modeling, the improvement gained from fully calibrated versus uncalibrated atomic data is marginal, as supported by Figs. 13–16, which show near-perfect overlap between calibrated and uncalibrated FAC opacity curves.

V. SUMMARY AND CONCLUSIONS

In this study, we present comprehensive atomic structure calculations for the energy levels and E1 permitted transitions of all 28 singly and doubly ionized lanthanide ions ($_{57}\text{La}$ to $_{70}\text{Yb}$), employing the FAC code. We use an innovative optimization technique for the local central potential in FAC [63], which significantly reduces discrepancies when compared to experimental atomic data. Furthermore, all experimentally confirmed energy levels available in the literature are utilized to calibrate our computed atomic structures and the corresponding transition energies. This calibration ensures improved accuracy in both level energies and radiative transition parameters. On average, we implemented corrections of 2950 and 2571 cm^{-1} for singly and doubly ionized lanthanides, respectively. The corrections for singly ionized species are generally greater due to the wider availability of highly excited experimental levels, for which the agreement between theory and experiment is lower. For the ions considered in this study, we identified a total of 146 849 energy levels below the ionization threshold, associated with 29 337 507 electric dipole transitions. Of these transitions, 66 722 have both upper and lower levels precisely calibrated against experimental data, permitting accurate determination of transition wavelengths.

We present an extensive comparison of the atomic energy level structure and oscillator strengths between our calculations and extant experimental and theoretical data. We find very good agreement with the majority of previously published lanthanide atomic structure calculations on the energy level densities. For the oscillator strengths of electric dipole allowed transitions, a strong correlation is observed between our results and both experimental and theoretical values for strong transitions [$\log(gf) > -1$]. Conversely, for weak transitions [$\log(gf) < -1$], the oscillator strengths calculated by us, as well as those from the semiempirical

calculations in the DREAM database using the HFR code, are markedly weaker than the experimental data.

We have also computed LTE opacities for our lanthanide ions by solving the Saha ionization and Boltzmann excitation equations. Our results show variations of ~ 2 orders of magnitude in the expansion opacity across the ions in our sample. Differences in expansion opacity among atomic structure calculations from varying codes for the same ion are generally within a factor of 2. In numerous instances, we detect a significant increase in opacity at short wavelengths, attributed to the substantially greater number of electronic configurations compared to previous studies. The calibration procedure implemented to enhance transition accuracy exerts only a marginal influence on the opacity. Gray opacities align well with previous findings, effectively reproducing the previously identified double-peaked structure of the lanthanide group. Our results agree well with published data using the GRASP and HULLAC (V2) codes but are in moderate disagreement with opacity results from HFR. We show that this disagreement is mainly caused by a difference in energy level density at intermediate energies ($\sim$ halfway to the ionization threshold).

While the atomic energy levels and permitted E1 transitions computed in this study suffice for LTE radiative transfer modeling, additional data are required to extend the modeling efforts to the nebular phase. We are currently computing forbidden M1 and E2 transitions between our calibrated energy levels, which are highly relevant for non-LTE radiative transfer, as well as electron-ion collision strengths required to obtain non-LTE occupation numbers. We will publish our non-LTE atomic data in a second paper.

ACKNOWLEDGMENTS

We thank G. Gaigalas, M. Tanaka, D. Kato, J. Deprince, and C. J. Fontes for making some or all of their calculated atomic data public, facilitating benchmarks with other codes. We want to especially thank Yuri Ralchenko, Alexander Kramida, Joseph N. Tan, Karen Olsen, and the whole NIST atomic spectroscopy group for their long-standing community work, without which this study would not have been possible. The authors thank the anonymous reviewer for their constructive feedback, which significantly improved the quality of this manuscript. A. F. and G. M.-P. acknowledge support by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation program (ERC Advanced Grant KILONOVA No. 885281), the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)—Project-ID No. 279384907—SFB 1245, and MA 4248/3-1. R. F. S. acknowledges the support from National funding by FCT (Portugal), through the

individual research Grant No. 2022.10009.BD. R. F. S., J. M. S., and J. P. M. acknowledge support through project funding 2023.14470.PEX “Spectral Analysis and Radiative Data for Elemental Kilonovae Identification (SPARKLE)” [197]. This research made use of Astropy, a community-developed core Python package for Astronomy [198,199], as well as NUMPY [200], SCIPY [201], PANDAS [202], and MATPLOTLIB [203].

DATA AVAILABILITY

The data that support the findings of this article are openly available [204].

APPENDIX A: DATASET

The complete dataset underlying this study is publicly available in machine-readable format on Zenodo [204]. It includes all calculated and calibrated energy levels, radiative transition data, and configuration information for singly and doubly ionized lanthanide ions as described in the text. This dataset is intended to support reproducibility and facilitate future applications in radiative transfer modeling, spectroscopic analysis, and atomic physics research. Tables IV and V provide representative excerpts of the published data, illustrating the structure and format included in the full release.

TABLE IV. Energy levels (in cm^{-1}) relative to the ground state for all ions in this study. This table is available in its entirety in machine-readable form. Part of the data are shown here for guidance regarding its form and content. The last column shows the type of calibration of the energy level: xmatch indicates that the levels were directly identified in experimental data, while “shifted” refers to a calibration based on other identified levels in the same J -parity group, configuration, or both (see Sec. II C).

Index	Z^a	Charge ^b	Energy ^c	J^d	Parity	Conf.	LS1	LS2	Method
0	57	1	0.00	2	0	5d2	3F	1D	Xmatch
1	57	1	1016.10	3	0	5d2	3F	3F	Xmatch
2	57	1	1394.46	2	0	5d2	1D	1D	Xmatch
3	57	1	1895.15	1	0	5d1.6s1	3D	3D	Xmatch
4	57	1	1970.70	4	0	5d2	3F	3F	Xmatch
5	57	1	2591.60	2	0	5d1.6s1	3D	3D	Xmatch
6	57	1	3250.35	3	0	5d1.6s1	3D	3D	Xmatch
7	57	1	5249.70	0	0	5d2	3P	3P	Xmatch
8	57	1	5718.12	1	0	5d2	3P	3P	Xmatch
9	57	1	6227.42	2	0	5d2	3P	3P	Xmatch
10	57	1	7394.57	0	0	6s2	1S	1S	Xmatch

^aAtomic number.

^bIon charge.

^cEnergy in cm^{-1} .

^dTotal angular momentum.

TABLE V. Transitions between levels for all singly and doubly ionized lanthanides in this study. This table is available in its entirety in machine-readable form. Part of the data are shown here for guidance regarding its form and content.

Z^a	C^b	Lower Level							Upper Level							Transition information				
		No.	E^c	J^d	P^e	Conf.	LS	Method	No.	E^c	J^d	P^e	Conf.	LS	Method	Type	Energy ^c	λ^f	Log(gf)	A value ^g
57	1	0	0.00	2	0	5d2	3F	Xmatch	14	14147.98	2	1	4f1.6s1	3F	Xmatch	E1	14147.98	7068.15	-1.0213	2.54(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	15	14375.17	3	1	4f1.6s1	3F	Xmatch	E1	14375.17	6956.44	-1.9309	2.31(5)
57	1	0	0.00	2	0	5d2	3F	Xmatch	17	15773.77	3	1	4f1.6s1	1F	Xmatch	E1	15773.77	6339.64	-3.6378	5.46(3)
57	1	0	0.00	2	0	5d2	3F	Xmatch	19	17211.93	2	1	4f1.5d1	3F	Xmatch	E1	17211.93	5809.92	-1.4129	1.53(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	21	18235.56	3	1	4f1.5d1	3F	Xmatch	E1	18235.56	5483.79	-2.0328	2.94(5)
57	1	0	0.00	2	0	5d2	3F	Xmatch	23	18895.41	2	1	4f1.5d1	1D	Xmatch	E1	18895.41	5292.29	-1.3232	2.26(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	26	20402.82	3	1	4f1.5d1	3G	Xmatch	E1	20402.82	4901.28	-0.2445	2.26(7)
57	1	0	0.00	2	0	5d2	3F	Xmatch	28	21441.73	1	1	4f1.5d1	3D	Xmatch	E1	21441.73	4663.80	-0.6398	2.34(7)
57	1	0	0.00	2	0	5d2	3F	Xmatch	29	22106.02	2	1	4f1.5d1	3D	Xmatch	E1	22106.02	4523.65	-1.3769	2.74(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	31	22537.30	3	1	4f1.5d1	3D	Xmatch	E1	22537.30	4437.09	-1.4071	1.90(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	33	22705.15	1	1	4f1.5d1	3P	Xmatch	E1	22705.15	4404.29	-1.6800	2.40(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	34	23246.93	2	1	4f1.5d1	3P	Xmatch	E1	23246.93	4301.64	-1.7556	1.27(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	35	24462.66	2	1	5d1.6p1	1D	Xmatch	E1	24462.66	4087.86	-0.1804	5.27(7)
57	1	0	0.00	2	0	5d2	3F	Xmatch	36	24522.70	3	1	4f1.5d1	1F	Xmatch	E1	24522.70	4077.85	-1.7765	9.59(5)
57	1	0	0.00	2	0	5d2	3F	Xmatch	37	25973.37	1	1	5d1.6p1	3D	Xmatch	E1	25973.37	3850.10	-0.2697	8.06(7)
57	1	0	0.00	2	0	5d2	3F	Xmatch	38	26414.01	2	1	5d1.6p1	3F	Xmatch	E1	26414.01	3785.87	-0.8328	1.37(7)
57	1	0	0.00	2	0	5d2	3F	Xmatch	39	26837.66	3	1	5d1.6p1	3F	Xmatch	E1	26837.66	3726.11	-1.3915	2.79(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	40	27388.11	2	1	5d1.6p1	3D	Xmatch	E1	27388.11	3651.22	-1.0682	8.55(6)
57	1	0	0.00	2	0	5d2	3F	Xmatch	42	28154.55	1	1	6s1.6p1	3P	Xmatch	E1	28154.55	3551.82	-2.7414	3.20(5)
57	1	0	0.00	2	0	5d2	3F	Xmatch	43	28315.25	3	1	5d1.6p1	3D	Xmatch	E1	28315.25	3531.67	-2.5111	2.36(5)

^aAtomic number.^bIon charge.^cEnergy in cm^{-1} .^dTotal angular momentum.^eParity.^fWavelength in $\text{\AA}$.^gValues given as $A(B) = A \times 10^B$.

APPENDIX B: ENERGY LEVELS OF CALCULATED IONS

In Figs. 17–44 we give an overview of the energy levels for all 28 ions studied in this work. Instead of showing the electronic configuration bands, we display energy levels split into parity and angular momentum J , as these are the true quantum numbers and they do not depend on mixing between configurations. Particularly, at high-level energies, multiple electronic configurations contribute on a similar level to the eigenvector compositions, making it challenging to assign the energy level to one specific configuration.

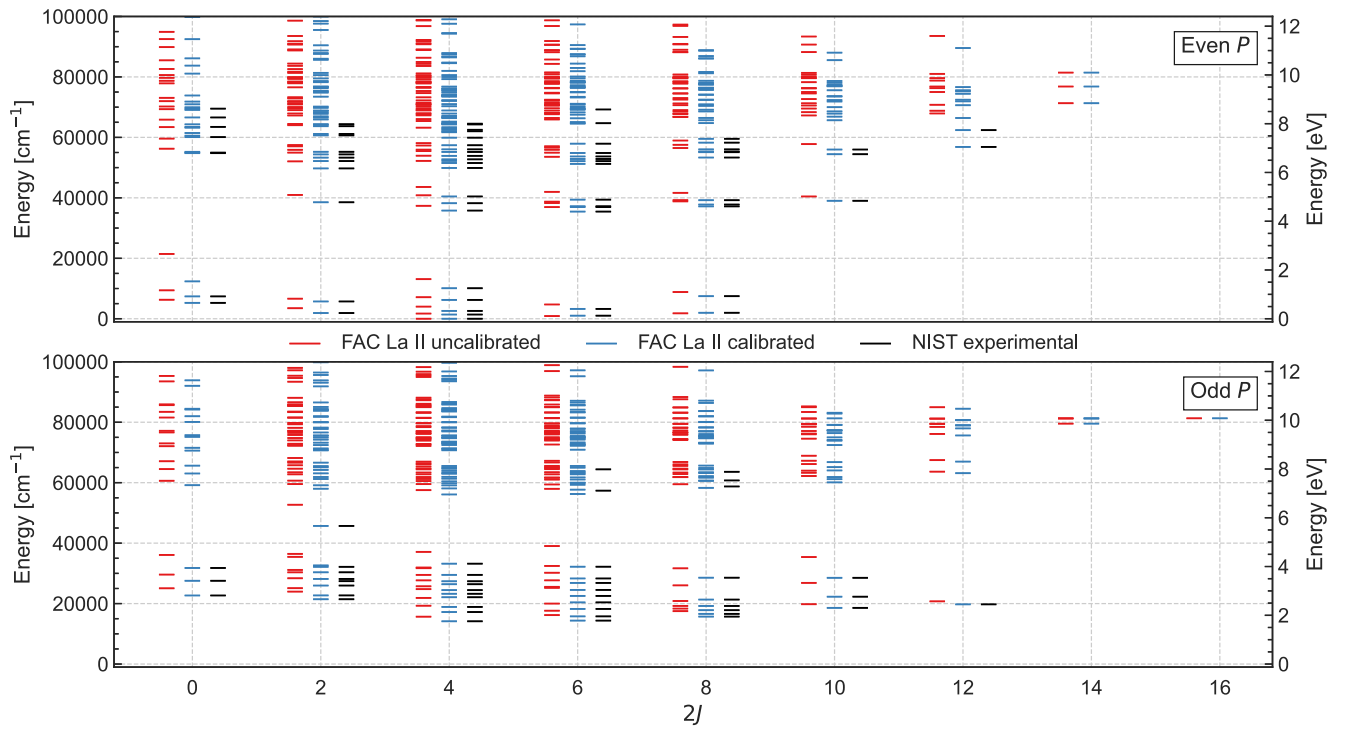


FIG. 17. Energy levels for La II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

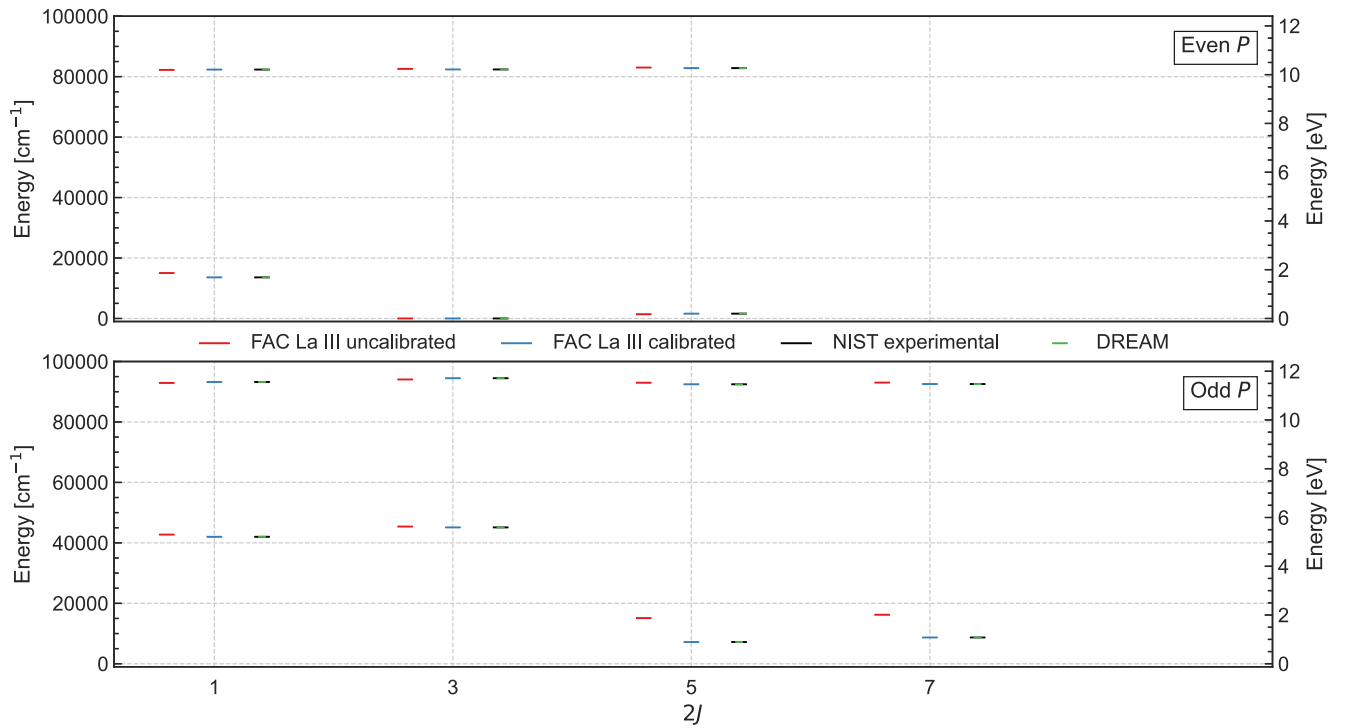


FIG. 18. Energy levels for La III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

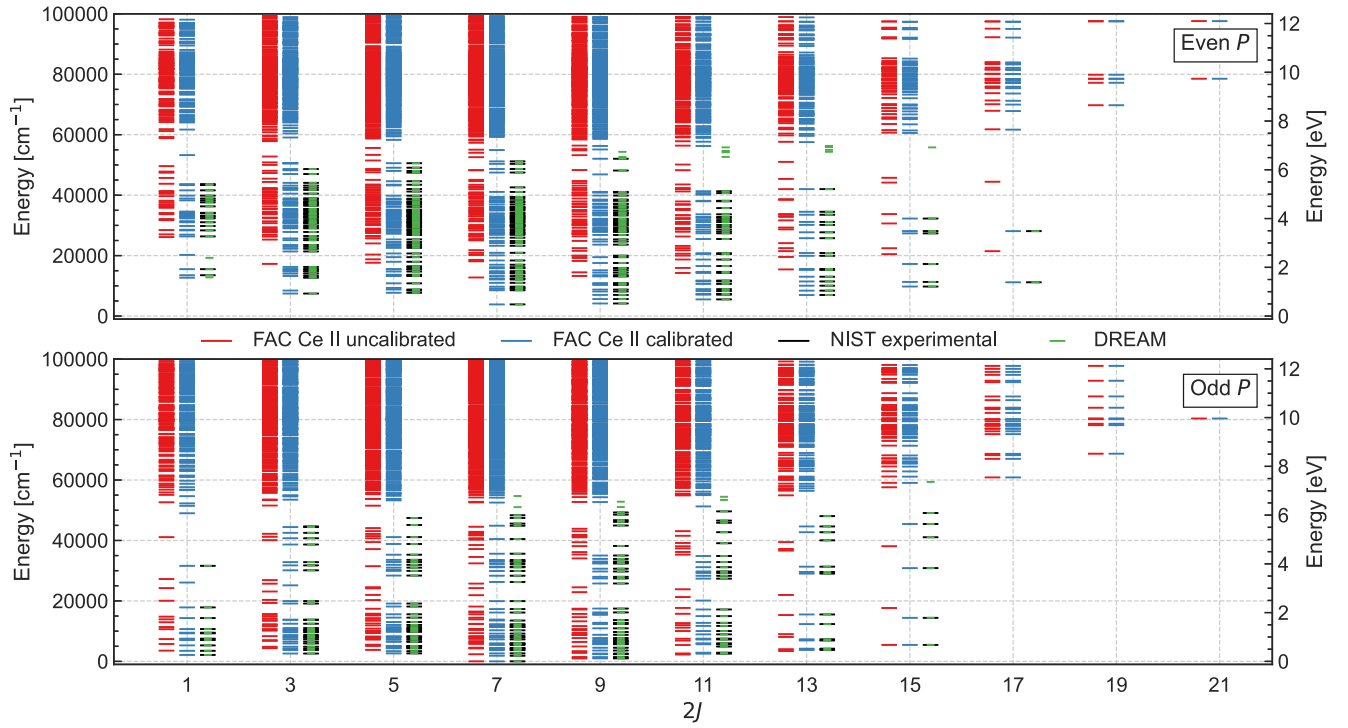


FIG. 19. Energy levels for Ce ii for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

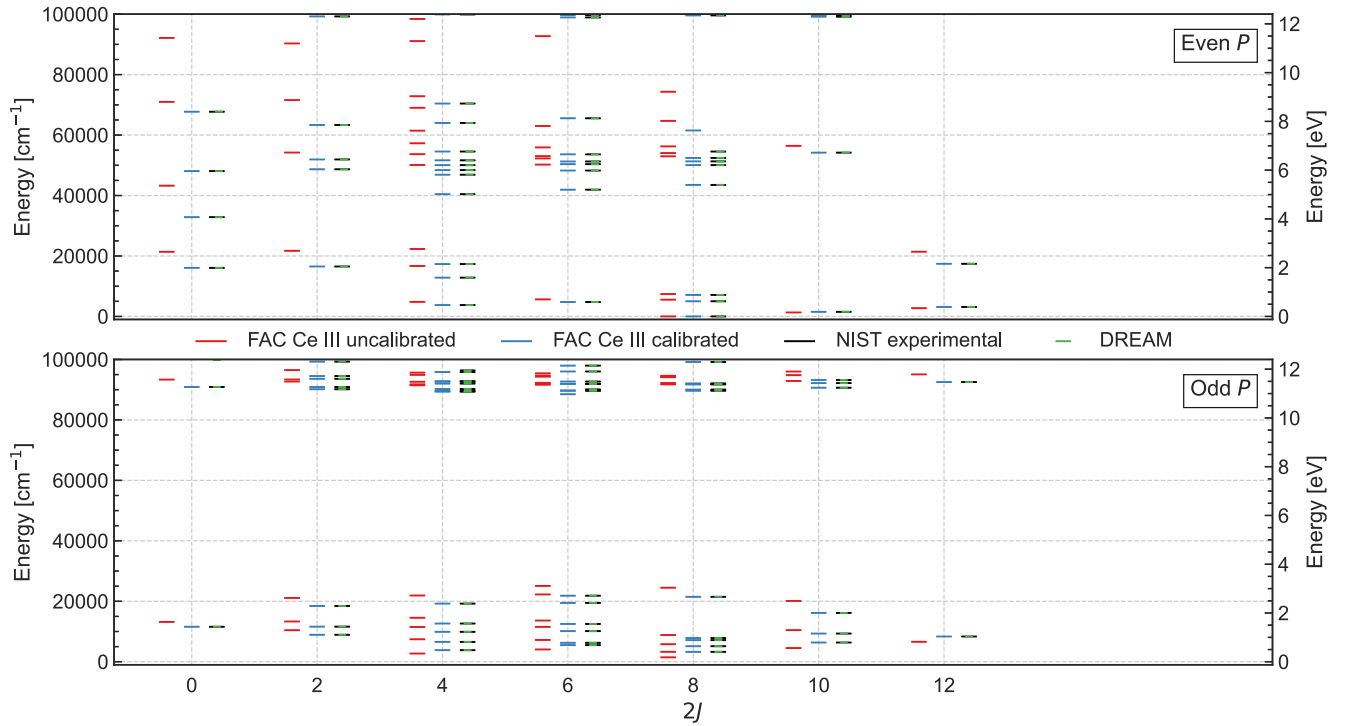


FIG. 20. Energy levels for Ce iii for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

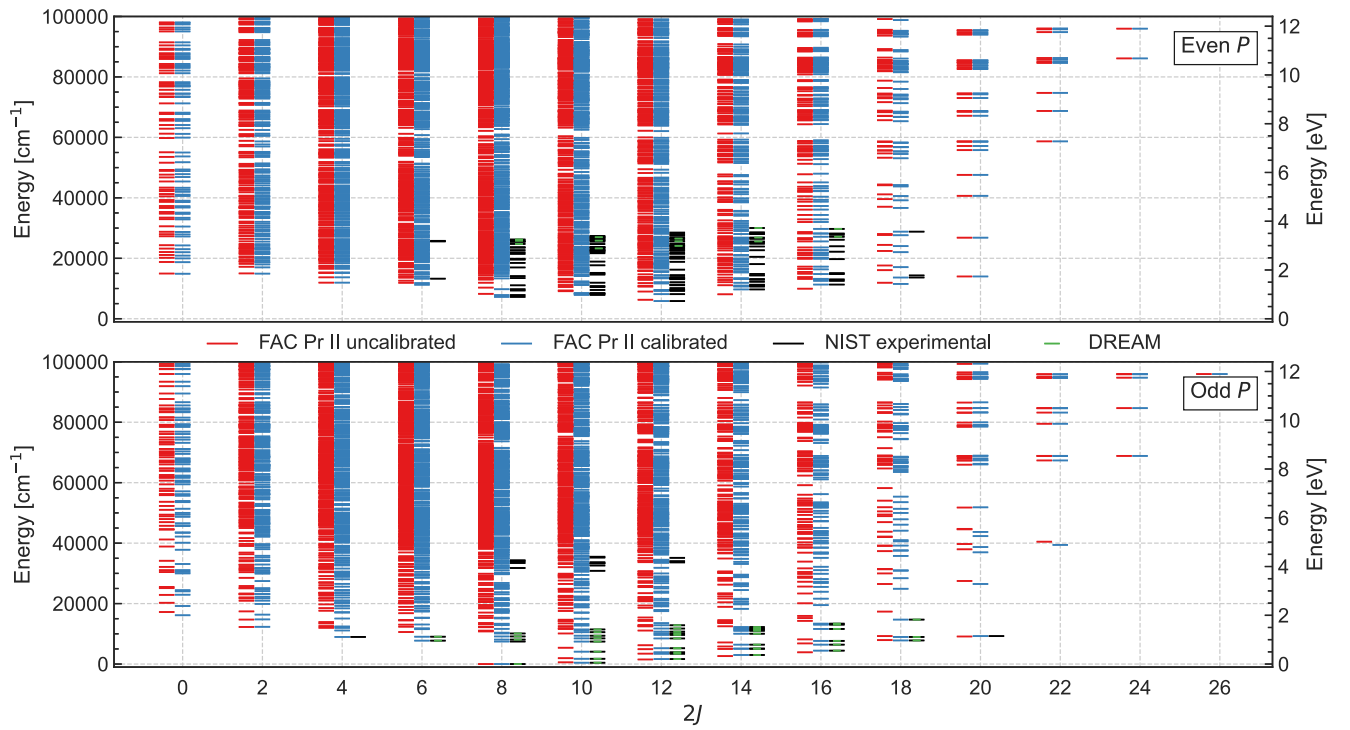


FIG. 21. Energy levels for Pr II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

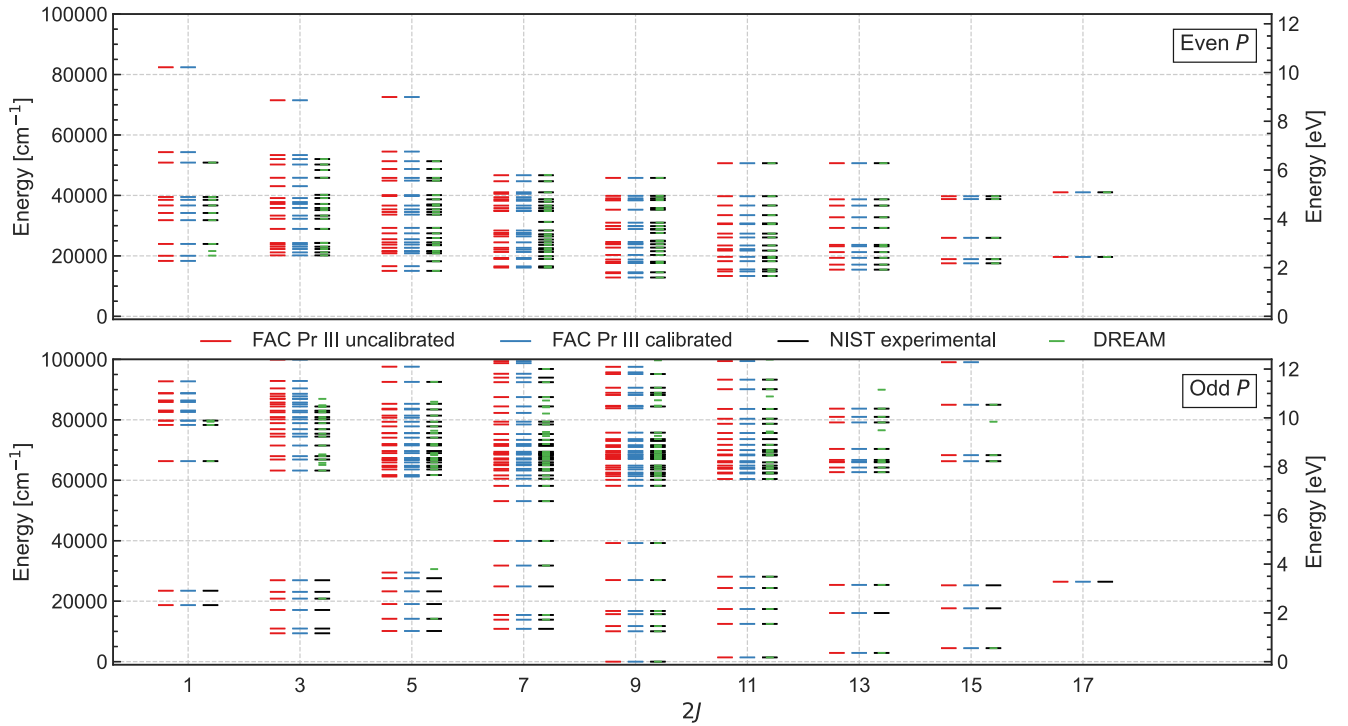


FIG. 22. Energy levels for Pr III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

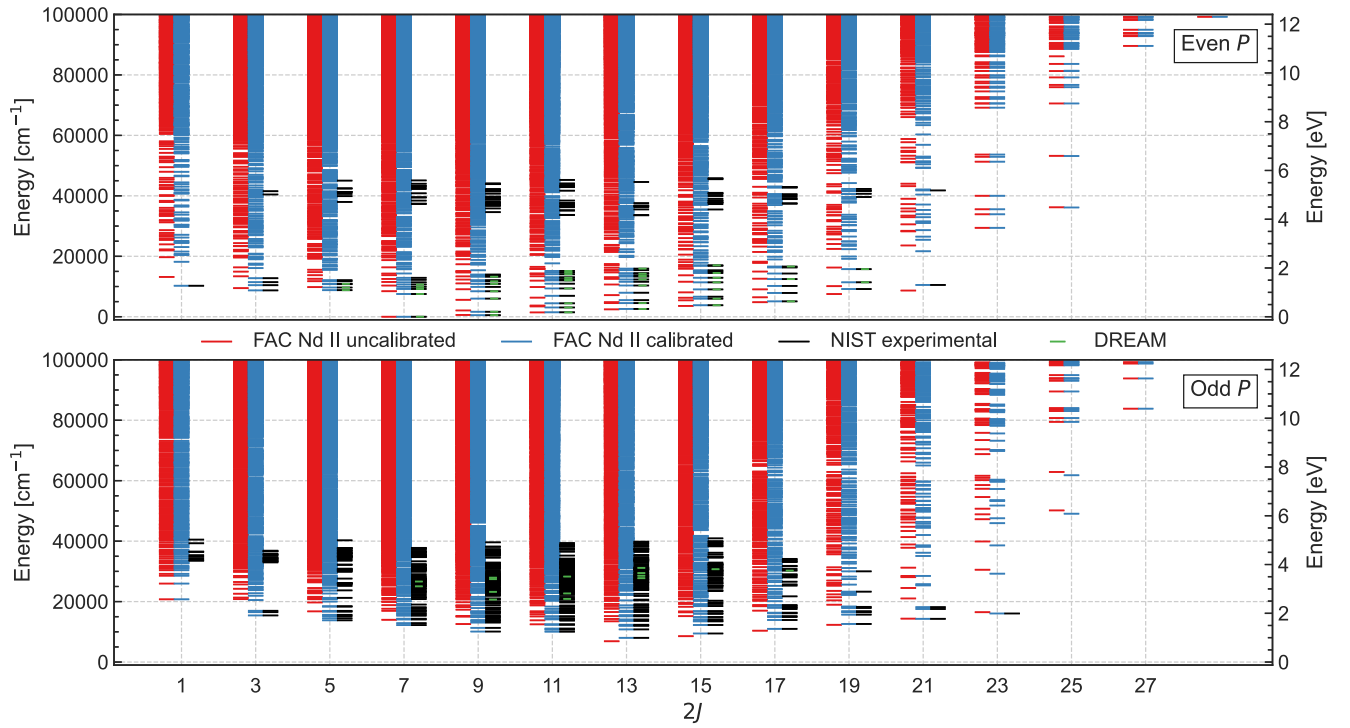


FIG. 23. Energy levels for Nd II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

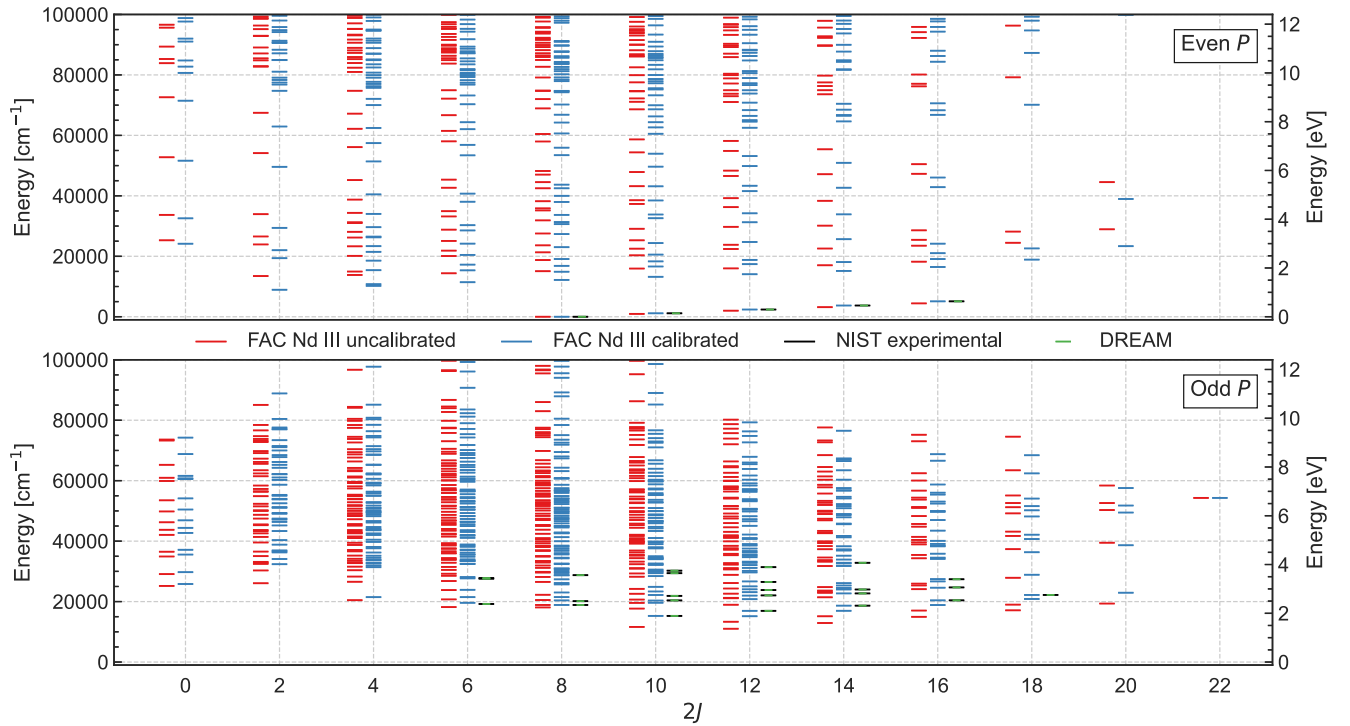


FIG. 24. Energy levels for Nd III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green. In contrast to Fig. 3, this shows the calibration to NIST data only.

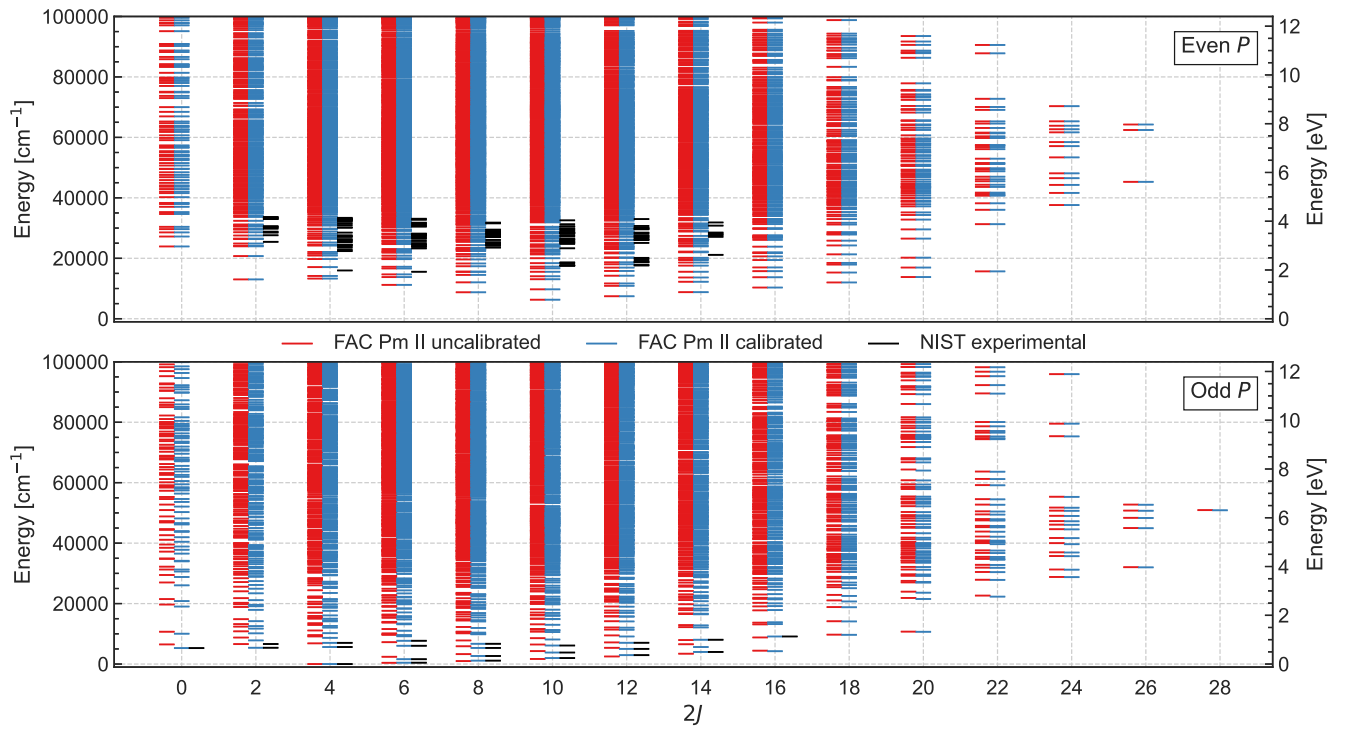


FIG. 25. Energy levels for Pm II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

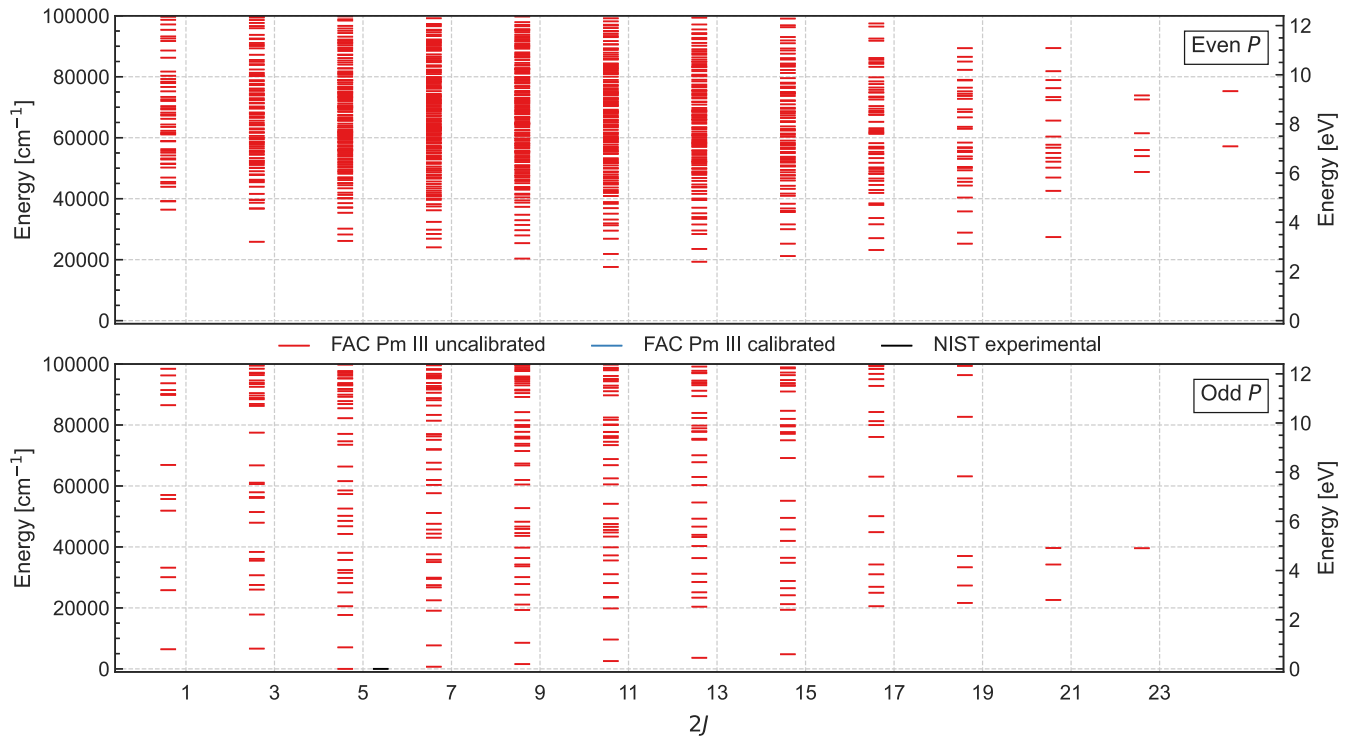


FIG. 26. Energy levels for Pm III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

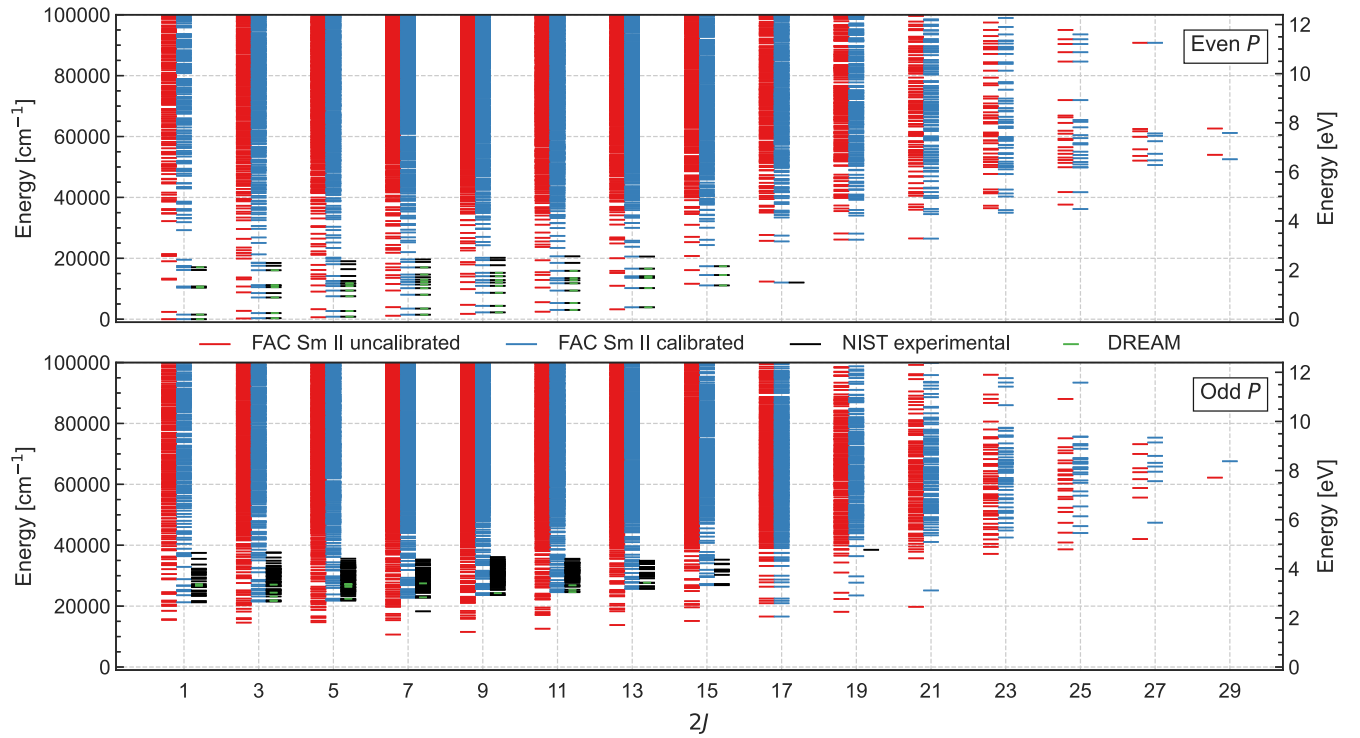


FIG. 27. Energy levels for Sm II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

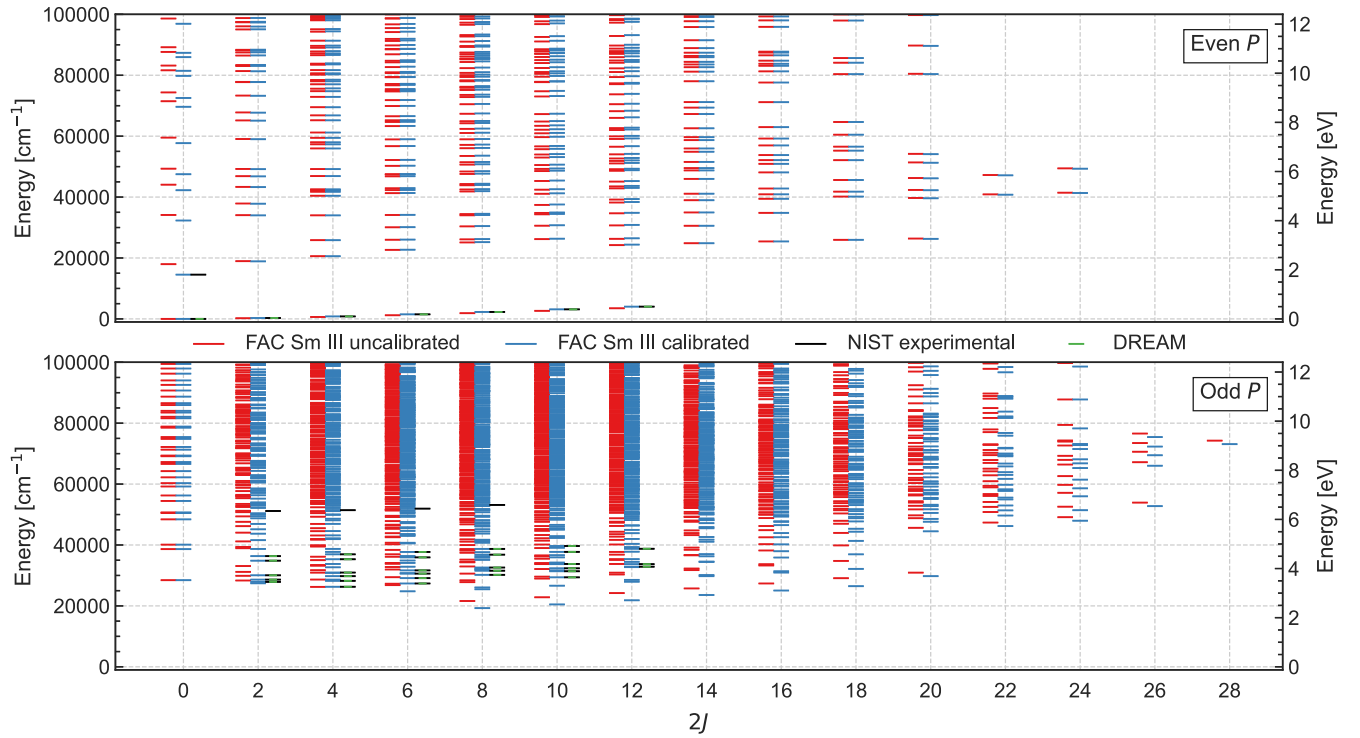


FIG. 28. Energy levels for Sm III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

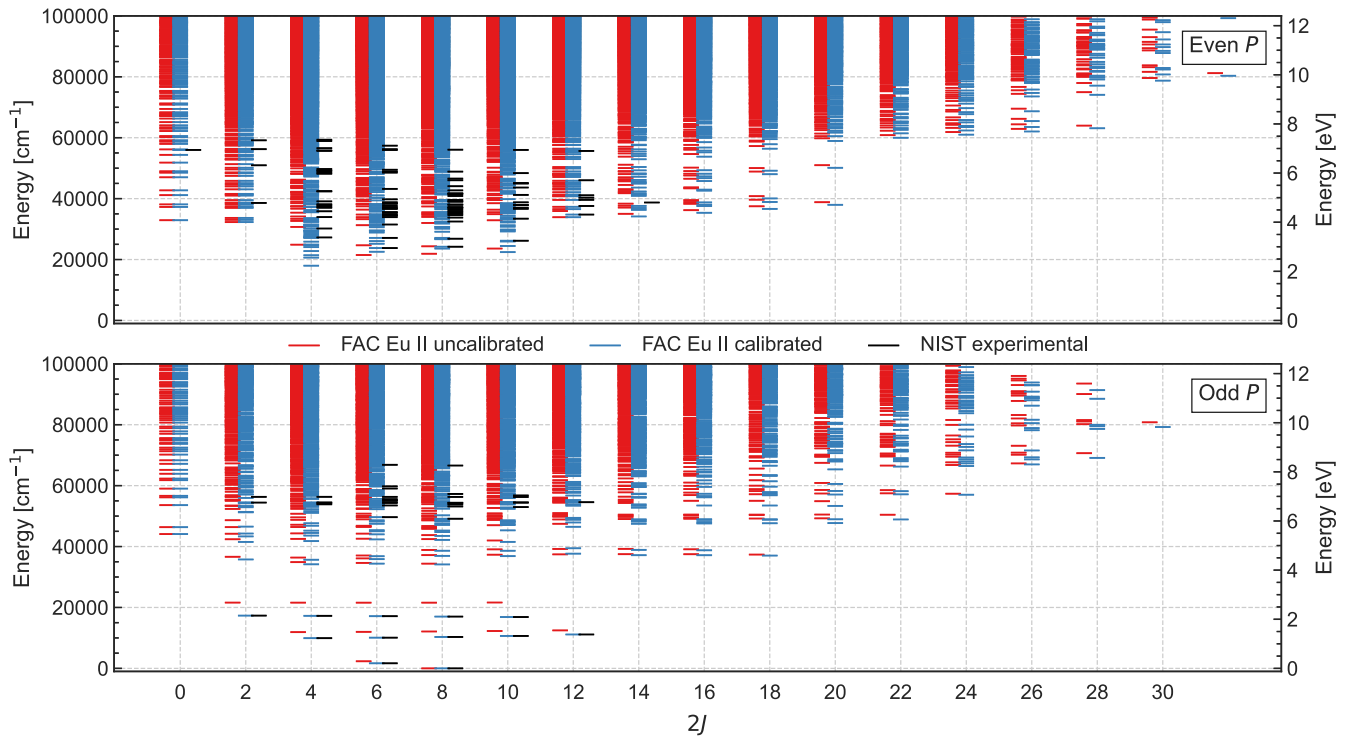


FIG. 29. Energy levels for Eu II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

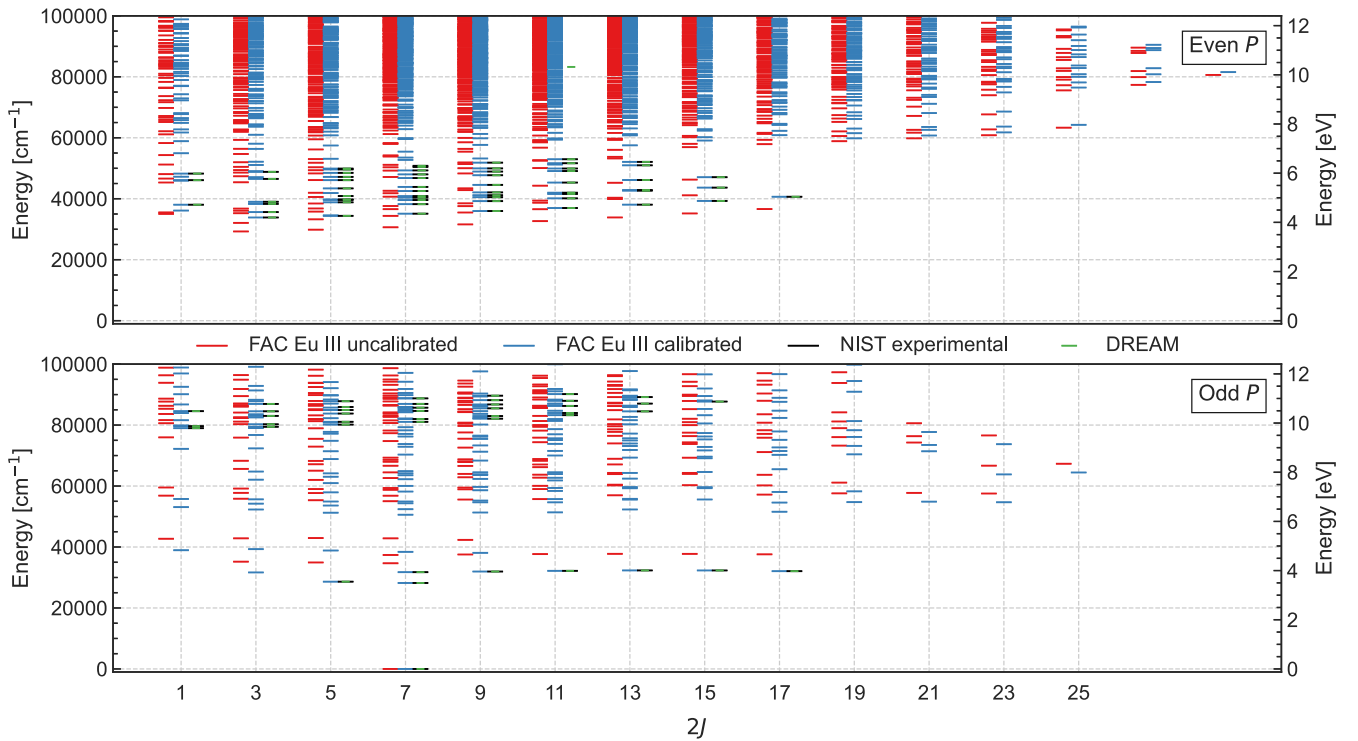


FIG. 30. Energy levels for Eu III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

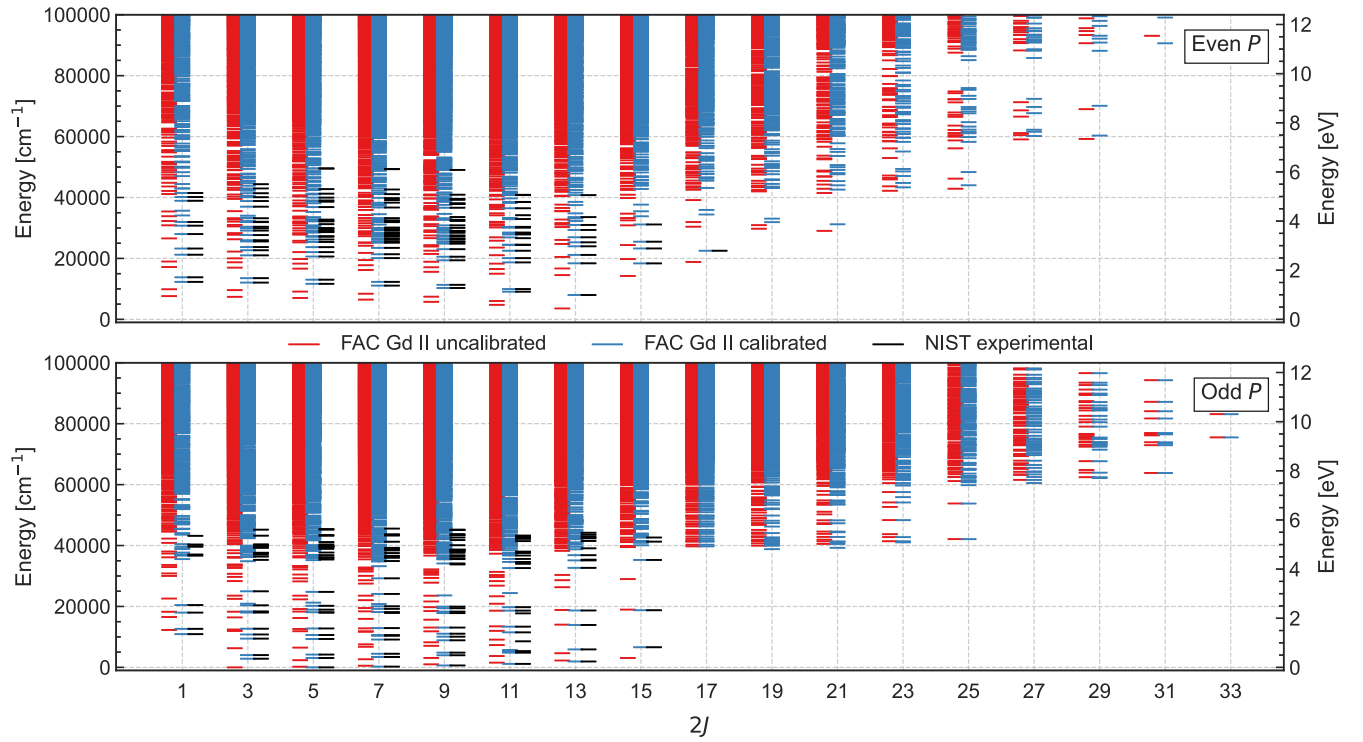


FIG. 31. Energy levels for Gd II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

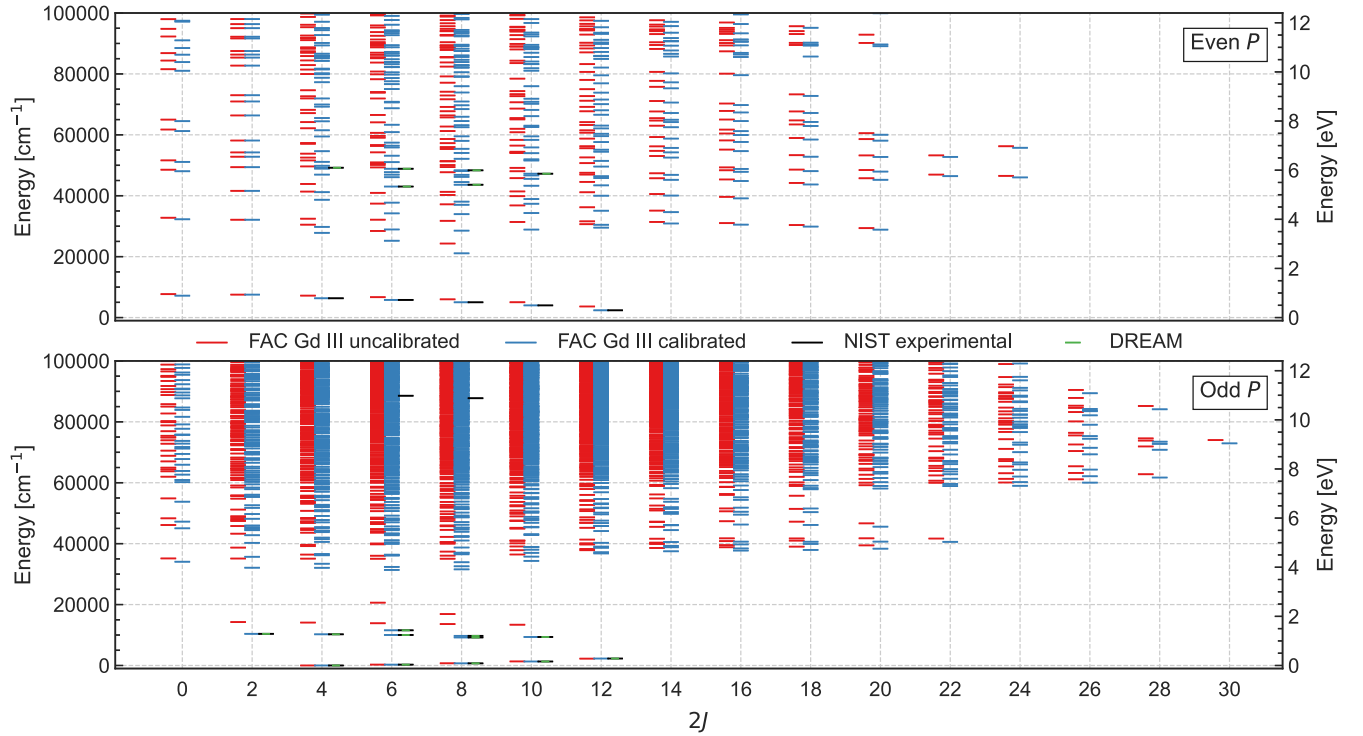


FIG. 32. Energy levels for Gd III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

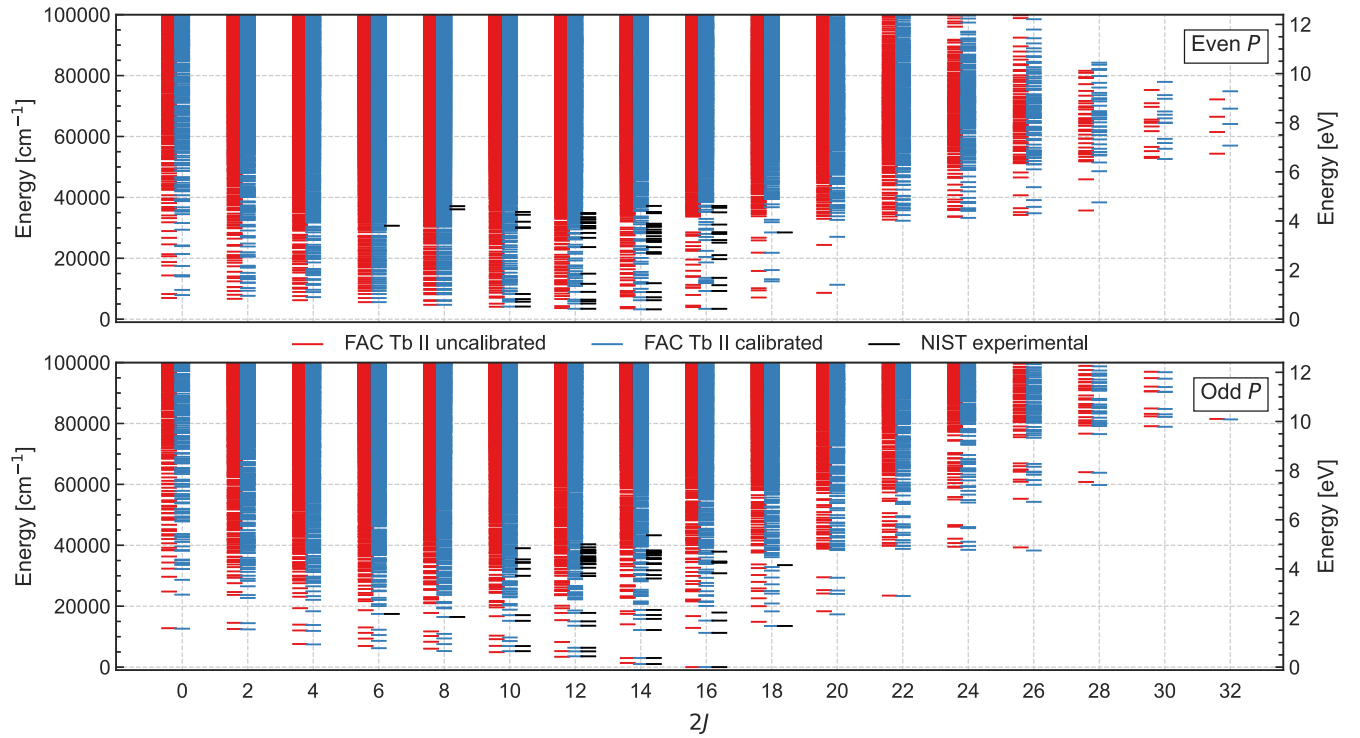


FIG. 33. Energy levels for Tb II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

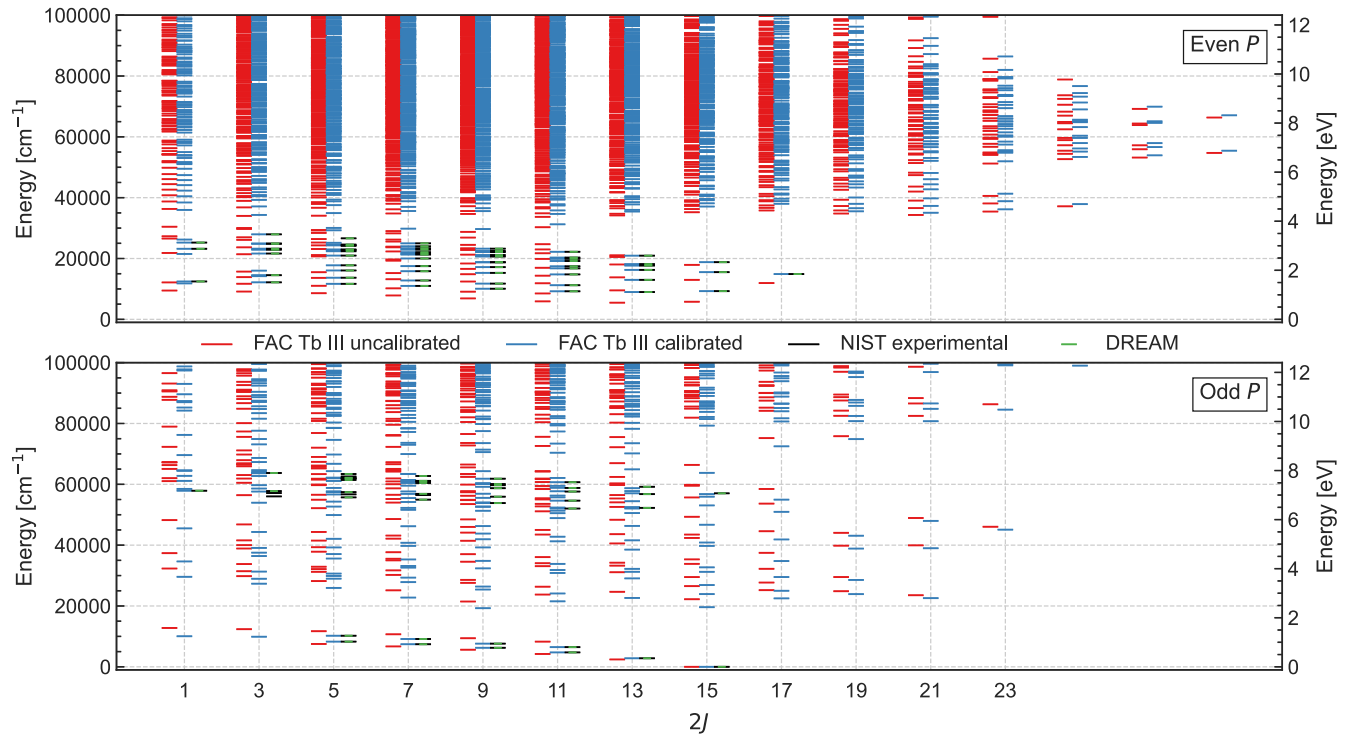


FIG. 34. Energy levels for Tb III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

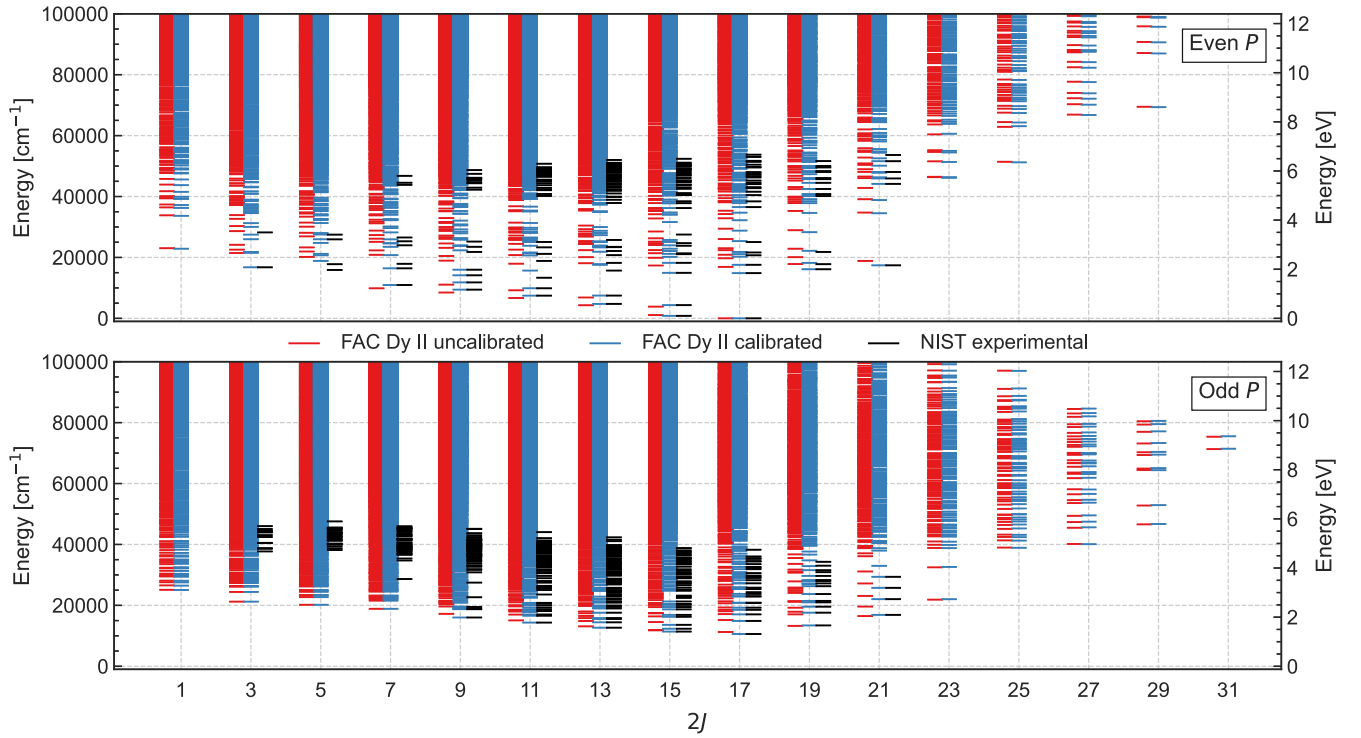


FIG. 35. Energy levels for Dy II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

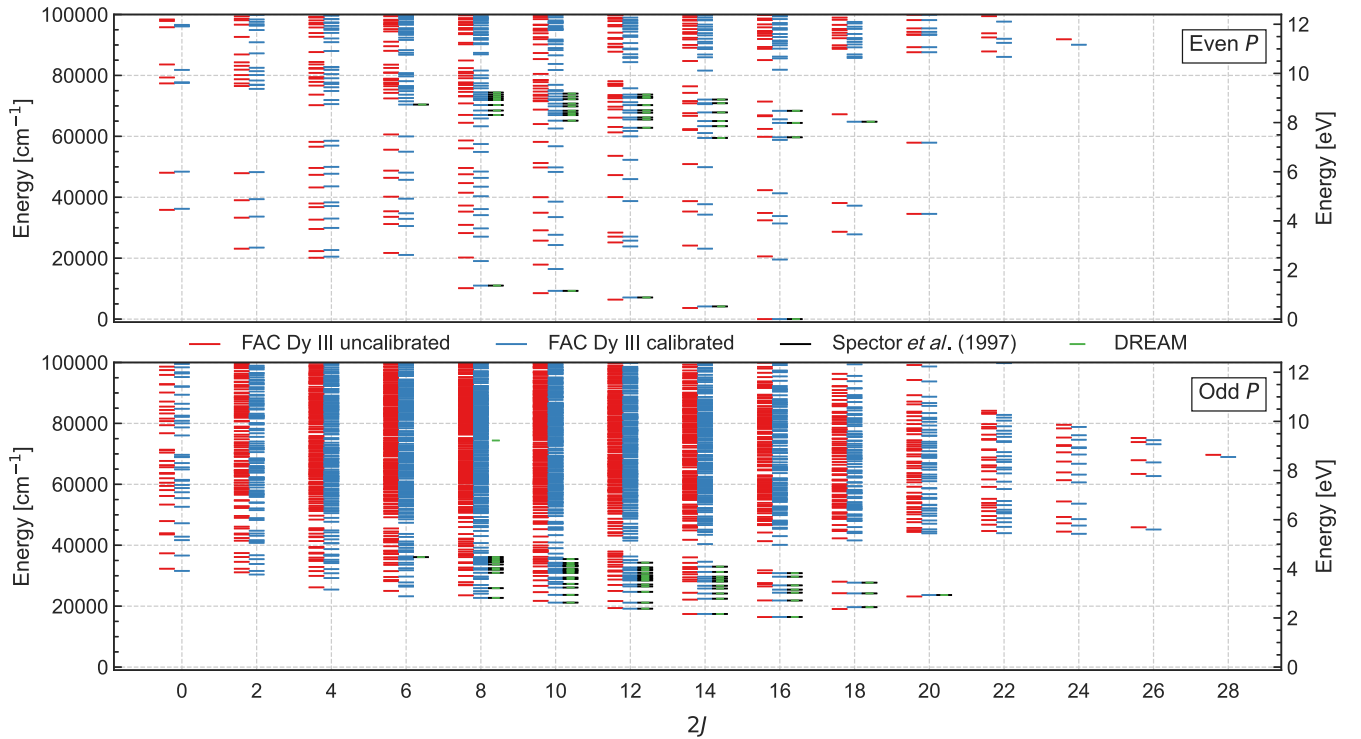


FIG. 36. Energy levels for Dy III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

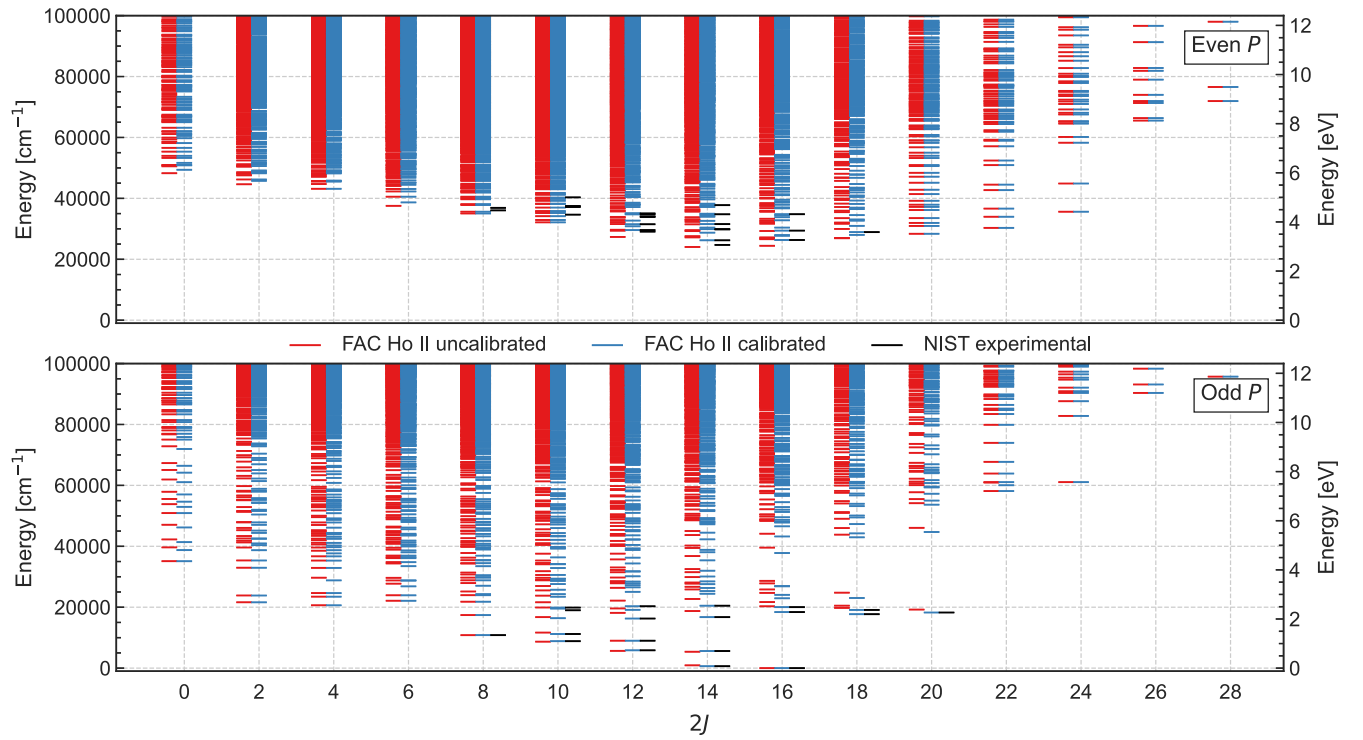


FIG. 37. Energy levels for Ho II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels.

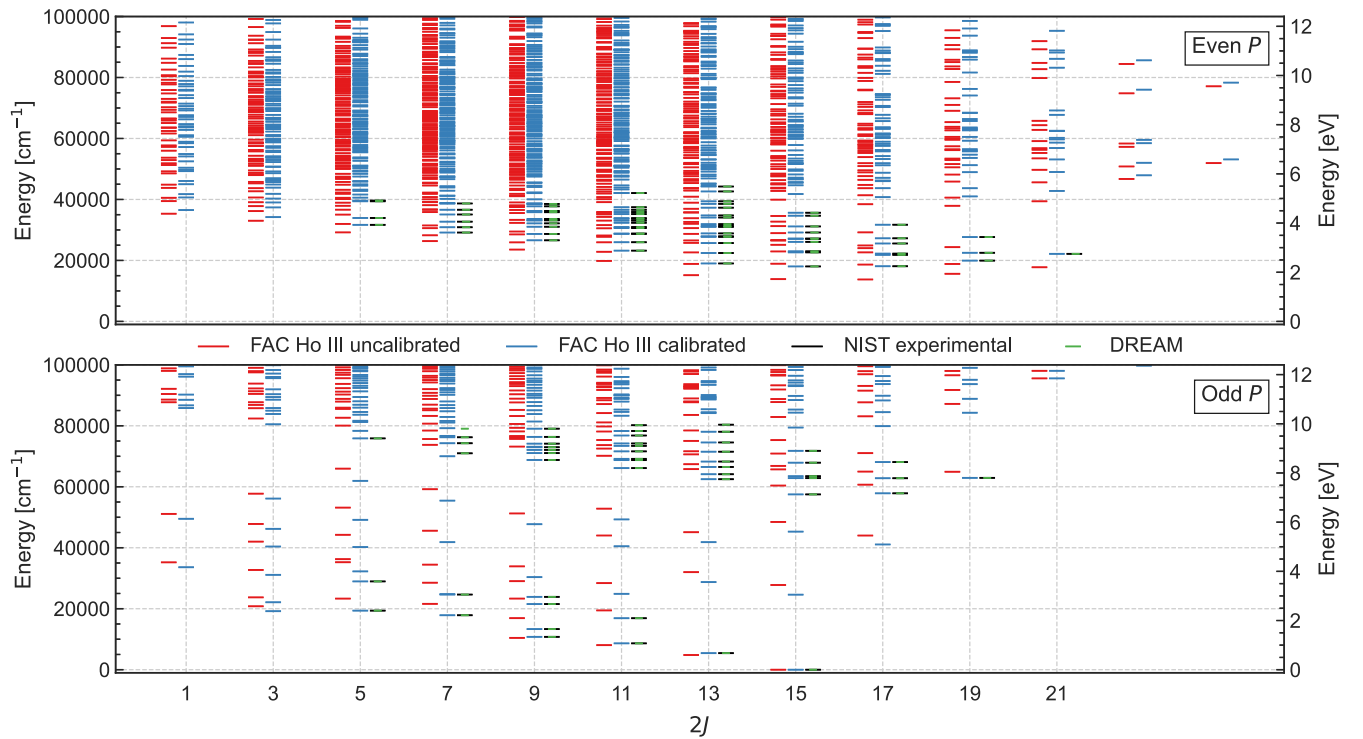


FIG. 38. Energy levels for Ho III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

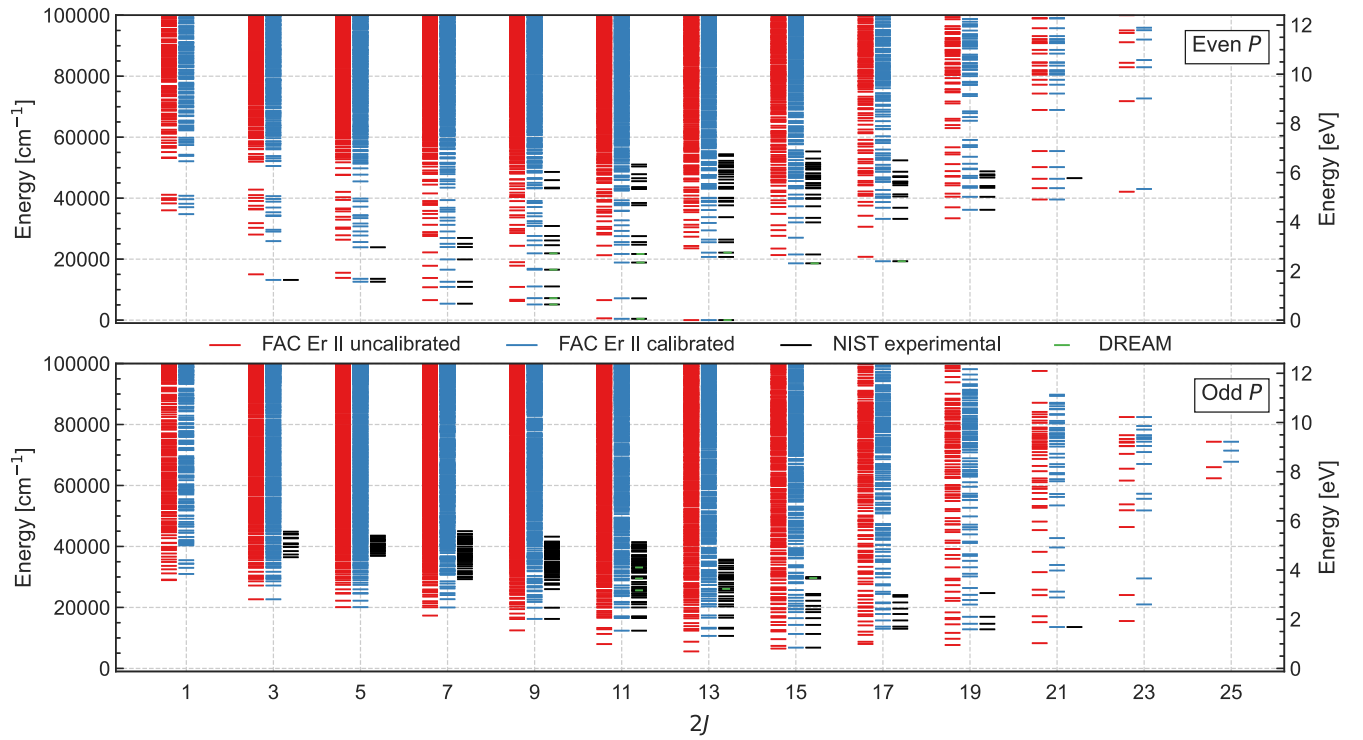


FIG. 39. Energy levels for Er II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

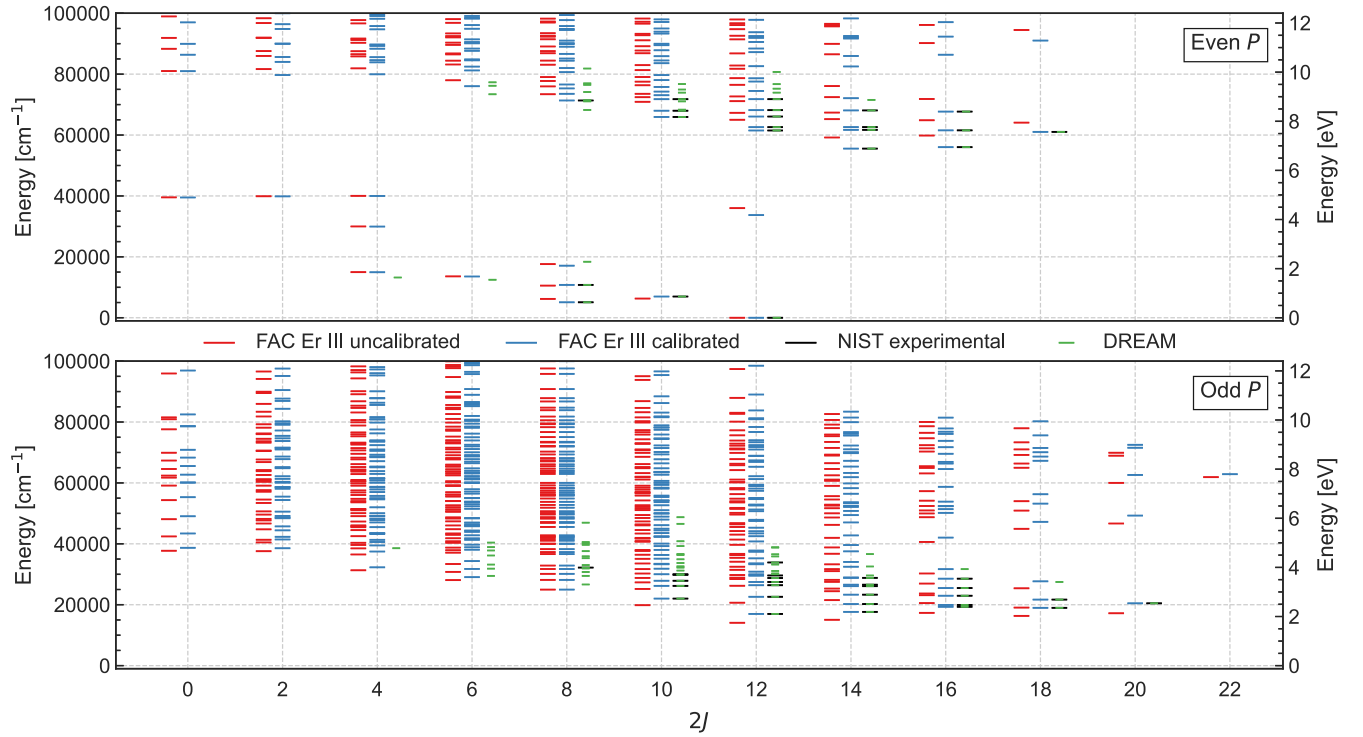


FIG. 40. Energy levels for Er III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

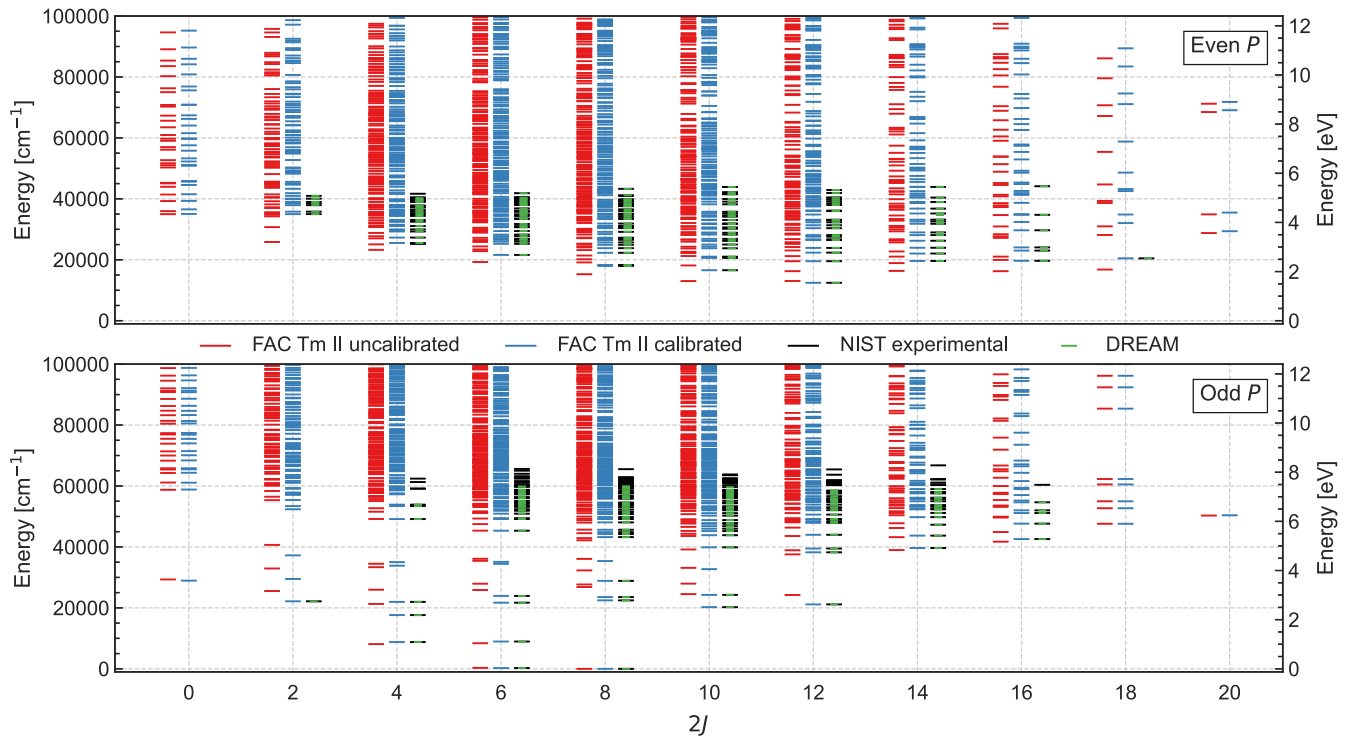


FIG. 41. Energy levels for Tm II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

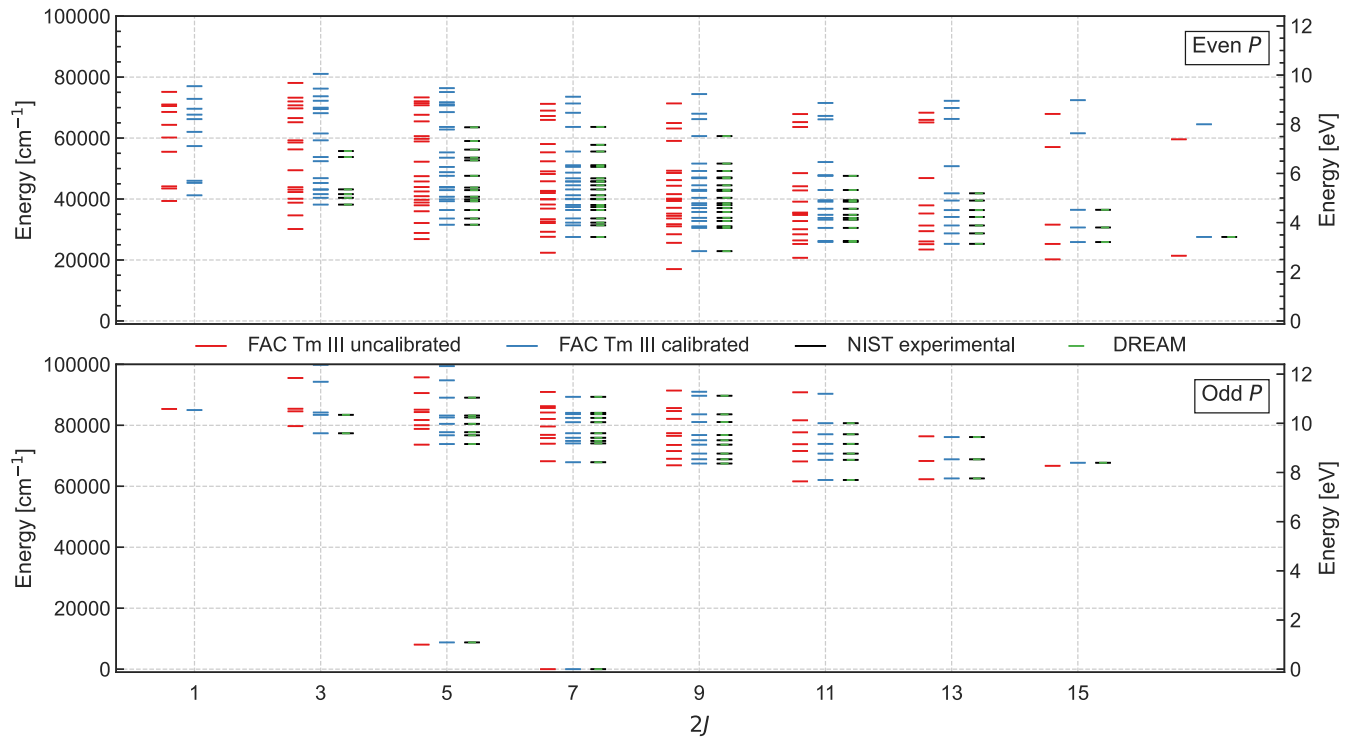


FIG. 42. Energy levels for Tm III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

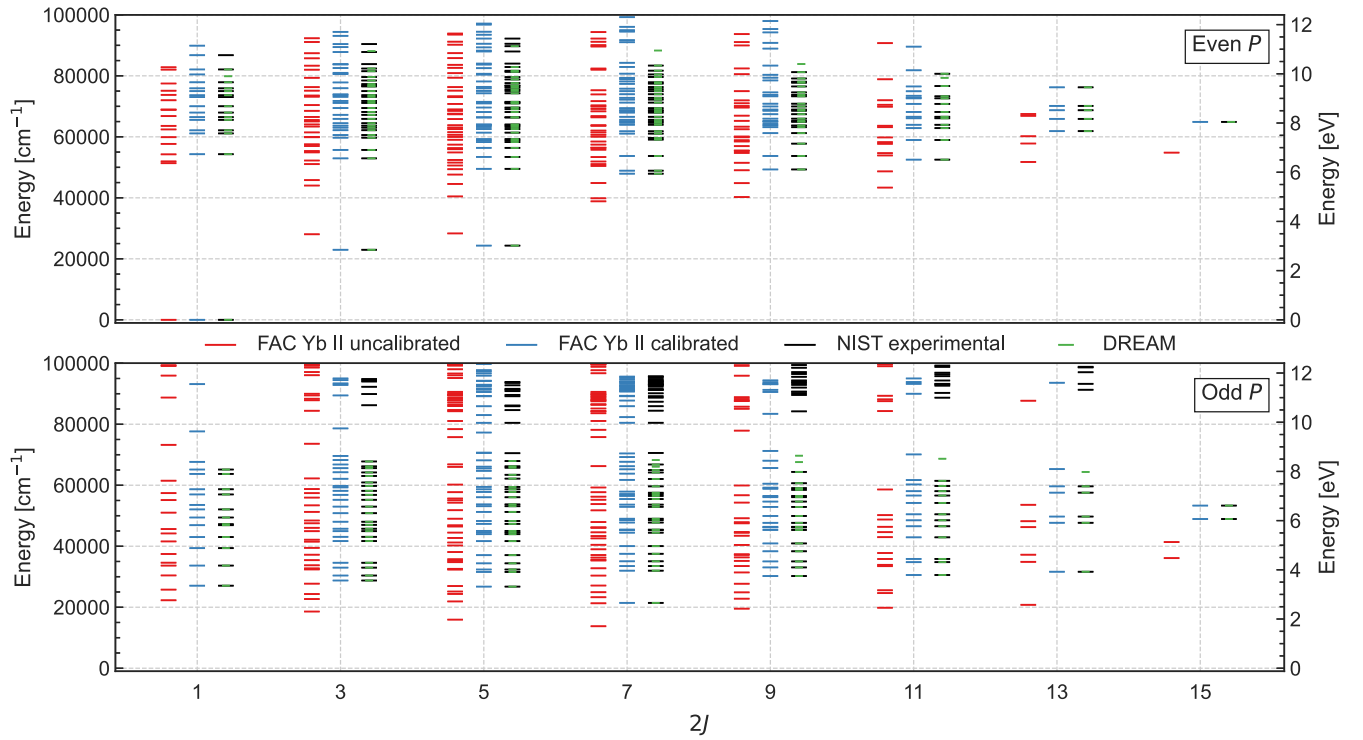


FIG. 43. Energy levels for Yb II for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

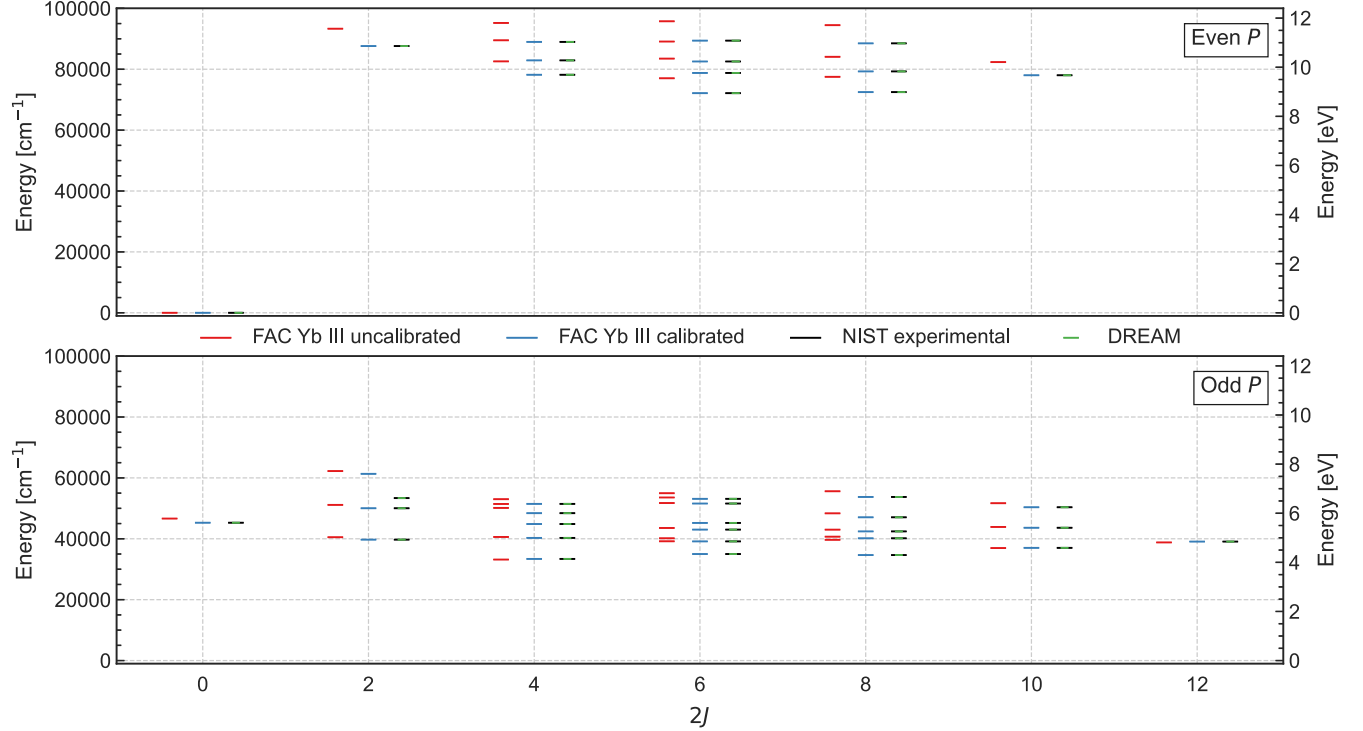


FIG. 44. Energy levels for Yb III for even (top) and odd (bottom) parity for the model given in Table I using the FAC code. Red horizontal lines indicate the initial model, while blue lines indicate the level energies of the calibrated model. Black horizontal lines show experimental data from the NIST database [65] used to calibrate the calculated levels. Levels present in the DREAM database are shown in green.

- [1] D. A. Coulter *et al.*, Swope Supernova Survey 2017a (SSS17a), The optical counterpart to a gravitational wave source, *Science* **358**, 1556 (2017).
- [2] P. S. Cowperthwaite *et al.*, The electromagnetic counterpart of the binary neutron star merger LIGO/Virgo GW170817. II. UV, Optical, and near-infrared light curves and comparison to kilonova models, *Astrophys. J. Lett.* **848**, L17 (2017).
- [3] S. J. Smartt *et al.*, A kilonova as the electromagnetic counterpart to a gravitational-wave source, *Nature (London)* **551**, 75 (2017).
- [4] M. R. Drout *et al.*, Light curves of the neutron star merger GW170817/SSS17a: Implications for r-process nucleosynthesis, *Science* **358**, 1570 (2017).
- [5] Y. Utsumi *et al.*, J-GEM observations of an electromagnetic counterpart to the neutron star merger GW170817, *Publ. Astron. Soc. Jpn.* **69**, 101 (2017).
- [6] B. P. Abbott *et al.*, Multi-messenger observations of a binary neutron star merger, *Astrophys. J. Lett.* **848**, L12 (2017).
- [7] B. P. Abbott *et al.*, GW170817: Observation of gravitational waves from a binary neutron star inspiral, *Phys. Rev. Lett.* **119**, 161101 (2017).
- [8] J. M. Lattimer and D. N. Schramm, Black-hole-neutron-star collisions, *Astrophys. J. Lett.* **192**, L145 (1974).
- [9] E. Symbalisty and D. N. Schramm, Neutron star collisions and the r-process, *Astrophys. Lett.* **22**, 143 (1982), <https://ui.adsabs.harvard.edu/abs/1982ApL....22..143S/abstract>.
- [10] D. Eichler, M. Livio, T. Piran, and D. N. Schramm, Nucleosynthesis, neutrino bursts and γ -rays from coalescing neutron stars, *Nature (London)* **340**, 126 (1989).
- [11] C. Freiburghaus, S. Rosswog, and F. K. Thielemann, R-process in neutron star mergers, *Astrophys. J. Lett.* **525**, L121 (1999).
- [12] S. Goriely, A. Bauswein, and H.-T. Janka, R-process nucleosynthesis in dynamically ejected matter of neutron star mergers, *Astrophys. J. Lett.* **738**, L32 (2011).
- [13] A. Bauswein, T. W. Baumgarte, and H. T. Janka, Prompt merger collapse and the maximum mass of neutron stars, *Phys. Rev. Lett.* **111**, 131101 (2013).
- [14] S. Wanajo, Y. Sekiguchi, N. Nishimura, K. Kiuchi, K. Kyutoku, and M. Shibata, Production of all the r-process nuclides in the dynamical ejecta of neutron star mergers, *Astrophys. J. Lett.* **789**, L39 (2014).
- [15] L.-X. Li and B. Paczyński, Transient events from neutron star mergers, *Astrophys. J. Lett.* **507**, L59 (1998).
- [16] S. R. Kulkarni, Modeling supernova-like explosions associated with gamma-ray bursts with short durations, *arXiv: astro-ph/0510256*.
- [17] B. D. Metzger, G. Martínez-Pinedo, S. Darbha, E. Quataert, A. Arcones, D. Kasen, R. Thomas, P. Nugent, I. V. Panov, and N. T. Zinner, Electromagnetic counterparts of compact object mergers powered by the radioactive decay of r-process nuclei, *Mon. Not. R. Astron. Soc.* **406**, 2650 (2010).
- [18] D. Kasen, N. R. Badnell, and J. Barnes, Opacities and spectra of the r-process ejecta from neutron star mergers, *Astrophys. J.* **774**, 25 (2013).
- [19] M. Tanaka and K. Hotokezaka, Radiative transfer simulations of neutron star merger ejecta, *Astrophys. J.* **775**, 113 (2013).
- [20] B. D. Metzger and R. Fernández, Red or blue? A potential kilonova imprint of the delay until black hole formation following a neutron star merger, *Mon. Not. R. Astron. Soc.* **441**, 3444 (2014).
- [21] D. Kasen, B. Metzger, J. Barnes, E. Quataert, and E. Ramirez-Ruiz, Origin of the heavy elements in binary neutron-star mergers from a gravitational-wave event, *Nature (London)* **551**, 80 (2017).
- [22] J. Barnes, D. Kasen, M.-R. Wu, and G. Martínez-Pinedo, Radioactivity and thermalization in the ejecta of compact object mergers and their impact on kilonova light curves, *Astrophys. J.* **829**, 110 (2016).
- [23] M. Tanaka, D. Kato, G. Gaigalas, P. Rynkun, L. Radžičūtė, S. Wanajo, Y. Sekiguchi, N. Nakamura, H. Tanuma, I. Murakami, and H. A. Sakaue, Properties of kilonovae from dynamical and post-merger ejecta of neutron star mergers, *Astrophys. J.* **852**, 109 (2018).
- [24] M. Tanaka, D. Kato, G. Gaigalas, and K. Kawaguchi, Systematic opacity calculations for kilonovae, *Mon. Not. R. Astron. Soc.* **496**, 1369 (2020).
- [25] M. Bulla, POSSIS: Predicting spectra, light curves, and polarization for multidimensional models of supernovae and kilonovae, *Mon. Not. R. Astron. Soc.* **489**, 5037 (2019).
- [26] L. J. Shingles, C. E. Collins, V. Vijayan, A. Flörs, O. Just, G. Leck, Z. Xiong, A. Bauswein, G. Martínez-Pinedo, and S. A. Sim, Self-consistent 3D radiative transfer for kilonovae: Directional spectra from merger simulations, *Astrophys. J. Lett.* **954**, L41 (2023).
- [27] C. E. Collins, L. J. Shingles, A. Bauswein, S. A. Sim, T. Soutanis, V. Vijayan, A. Flörs, O. Just, G. Leck, G. Lioutas, G. Martínez-Pinedo, A. Snepken, D. Watson, and Z. Xiong, Towards inferring the geometry of kilonovae, *Mon. Not. R. Astron. Soc.* **529**, 1333 (2024).
- [28] A. Kitamura, K. Kawaguchi, M. Tanaka, and S. Fujibayashi, Linking analytic light-curve models to physical properties of kilonovae, *Astrophys. J.* **982**, 97 (2025).
- [29] J. Barnes, Y. L. Zhu, K. A. Lund, T. M. Sprouse, N. Vassh, G. C. McLaughlin, M. R. Mumpower, and R. Surman, Kilonovae across the nuclear physics landscape: The impact of nuclear physics uncertainties on r-process-powered emission, *Astrophys. J.* **918**, 44 (2021).
- [30] J. Barnes and D. Kasen, Effect of a high opacity on the light curves of radioactively powered transients from compact object mergers, *Astrophys. J.* **775**, 18 (2013).
- [31] D. Kasen, R. Fernández, and B. D. Metzger, Kilonova light curves from the disc wind outflows of compact object mergers, *Mon. Not. R. Astron. Soc.* **450**, 1777 (2015).
- [32] C. J. Fontes, C. L. Fryer, A. L. Hungerford, P. Hakel, J. Colgan, D. P. Kilcrease, and M. E. Sherrill, Relativistic opacities for astrophysical applications, *High Energy Density Phys.* **16**, 53 (2015).
- [33] S. Banerjee, M. Tanaka, K. Kawaguchi, D. Kato, and G. Gaigalas, Simulations of early kilonova emission from neutron star mergers, *Astrophys. J.* **901**, 29 (2020).
- [34] H. Carvajal Gallego, J. C. Berengut, P. Palmeri, and P. Quinet, Large-scale atomic data calculations in Ce V—X ions for application to early kilonova emission from neutron star mergers, *Mon. Not. R. Astron. Soc.* **509**, 6138 (2022).

- [35] H. Carvajal Gallego, J. C. Berengut, P. Palmeri, and P. Quinet, Atomic data and opacity calculations in La V-X ions for the investigation of kilonova emission spectra, *Mon. Not. R. Astron. Soc.* **513**, 2302 (2022).
- [36] S. Banerjee, M. Tanaka, D. Kato, G. Gaigalas, K. Kawaguchi, and N. Domoto, Opacity of the highly ionized lanthanides and the effect on the early eilonova, *Astrophys. J.* **934**, 117 (2022).
- [37] H. Carvajal Gallego, J. Deprince, J. C. Berengut, P. Palmeri, and P. Quinet, Opacity calculations in four to nine times ionized Pr, Nd, and Pm atoms for the spectral analysis of kilonovae, *Mon. Not. R. Astron. Soc.* **518**, 332 (2023).
- [38] S. Banerjee, M. Tanaka, D. Kato, and G. Gaigalas, Diversity of early kilonova with the realistic opacities of highly ionized heavy elements, *Astrophys. J.* **968**, 64 (2024).
- [39] H. Carvajal Gallego, J. Deprince, L. Maison, P. Palmeri, and P. Quinet, Overview of the contributions from all lanthanide elements to kilonova opacity in the temperature range from 25 000 to 40 000 K, *Astron. Astrophys.* **685**, A91 (2024).
- [40] G. Gaigalas, P. Rynkun, L. Radžiūtė, D. Kato, M. Tanaka, and P. Jönsson, Energy level structure and transition data of Er^{2+} , *Astrophys. J. Suppl. Ser.* **248**, 13 (2020).
- [41] H. Carvajal Gallego, P. Palmeri, and P. Quinet, Multi-configuration Dirac-Hartree-Fock radiative parameters for emission lines in Ce II-IV ions and cerium opacity calculations for kilonovae, *Mon. Not. R. Astron. Soc.* **501**, 1440 (2021).
- [42] J. H. Gillanders, M. McCann, S. A. Sim, S. J. Smartt, and C. P. Ballance, Constraints on the presence of platinum and gold in the spectra of the kilonova AT2017gfo, *Mon. Not. R. Astron. Soc.* **506**, 3560 (2021).
- [43] R. F. Silva, J. M. Sampaio, P. Amaro, A. Flörs, G. Martínez-Pinedo, and J. P. Marques, Structure calculations in Nd III and U III relevant for kilonovae modelling, *Atoms* **10**, 18 (2022).
- [44] A. Flörs, R. F. Silva, J. Deprince, H. Carvajal Gallego, G. Leck, L. J. Shingles, G. Martínez-Pinedo, J. M. Sampaio, P. Amaro, J. P. Marques, S. Goriely, P. Quinet, P. Palmeri, and M. Godefroid, Opacities of singly and doubly ionized neodymium and uranium for kilonova emission modeling, *Mon. Not. R. Astron. Soc.* **524**, 3083 (2023).
- [45] G. Gaigalas, P. Rynkun, N. Domoto, M. Tanaka, D. Kato, and L. Kitovienė, Theoretical investigation of energy levels and transitions for Ce III with applications to kilonova spectra, *Mon. Not. R. Astron. Soc.* **530**, 5220 (2024).
- [46] C. J. Fontes, C. L. Fryer, A. L. Hungerford, R. T. Wollaeger, and O. Korobkin, A line-binned treatment of opacities for the spectra and light curves from neutron star mergers, *Mon. Not. R. Astron. Soc.* **493**, 4143 (2020).
- [47] L. Radžiūtė, G. Gaigalas, D. Kato, P. Rynkun, and M. Tanaka, Extended calculations of energy levels and transition rates for singly ionized lanthanide elements. I. Pr-Gd, *Astrophys. J. Suppl. Ser.* **248**, 17 (2020).
- [48] L. Radžiūtė, G. Gaigalas, D. Kato, P. Rynkun, and M. Tanaka, Extended calculations of energy levels and transition rates for singly ionized lanthanide elements. II. Tb-Yb, *Astrophys. J. Suppl. Ser.* **257**, 29 (2021).
- [49] C. J. Fontes, C. L. Fryer, R. T. Wollaeger, M. R. Mumpower, and T. M. Sprouse, Actinide opacities for modelling the spectra and light curves of kilonovae, *Mon. Not. R. Astron. Soc.* **519**, 2862 (2023).
- [50] D. Kato, M. Tanaka, G. Gaigalas, L. Kitovienė, and P. Rynkun, Systematic opacity calculations for kilonovae—II. Improved atomic data for singly ionized lanthanides, *Mon. Not. R. Astron. Soc.* **535**, 2670 (2024).
- [51] J. Deprince, G. Wagle, S. Ben Nasr, H. Carvajal Gallego, M. Godefroid, S. Goriely, O. Just, P. Palmeri, P. Quinet, and S. Van Eck, Kilonova ejecta opacity inferred from new large-scale HFR atomic calculations in all elements between Ca ($Z = 20$) and Lr ($Z = 103$), *Astron. Astrophys.* **696**, A32 (2025).
- [52] W. Even, O. Korobkin, C. L. Fryer, C. J. Fontes, R. T. Wollaeger, A. Hungerford, J. Lippuner, J. Miller, M. R. Mumpower, and G. W. Misch, Composition effects on kilonova spectra and light curves. I, *Astrophys. J.* **899**, 24 (2020).
- [53] N. R. Badnell, AUTOSTRUCTURE: General program for calculation of atomic and ionic properties, Astrophysics Source Code Library, record ascl:1612.014 (2016), <https://ascl.net/1612.014>.
- [54] M. F. Gu, The flexible atomic code, *Can. J. Phys.* **86**, 675 (2008).
- [55] C. Froese Fischer, G. Gaigalas, P. Jönsson, and J. Bieroń, GRASP2018-A Fortran 95 version of the general relativistic atomic structure package, *Comput. Phys. Commun.* **237**, 184 (2019).
- [56] A. Bar-Shalom, M. Klapisch, and J. Oreg, HULLAC, An integrated computer package for atomic processes in plasmas, *J. Quant. Spectrosc. Radiat. Transfer* **71**, 169 (2001).
- [57] R. D. Cowan, *The Theory of Atomic Structure and Spectra*, Los Alamos Series in Basic and Applied Sciences (University of California Press, Ltd., Berkeley, 1981).
- [58] C. J. Fontes, H. L. Zhang, J. Abdallah, Jr., R. E. H. Clark, D. P. Kilcrease, J. Colgan, R. T. Cunningham, P. Hakel, N. H. Magee, and M. E. Sherrill, The Los Alamos suite of relativistic atomic physics codes, *J. Phys. B* **48**, 144014 (2015).
- [59] J. P. Desclaux, A multiconfiguration relativistic DIRAC-FOCK program, *Comput. Phys. Commun.* **9**, 31 (1975).
- [60] N. Domoto, M. Tanaka, D. Kato, K. Kawaguchi, K. Hotokezaka, and S. Wanajo, Lanthanide features in near-infrared spectra of kilonovae, *Astrophys. J.* **939**, 8 (2022).
- [61] Q. Lu, C. L. Yan, J. Meng, G. Q. Xu, Y. Yang, C. Y. Chen, J. Xiao, J. G. Li, J. G. Wang, and Y. Zou, Visible spectra of W^{8+} in an electron-beam ion trap, *Phys. Rev. A* **103**, 022808 (2021).
- [62] M. McCann, S. Bromley, S. D. Loch, and C. P. Ballance, Atomic data calculations for Au I-Au III and exploration in the application of collisional-radiative theory to laboratory and neutron star merger plasmas, *Mon. Not. R. Astron. Soc.* **509**, 4723 (2022).
- [63] R. Ferreira da Silva, A. Flörs, L. Leitão, J. P. Marques, G. Martínez-Pinedo, and J. M. Sampaio, Systematic bayesian optimization for atomic structure calculations of heavy elements, *Phys. Rev. A* **112**, 012802 (2025).
- [64] M. Hoffman, E. Brochu, and N. de Freitas, Portfolio allocation for bayesian optimization, in *Proceedings of the Twenty-Seventh Conference on Uncertainty in*

- Artificial Intelligence*, UAI'11 (AUAI Press, Arlington, Virginia, 2011), pp. 327–336.
- [65] A. Kramida, Yu. Ralchenko, and J. Reader (NIST ASD Team), NIST Atomic Spectra Database (ver. 5.9) (2021), national Institute of Standards and Technology, Gaithersburg, MD.
- [66] P. Quinet and P. Palmeri, Current status and developments of the atomic Database on Rare-Earths at Mons University (DREAM), *Atoms* **8**, 18 (2020).
- [67] M. Ding, A. N. Ryabtsev, E. Y. Kononov, T. Ryabchikova, C. P. Clear, F. Concepcion, and J. C. Pickering, Spectrum and energy levels of the low-lying configurations of Nd III, *Astron. Astrophys.* **684**, A149 (2024).
- [68] N. Spector, J. Sugar, and J.-F. Wyart, Analysis of the third spectrum of dysprosium (Dy III), *J. Opt. Soc. Am. B* **14**, 511 (1997).
- [69] G. Gaigalas, C. Fischer, P. Rynkun, and P. Jönsson, JJ2LSJ transformation and unique labeling for energy levels, *Atoms* **5**, 6 (2017).
- [70] C. Ferrara, M. Giarrusso, and F. Leone, Experimental atomic data of spectral lines—I. Cs, Ba, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Re, and Os in the 370–1000 nm interval, *Mon. Not. R. Astron. Soc.* **527**, 4440 (2024).
- [71] E. A. Den Hartog, G. T. Voith, and I. U. Roederer, Atomic transition probabilities for ultraviolet and optical lines of Tm II, *Astrophys. J. Suppl. Ser.* **274**, 9 (2024).
- [72] G. T. Voith, E. A. Den Hartog, and I. U. Roederer, Atomic transition probabilities for UV and optical lines of Gd II, *Astrophys. J. Suppl. Ser.* **278**, 7 (2025).
- [73] W. F. Meggers, Regularities in the arc spectrum of lanthanum, *J. Wash. Acad. Sci.* **17**, 25 (1927), <https://www.jstor.org/stable/24522554?seq=11>.
- [74] H. N. Russell and W. F. Meggers, An analysis of lanthanum spectra (La I, La II, La III), *Bur Stand J Res* **9**, 625 (1932).
- [75] G. R. Harrison, N. Rosen, and J. Rand McNally, Zeeman effect data for the spectra of Lanthanum—La I and La II, *J. Opt. Soc. Am.* **35**, 658 (1945).
- [76] F. Güzelçimen, M. Tonka, Z. Uddin, N. A. Bhatti, L. Windholz, S. Kröger, and G. Başar, Revised energy levels of singly ionized lanthanum, *J. Quant. Spectrosc. Radiat. Transfer* **211**, 188 (2018).
- [77] R. C. Gibbs and H. E. White, Rubidium and caesium-like doublets of stripped atoms, *Proc. Natl. Acad. Sci. U.S.A.* **12**, 551 (1926).
- [78] J. S. Badami, The spectrum of trebly-ionized cerium (Ce IV), *Proc. Phys. Soc.* **43**, 53 (1931).
- [79] R. J. Lang, The spectrum of trebly ionized cerium, *Can. J. Res.* **13**, 1 (1935).
- [80] J. Sugar, Analyses of lanthanide and actinide spectra, *J. Opt. Soc. Am.* **55**, 1283 (1965).
- [81] H. Odabasi, Spectrum of doubly ionized Lanthanum (La iii)*, *J. Opt. Soc. Am.* **57**, 1459 (1967).
- [82] W. C. Martin, R. Zalubas, and L. Hagan, *Atomic Energy Levels: The Rare Earth Elements (The Spectra of Lanthanum, Cerium, Praseodymium, Neodymium, Promethium, Samarium, Europium, Gadolinium, Terbium, Dysprosium, Holmium, Erbium, Thulium, Ytterbium, and Lutetium)*, National Standard Reference Data Series Vol. NSRDS-NBS 60 (National Bureau of Standards, Washington, DC, 1978), [10.6028/NBS.NSRDS.60](https://doi.org/10.6028/NBS.NSRDS.60).
- [83] W. E. Albertson and G. R. Harrison, Preliminary analysis of the first spark spectrum of Cerium—Ce II, *Phys. Rev.* **52**, 1209 (1937).
- [84] G. R. Harrison, W. E. Albertson, and N. F. Hosford, Zeeman effect data and further classification of the first spark spectrum of Cerium—Ce II, *J. Opt. Soc. Am.* **31**, 439 (1941).
- [85] C. H. Corliss, Wavelengths and energy levels of the second spectrum of Cerium (Ce II), *J. Res. Natl. Bur. Stand.* **77A**, 419 (1973).
- [86] T. L. Bruin, J. N. Lier, and H. J. van de Vliet, The Zeeman-effect of doubly ionized cerium, *Proc. R. Acad. Amsterdam* **40**, 334 (1937), <https://nvlpubs.nist.gov/nistpubs/Legacy/NSRDS/nbsnsrds60.pdf>.
- [87] H. N. Russell, R. B. King, and R. J. Lang, The third spectrum of cerium (Ce III), *Phys. Rev.* **52**, 456 (1937).
- [88] S. Johansson and U. Litzén, The $4f^2$ – $4f5d$ lines of Ce III, *Phys. Scr.* **6**, 139 (1972).
- [89] N. Rosen, G. R. Harrison, and J. R. McNally, Zeeman effect data and preliminary classification of the spark spectrum of Praseodymium—Pr II, *Phys. Rev.* **60**, 722 (1941).
- [90] A. Ginibre, Fine and hyperfine structures of singly ionized praseodymium: I. Energy levels, hyperfine structures and Zeeman effect, classified lines, *Phys. Scr.* **39**, 694 (1989).
- [91] A. Ginibre, Fine and hyperfine structures of singly ionised praseodymium: II. Parametric interpretation of fine and hyperfine structures for the even levels of singly ionised praseodymium, *Phys. Scr.* **39**, 710 (1989).
- [92] S. Ivarsson, U. Litzén, and G. M. Wahlgren, Accurate wavelengths, oscillator strengths and hyperfine structure in selected praseodymium lines of astrophysical interest, *Phys. Scr.* **64**, 455 (2001).
- [93] B. Furmann, D. Stefańska, E. Stachowska, J. Ruczkowski, and J. Dembczyński, Hyperfine-structure measurements and new levels evaluation in singly ionized praseodymium, *Eur. Phys. J. D* **17**, 275 (2001).
- [94] B. Furmann, D. Stefańska, J. Dembczyński, and E. Stachowska, New levels and hyperfine structure evaluation in singly ionized praseodymium, *Phys. Scr.* **72**, 300 (2005).
- [95] B. Furmann, D. Stefańska, J. Dembczyński, and E. Stachowska, New electron levels and classified lines in Pr II from hyperfine structure measurements, *At. Data Nucl. Data Tables* **93**, 127 (2007).
- [96] J. Sugar, Analysis of the third spectrum of praseodymium*, *J. Opt. Soc. Am.* **53**, 831 (1963).
- [97] J. Sugar, The third spectrum of Praseodymium (Pr (III) in the vacuum ultraviolet, *J. Res. Natl. Bur. Stand., Sect. A* **73A**, 333 (1969).
- [98] H. Crosswhite, H. M. Crosswhite, and B. R. Judd, Magnetic parameters for the configuration f^3 , *Phys. Rev.* **174**, 89 (1968).
- [99] J. Sugar, Spectrum of doubly ionized praseodymium from 2107 Å to 10716 Å, *J. Res. Natl. Bur. Stand., Sect. A* **78A**, 555 (1974).
- [100] J. F. Wyart, J. Blaise, and P. Camus, Progrès Récents dans l'Interprétation des configurations $4f^N(5d + 6s)$ des Lanthanides II. Etude Paramétrique des configurations, *Phys. Scr.* **9**, 325 (1974).

- [101] W. E. Albertson, G. R. Harrison, and J. R. McNally, First spark spectrum of neodymium—preliminary classification and Zeeman effect data, *Phys. Rev.* **61**, 167 (1942).
- [102] J. F. Wyart, Ph.D. thesis, University of Paris, Orsay, 1968.
- [103] R. Kielkopf, Ph.D. thesis, University of Amsterdam, 1969.
- [104] J. Blaise, J. Chevillard, J. Vergès, and J. F. Wyart, Etude des spectres d'émission dans l'infrarouge par l'emploi d'un SISAM—IV. spectre d'émission du néodyme, *Spectrochim. Acta B Atom. Spectros.* **25**, 333 (1970).
- [105] J. Blaise, J. F. Wyart, R. Hoekstra, and P. J. G. Kruiver, Present state of the analysis of Nd I and Nd II, *J. Opt. Soc. Am.* **61**, 1335 (1971).
- [106] J. Blaise (unpublished analysis, 2002).
- [107] H. Crosswhite (unpublished analysis, 1976).
- [108] G. H. Dieke, H. M. Crosswhite, and B. Dunn, Emission spectra of the doubly and triply ionized rare earths*, *J. Opt. Soc. Am.* **51**, 820 (1961).
- [109] G. H. Dieke and H. M. Crosswhite, The spectra of the doubly and triply ionized rare earths, *Appl. Opt.* **2**, 675 (1963).
- [110] M. Aldenius, Ph.D. thesis, University of Lund, 2001.
- [111] T. Ryabchikova, A. Ryabtsev, O. Kochukhov, and S. Bagnulo, Rare-earth elements in the atmosphere of the magnetic chemically peculiar star HD 144897. New classification of the Nd III spectrum, *Astron. Astrophys.* **456**, 329 (2006).
- [112] J. A. Weinman, Promethium spectra: Pm II and Pm III, *Phys. Rev.* **78**, 628 (1950).
- [113] R. G. Gutmacher, J. G. Conway, and C. E. Moore, The second spectrum of promethium, *J. Opt. Soc. Am.* **48**, 389 (1958).
- [114] R. Otto, H. Huhnermann, J. Reader, and J. F. Wyart, Hyperfine structure investigations and identification of new energy levels in the ionic spectrum of ^{147}Pm , *J. Phys. B* **28**, 3615 (1995).
- [115] W. C. Martin, Energy levels and classified lines in the second spectrum of thorium (Th II), *J. Opt. Soc. Am.* **61**, 1682 (1971).
- [116] W. Albertson, Analysis of the spectrum of singly ionized samarium, *Astrophys. J.* **84**, 26 (1936).
- [117] J. Blaise, C. Morillon, M.-G. Schweighofer, and J. Vergès, Etude des spectres d'émission dans l'infrarouge par l'emploi d'un SISAM—III. Spectre d'émission du samarium, *Spectrochim. Acta B Atom. Spectros.* **24**, 405 (1969).
- [118] A. Dupont, Spectrum of Sm III*, *J. Opt. Soc. Am.* **57**, 867 (1967).
- [119] W. Albertson, The spectrum of singly ionized europium, *Phys. Rev.* **45**, 499 (1934).
- [120] H. N. Russell, W. Albertson, and D. N. Davis, The spark spectrum of europium, Eu II, *Phys. Rev.* **60**, 641 (1941).
- [121] B. Furmann and D. Stefańska, Experimental determination of core relaxation and screening effects on the wavefunction at a nucleus for stable isotopes of $^{151,153}\text{Eu}$ II, *Eur. Phys. J. Special Topics* **222**, 2279 (2013).
- [122] J. Sugar and N. Spector, Spectrum and energy levels of doubly ionized europium (Eu III), *J. Opt. Soc. Am.* **64**, 1484 (1974).
- [123] J. F. Wyart, W. Ü. L. Tchang-Brillet, S. S. Churilov, and A. N. Ryabtsev, Extended analysis of the Eu III spectrum, *Astron. Astrophys.* **483**, 339 (2008).
- [124] W. E. Albertson, H. Bruynes, and R. Hanau, The normal electron configuration of singly ionized gadolinium, *Phys. Rev.* **57**, 292 (1940).
- [125] H. N. Russell, The arc and spark spectra of gadolinium, *J. Opt. Soc. Am.* **40**, 550 (1950).
- [126] J. Blaise, J. Chevillard, J. Vergès, J. F. Wyart, and T. A. M. van Kleef, Etude des spectres d'émission dans l'infrarouge par l'emploi d'un SISAM—V. Spectre d'émission du gadolinium, *Spectrochim. Acta B Atom. Spectros.* **26**, 1 (1971).
- [127] A. Venugopalan, S. M. Afzal, and S. A. Ahmad, Isotope shift studies in the UV spectrum of singly ionised gadolinium, *Spectrochim. Acta B Atom. Spectros.* **53**, 633 (1998).
- [128] N. Spector, Analysis of even configurations in the second spectrum of gadolinium (Gd II), *J. Opt. Soc. Am.* **60**, 763 (1970).
- [129] W. R. Callahan, The spectrum of doubly ionized gadolinium, Ph.D. thesis, Johns Hopkins University, Maryland, 1962.
- [130] W. R. Callahan, Spectrum of doubly ionized gadolinium*, *J. Opt. Soc. Am.* **53**, 695 (1963).
- [131] J. F. J. Kielkopf, Ph.D. thesis, Johns Hopkins University, 1969.
- [132] E. Meinders, Classification of Tb II-lines in connection with hyperfine structure, *Physica (Utrecht)* **42**, 427 (1969).
- [133] P. F. A. Klinkenberg, Interpretation of Zeeman patterns of Tb II-lines, *Opt. Pura Apl.* **10** (1977), https://sedoptica.es/Menu_Volumenes/Pdfs/OPA_10_3_10.pdf.
- [134] J. Blaise, P. Camus, and J. Wyart, *Gmelin Handbuch der Anorganischen Chemie*, Vol. 39 (Springer-Verlag, Berlin, 1976).
- [135] E. Meinders, T. A. M. Van Kleef, and J. F. Wyart, The analysis of doubly ionized terbium (Tb III), *Physica (Utrecht)* **61**, 443 (1972).
- [136] E. Paulson, Wave-lengths of elements at high temperatures, *Astrophys. J.* **40**, 298 (1914).
- [137] W. F. Meggers, Series regularities in the spectra of the lanthanide rare earths, *Rev. Mod. Phys.* **14**, 96 (1942).
- [138] J. M. Blank, Zeeman effect of Dy II, *J. Opt. Soc. Am.* **42**, 117 (1952).
- [139] V. G. Mossotti and V. A. Fassel, Emission flame spectrometry of the rare earths, *Spectrochim. Acta* **20**, 1117 (1964).
- [140] K. L. Vander Sluis and J. R. McNally, Zeeman effect in Dy II, *J. Opt. Soc. Am.* **60**, 1209 (1970).
- [141] J. G. Conway and E. F. Worden, Preliminary level analysis of the first and second spectra of dysprosium, Dy I and Dy II*, *J. Opt. Soc. Am.* **61**, 704 (1971).
- [142] J.-F. Wyart, Dysprosium levels II: Odd configurations, *Spectrochim. Acta B Atom. Spectros.* **27**, 443 (1972).
- [143] J.-F. Wyart, Dysprosium levels III: Even configurations, *Spectrochim. Acta B Atom. Spectros.* **27**, 616 (1972).
- [144] J.-F. Wyart, Analyse paramétrique de la configuration $4f^9 5d 6s$ de Dy II, *Physica (Utrecht)* **89**, 361 (1976).
- [145] G. Nave and U. Griesmann, New energy levels and classifications of spectral lines from neutral and singly-ionized dysprosium (Dy I and Dy II), *Phys. Scr.* **62**, 463 (2000).

- [146] H. M. Crosswhite, Spectra of quadruply ionized praseodymium (Pr V), doubly and triply ionized neodymium (Nd III and Nd IV), and doubly ionized dysprosium (Dy III), *J. Opt. Soc. Am.* **53**, 202 (1963).
- [147] J. Sugar, Energy levels of neutral and singly ionized holmium (Ho I and Ho II), *J. Opt. Soc. Am.* **58**, 1519 (1968).
- [148] A. E. J. Livingston and E. H. Pinnington, Spectrum of singly-ionized holmium (Ho II), *J. Opt. Soc. Am.* **61**, 1429 (1971).
- [149] J.-F. Wyart, J. Blaise, and T. A. M. Van Kleef, A parametric study of the $4f^{11}6p$ configuration of Ho II, *J. Phys. B* **7**, 1111 (1974).
- [150] J. Gurell, G. M. Wahlgren, G. Nave, and J.-F. Wyart, The spectrum of singly ionized holmium (Ho II), *Phys. Scr.* **79**, 035306 (2009).
- [151] J. H. McElaney, The spectrum of doubly ionized homium, Ph.D. thesis, Johns Hopkins University, Maryland, 1966.
- [152] J. H. McElaney, Spectrum of Ho III*, *J. Opt. Soc. Am.* **57**, 870 (1967).
- [153] J. Becher, Theoretical Investigation of Doubly-Ionized and Triply-Ionized Lanthanides, and the Empirical Analysis of Erbium, Ph.D. thesis, Johns Hopkins University, Maryland, 1965.
- [154] R. Hussain, The Spectra of Dysprosium-IV and Holmium-III, Ph.D. thesis, Johns Hopkins University, Maryland, 1973.
- [155] J. F. Wyart, H. M. Crosswhite, and R. Hussain, Energy levels of Ho III, *Physica (Amsterdam)* **85B+C**, 386 (1976).
- [156] J. R. McNally and K. L. V. Sluis, Low levels of the arc spectrum of erbium (Er II), *J. Opt. Soc. Am.* **49**, 200 (1959).
- [157] J. W. Lindner and S. P. Davis, Zeeman effect in the arc spectrum of erbium, *J. Opt. Soc. Am.* **48**, 542 (1958).
- [158] A. Gatterer and J. Junkes, *Spektren der Seltenen Erden* (Specola Vaticana, Vatican City, 1945).
- [159] B. R. Judd and L. C. Marquet, A pair coupling scheme for $f4^{12}6s$, *J. Opt. Soc. Am.* **52**, 504 (1962).
- [160] C. H. Corliss, Electrostatic parameters for erbium in the spectra Er II and Er III, *Astrophys. J.* **138**, 272 (1963).
- [161] L. C. Marquet and S. P. Davis, Atomic energy levels of neutral erbium*, *J. Opt. Soc. Am.* **55**, 471 (1965).
- [162] K. L. V. Sluis and J. R. McNally, Zeeman effect of Er II, *J. Opt. Soc. Am.* **60**, 94 (1970).
- [163] N. Spector, New low even levels of singly ionized Erbium (Er II), *Astrophys. J.* **167**, 205 (1971).
- [164] N. Spector, A study of infrared spectra of lanthanide and actinide free ions in yttrium and lanthanum trichloride matrices, *J. Opt. Soc. Am.* **61**, 1495 (1971).
- [165] J.-F. Wyart and J. E. Lawler, Assessment and optimization of the Er II spectroscopic data, *Phys. Scr.* **79**, 035301 (2009).
- [166] G. H. Dieke, H. M. Crosswhite, and B. Dunn, Interpretations of the spectra of the third spectra of the rare earths, *J. Opt. Soc. Am.* **51**, 337 (1961).
- [167] N. Spector, Level structure of doubly ionized erbium (Er III), *J. Opt. Soc. Am.* **63**, 358 (1973).
- [168] J. F. Wyart, J. J. A. Koot, and T. A. M. Van Kleef, The configuration $4f^{11}6p$ in the lanthanide spectra, *Physica (Utrecht)* **77**, 159 (1974).
- [169] J. F. Wyart and C. Bauche-Arnoult, Interprétation des configurations $4f^N 5d$ et $4f^N 6s$ par la Méthode paramétrique généralisée, *Phys. Scr.* **22**, 583 (1980).
- [170] J. F. Wyart, J. Blaise, W. P. Bidelman, and C. R. Cowley, Energy levels and transition probabilities in doubly-ionized erbium (Er III), *Phys. Scr.* **56**, 446 (1997).
- [171] J. Blaise and P. Camus, Spectre d'arc du thulium, *J. Phys. (Paris)* **26**, 605 (1965).
- [172] P. Camus, A. Gatterer, and J. Junkes, The spectrum of the singly ionized thulium atom (Tm II), *Spectrochim. Acta B Atom. Spectros.* **24**, 367 (1969).
- [173] N. Spector, Spectrum of singly ionized thulium (Tm II), *J. Opt. Soc. Am.* **57**, 1358 (1967).
- [174] P. Camus and J. Sugar, Analysis of the even-parity configurations in the second spectrum of thulium, *Phys. Scr.* **3**, 231 (1971).
- [175] J.-F. Wyart, J. Blaise, and P. Camus, A parametric study of the $4f^{13}6p$ configuration of Tm II, *J. Phys. B* **7**, 1112 (1974).
- [176] J.-F. Wyart, Analysis of the low-lying levels of doubly ionized thulium (Tm III), *Can. J. Phys.* **89**, 451 (2011).
- [177] J.-G. Li and V. A. Dzuba, Testing Bohr–Weisskopf effect and accuracy of electronic structure calculations with hyperfine structure of Tm II, *J. Phys. B* **53**, 035004 (2020).
- [178] J. Sugar, Energy levels of doubly ionized thulium (Tm III), *J. Opt. Soc. Am.* **59**, 1383 (1969).
- [179] J. Sugar, Spectrum of doubly ionized thulium (Tm III)*, *J. Opt. Soc. Am.* **60**, 454 (1970).
- [180] J.-F. Wyart, Analysis of the third spectrum of thulium (Tm III), *Phys. Scr.* **4**, 53 (1971).
- [181] W. F. Meggers, Spectra of the singly ionized rare earths, *J. Opt. Soc. Am.* **57**, 396 (1967).
- [182] N. Spector, The spectrum of singly ionized ytterbium (Yb II), *J. Opt. Soc. Am.* **58**, 837 (1968).
- [183] J.-F. Wyart and P. Camus, Interpretation of $4f^{13}5d6p$, $4f^{13}5d^2$, and $4f^{13}6p^2$ configurations of Yb II, *J. Quant. Spectrosc. Radiat. Transfer* **21**, 115 (1979).
- [184] B. W. Bryant, The spectra of doubly and triply ionized ytterbium, Johns Hopkins Spectroscopic Report No. 21 (1961).
- [185] B. W. Bryant, Spectra of doubly and triply ionized ytterbium, Yb III and Yb IV⁺, *J. Opt. Soc. Am.* **55**, 771 (1965).
- [186] J. Sugar, Configuration $4f\hat{1}35d$ of doubly ionized Ytterbium, *J. Opt. Soc. Am.* **60**, 571 (1970).
- [187] G. Gaigalas, D. Kato, P. Rynkun, L. Radžiūtė, and M. Tanaka, Extended calculations of energy levels and transition rates of Nd II-IV ions for application to neutron star mergers, *Astrophys. J. Suppl. Ser.* **240**, 29 (2019).
- [188] R. G. Eastman and P. A. Pinto, Spectrum formation in supernovae: Numerical techniques, *Astrophys. J.* **412**, 731 (1993).
- [189] V. V. Sobolev, *Moving Envelopes of Stars* (Harvard University Press, Cambridge, MA; London, England, 1960).
- [190] H. J. G. L. M. Lamers and J. P. Cassinelli, *Introduction to Stellar Winds* (Cambridge University Press, Cambridge, England, 1999), 10.1017/CBO9781139175012.
- [191] Q. Pognan, A. Jerkstrand, and J. Grumer, NLTE effects on kilonova expansion opacities, *Mon. Not. R. Astron. Soc.* **513**, 5174 (2022).

- [192] K. Hotokezaka, M. Tanaka, D. Kato, and G. Gaigalas, Nebular emission from lanthanide-rich ejecta of neutron star merger, *Mon. Not. R. Astron. Soc.* **506**, 5863 (2021).
- [193] J. H. Gillanders, S. J. Smartt, S. A. Sim, A. Bauswein, and S. Goriely, Modelling the spectra of the kilonova AT2017gfo—I. The photospheric epochs, *Mon. Not. R. Astron. Soc.* **515**, 631 (2022).
- [194] E. Pian, Binary neutron star mergers: A multi-messenger revolution, *Front. Astron. Space Sci.* **7**, 108 (2021).
- [195] D. Watson, C. J. Hansen, J. Selsing, A. Koch, D. B. Malesani, A. C. Andersen, J. P. U. Fynbo, A. Arcones, A. Bauswein, S. Covino, A. Grado, K. E. Heintz, L. Hunt, C. Kouveliotou, G. Leloudas, A. J. Levan, P. Mazzali, and E. Pian, Identification of strontium in the merger of two neutron stars, *Nature (London)* **574**, 497 (2019).
- [196] C. E. Collins, A. Bauswein, S. A. Sim, V. Vijayan, G. Martínez-Pinedo, O. Just, L. J. Shingles, and M. Kromer, 3D radiative transfer kilonova modelling for binary neutron star merger simulations, *Mon. Not. R. Astron. Soc.* **521**, 1858 (2023).
- [197] Spectral analysis and radiative data for elemental kilonovae identification (sparkle), [10.54499/2023.14470.PEX](https://doi.org/10.54499/2023.14470.PEX) (2025), this project has received funding from Fundação para a Ciência e a Tecnologia (FCT).
- [198] Astropy Collaboration, T. P. Robitaille, E. J. Tollerud, P. Greenfield, M. Droettboom, E. Bray, T. Aldcroft, M. Davis, A. Ginsburg, and A. M. Price-Whelan, Astropy: A community Python package for Astronomy, *Astron. Astrophys.* **558**, A33 (2013).
- [199] Astropy Collaboration, A. M. Price-Whelan, B. M. Sipőcz, H. M. Günther, P. L. Lim, S. M. Crawford, S. Conseil, D. L. Shupe, M. W. Craig, and N. Dencheva, The Astropy Project: Building an open-science project and status of the v2.0 core package, *Astron. J.* **156**, 123 (2018).
- [200] S. van der Walt, S. C. Colbert, and G. Varoquaux, The NumPy array: A structure for efficient numerical computation, *Comput. Sci. Eng.* **13**, 22 (2011).
- [201] E. Jones, T. Oliphant, P. Peterson *et al.*, SciPy: Open source scientific tools for Python <http://www.scipy.org/> (2001).
- [202] W. McKinney, Data structures for statistical computing in Python, in *Proceedings of the 9th Python in Science Conference*, edited by S. van der Walt and J. Millman (2010), pp. 51–56, [10.25080/Majora-92bf1922-00a](https://doi.org/10.25080/Majora-92bf1922-00a).
- [203] J. D. Hunter, Matplotlib: A 2D graphics environment, *Comput. Sci. Eng.* **9**, 90 (2007).
- [204] A. Flörs, GSI database for kilonova radiative transfer, [10.5281/zenodo.15835361](https://doi.org/10.5281/zenodo.15835361) (2025).