Insights on the complexity of the excited states of Eu-doped luminescent materials Electronic Supplementary Information (ESI)

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I. INTRODUCTION

Here we describe the details and collect the results of *ab initio* calculations on the electronic structure of Eu^{2+} and Eu^{3+} ions in alkaline earth fluoride, MeF_2, and sulfide, MeF, host crystals (Me = Ca, Sr, Ba). They use wave function theory and the embedded cluster approximation and have been performed with the MOLCAS package.[1]

The relativistic second-order Douglas-Kroll-Hess (DKH) many-electron Hamiltonian[2,3] has been used in all calculations. In a first step, the spin-orbit coupling operator is removed from the Hamiltonian so that spin-orbit free state-average restricted-active-space self-consistent-field (SA-RASSCF) variational calculations[4–8] are done on a many-electron active configurational space. The definition of the active spaces are detailed below. These SA-RASSCF calculations take care of the non-dynamic electron correlation. They are in fact multi-configurational SCF calculations in which the molecular orbital coefficients and the configuration interaction expansion coefficients are variational. Subsequently, the SA-RASSCF wave functions are used in multi-state second-order perturbation theory (MS-RASPT2) calculations.[9–13] In this way, dynamic correlation effects in the ground and excited states of the embedded clusters are taken into account. The MS-RASPT2 calculations use the (occupied and empty) molecular orbitals optimized in the SA-RASSCF calculations and some selected electron shells are correlated as described below.

In a second step, the full DKH Hamiltonian is used, the atomic mean-field integrals approximation (AMFI)[14] is adopted for its spin-orbit coupling part, and restricted-active-space state-interaction spin-orbit calculations (RASSI-SO)[15] are done. The RASSI-SO calculations are a particular means to use the spin-free-state-shifting operator (SFSS)[16] in order to efficiently and effectively combine spin-orbit couplings calculated with non-dynamically correlated wave functions (e.g. RASSCF), together with spin-orbit coupling free energies calculated with dynamic correlation (e.g. RASPT2). In them, we chose the transformed RASSCF wave functions (first-order wave functions of the MS-RASPT2 method) of the spin-orbit-free states of interest as a many-electron basis, and the MS-RASPT2 energies as shifting factors.

A. MeF_2 and MeS AIMP embedding potentials

The Hamiltonians of the otherwise isolated clusters are supplemented with the *ab initio* model potential (AIMP) embedding operators[17] of MeF_2 and MeS (Me = Ca, Sr, Ba). Those of the MeF_2 fluorides have been obtained elsewhere;[18] those of the MeS rock-salts have been obtained in this work and are available from the authors. The MeS embedding potentials have been calculated in self-consistent embedded-ions (SCEI)[19] Hartree-Fock (HF) calculations and they are made of: 1) total-ion embedding AIMPs representing Ca^{2+}, Sr^{2+}, or Ba^{2+} cations and S^{2-} anions, which are located at experimental sites of the MeS host lattices within a cube made of $5 \times 5 \times 5$ unit cells centered on Ca^{2+}, Sr^{2+}, or Ba^{2+}, depending on the case; and 2) a set of 3309 additional point charges at lattice sites are generated by the zero-multipole method of Gellé and Lepetit,[20] which closely reproduce the Ewald potential[21] within the clusters. The experimental crystal structures of CaS,[22] SrS,[23] and BaS[23] are: space group number 225, *Fm-3m* cubic, with lattice constants a = 5.710 Å (CaS), 6.021 Å (SrS), 6.3748 Å (BaS).

The effect of the AIMP embedding potentials of the MeF_2 and MeS hosts on the studied clusters is to include: 1) host electrostatic interactions (made of long-range point-charge or Madelung contributions and short-range charge density Coulomb contributions), 2) host-cluster exchange interactions, and 3) Pauli repulsion interactions from the host (non-orthogonality repulsive contributions due to cluster-host antisymmetry requirements). The Pauli repulsions from the S $3p$ shells as obtained in the SCEI calculations are known to be underestimated[24] and they are corrected following the prescriptions in Ref. 24, increasing their associated projection constants in order to achieve the experimental M-S bond length within less than 0.01 Å.

B. Eu^{2+} in MeF_2 and MeS

Eu^{2+} and Eu^{3+} ions are assumed to substitute for the alkaline earth Ca^{2+}, Sr^{2+}, or Ba^{2+} in the fluoride and sulfide hosts leading to 8-fold cubic and 6-fold octahedral coordination, respectively. Non-local charge compensation is assumed for the trivalent dopant in this work.

The Hamiltonian and wave functions of the clusters,

embedded in MeF_2 or MeS, comprise the Eu impurity ion at (0, 0, 0), eight F or six S ligands at variable (x,x,x) or (0,0,x) positions, and twelve or six Me second neighbors at fixed positions, $(\frac{1}{2},\frac{1}{2},0)$ or (1,0,0), respectively, as follows: $(EuF_8Me_{12})^{18+}$, $(EuF_8Me_{12})^{19+}$, or $(EuS_6Me_6)^{2+}$, $(EuS_6Me_6)^{3+}$, for Eu^{2+}, Eu^{3+} containing clusters. The embedded cluster calculations include all the electrons of the dopant and ligands and limited representations of the Me^{2+} second neighbors, as described next.

The following Gaussian atomic natural orbital relativistic basis sets ANO-RCC for the Europium[25] dopant and the Fluorine or Sulfur ligands,[26] were used to expand the clusters molecular orbitals: Eu($25s22p15d11f4g2h$)[$9s8p5d4f3g2h$] (quadruple-zeta with polarization quality) and F($14s9p4d$)[$5s4p3d$] or S($17s12p5d$)[$6s5p3d$] (quadruple-zeta with polarization without f nor g-functions quality). In the Eu-doped MeF_2 calculations, all occupied shells of the Me^{2+} second neighbor ions were considered frozen and their outermost s and p orbitals were used, contracted as [$1s1p$] orthogonalization functions, for which the Me^{2+} embedding AIMP data were used. Five s-type Gaussian functions were also added to the cluster bases at the next six neighboring interstitial sites.[18] In the Eu-doped MeS calculations, the description of the six Me^{2+} ions located next to the sulfur ligands in the (100) axes was improved further: only the inner shells of the Me^{2+} ions were frozen ([Mg] core for Ca^{2+}, [Zn] core for Sr^{2+}, and [Cd] core for Ba^{2+}); the corresponding atomic natural orbitals of the ANO-RCC set were used to build the core AIMP operators;[27] the 6-electron valence of the Me^{2+} were treated explicitly using the following valence bases, adapted from the ANO-RCC sets: Ca($20s16p6d$)[$3s4p1d$], Sr($23s19p12d$)[$3s4p1d$], Ba($26s22p15d$)[$3s4p1d$]. Using the D_{2h} point group in the calculations the number of symmetry adapted basis functions of the fluoride and sulfide clusters is: 469 and 471, respectively.

In the SA-RASSCF calculations on the Eu^{2+} clusters we used a restricted active space made of 7 electrons in 20 molecular orbitals of main character Eu-$4f$, Eu-$5d$, Eu-$6s$, and Eu-$5f$ (6 electrons in 20 MOs for Eu^{3+} clusters). We computed the following terms and used the following state-averages for the molecular orbital optimizations: For states in the $4f^7$ configuration of Eu^{2+}, 1 $^8A_{1u}$ term; 2 $^6A_{1u}$, 2 $^6A_{2u}$, and 4 ^6E_u; and 6 $^6T_{1u}$ and 6 $^6T_{2u}$ terms. For the $4f^65d$ and $4f^66s$ configurations of Eu^{2+}, 1 $^8A_{1g}$, 2 $^8A_{2g}$, and 3 ^8E_g; 6 $^8T_{1g}$ and 5 $^8T_{2g}$; 39 $^6A_{1g}$, 36 $^6A_{2g}$, and 75 ^6E_g; and 108 $^6T_{1g}$ and 111 $^6T_{2g}$ terms. For the $4f^6$ configuration of Eu^{3+}, 1 $^7A_{2g}$; 1 $^7T_{1g}$ and 1 $^7T_{2g}$; and 7 $^5A_{1g}$, 5 $^5A_{2g}$, and 13 ^5E_g; 16 $^5T_{1g}$ and 18 $^5T_{2g}$ terms. In all cases, all possible occupations were allowed in the Eu-$4f$ shells and up to four electrons were allowed in the Eu-$5d$, Eu-$6s$, and Eu-$5f$ shells (we refer to this calculations as SA-RASSCF($4f/5d6s5f-4e$)); this restricted active space should be fairly close to a complete 7-electron (or 6-electron) active space where all possible occupations of the 20 molecular orbitals would be allowed. Inclusion of the Eu $5f$-shells in the active space is needed for a better account of the large radial correlation effects in the 4f-shell, which strongly affect interconfigurational transitions also in the first half of the lanthanide series.[28] The number of configuration state functions (CSF) generated in each spin and D_{2h} symmetry block range between 4500 and 41500 CSF, for the Eu^{2+} clusters, and between 3400 and 24000 CSF, for the Eu^{3+} clusters.

In the MS-RASPT2 calculations we correlated all cluster valence electrons except those with main character Eu-$4d$. We used the standard IPEA value (0.25 au)[29] and an imaginary level shift of 0.15 to avoid intruder states.[30] Symmetry analyses of the SA-RASSCF multiconfigurational reference wave functions allowed us to perform MS-RASPT2 calculations over actual spin and O_h symmetry blocks, which avoids symmetry breakings at the MS-RASPT2 level of calculations and beyond. In the case of the MeF_2 hosts, small spikes or irregularities in the potential energy surfaces were found coinciding with sharp avoided crossings between some high energy lying spin sextet excited states of the $4f^65dt^1_{2g}$ and $4f^6ITE^1_{a_{1g}}$ configurations, which did not disappear using different and reasonable values of MS-RASPT2 parameters. These high energy sextet states were excluded from the subsequent RASSI-SO calculations.

The results of the SA-RASSCF and MS-CASPT2 spin-orbit free calculations for Eu^{2+} and Eu^{3+} clusters are collected in Tables S1–S3 for the MeF_2 hosts, and Tables S4–S6 for the MeS hosts. Figures S1 and S2 show the corresponding MS-CASPT2 energy curves.

Finally, the spin-orbit coupling calculations (RASSI-SO) were done allowing the coupling of all MS-RASPT2 states of spin multiplicity $2S+1 \geq 6$ for Eu^{2+} and $2S+1 \geq 5$ for Eu^{3+} mentioned above. Ultimately, the quality of all of the limitations imposed on the extent of spin-orbit coupling should be revealed by the comparisons between theoretical and experimental spectra discussed in the main body of this paper.

The results of the spin-orbit coupling RASSI-SO calculations for Eu^{2+} and Eu^{3+} cluster are collected in Tables S9–S11 for the MeF_2 hosts, and Tables S12–S14 for the MeS hosts. The corresponding energy curves for Eu^{2+} and Eu^{3+} are in Fig. 3 of the paper and here in Fig. S3, respectively.

C. Accuracy of the computed energies

Calculated and experimental energies are compared in Table S15 and Fig. 2. It is based on the results of this work and experimental excitation energies for the Eu^{2+}- and Eu^{3+}-doped fluoride and sulfide crystals. This table displays only those levels for which experimental spectroscopic data is available. All computed energies can be found in Tables S9–S14.

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TABLE S1: Spectroscopic constants of the ground and excited states of Eu^{2+} and Eu^{3+} -doped CaF_2 cubic defects calculated using the relativistic spin-free second order Douglas-Kroll-Hess Hamiltonian with AIMP CaF_2 embedding. The embedded cluster RASSCF results include basic bonding interactions and $4f$–shell radial correlation; the MS-RASPT2 ones include also dynamic correlation of 79 or 78 valence electrons in the Eu $5s, 5p$, F $2s, 2p$, closed shells and Eu $4f, 5d, 6s$ open shells. Eu–F bond distances ($d_{\mathrm{Eu-F},e}$ in Å), EuF_8 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), and minimum-to-minimum energy differences (T_e in cm^{-1}) are given. See Figs. S1, S2 and text for details.

	RASSCF			MS-RASPT2		
term	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e
			Eu^{2+}-doped CaF_2			
$4f^7(^8F)$						
$1\ ^8A_{1u}$	2.433	416	0	2.388	423	0
			$4f^6(5d + ITE_{a_{1g}})^1$ excited states			
$4f^6(^7F)5de_g^1$						
Octets						
$1\ ^8T_{2g}$	2.419	420	24344	2.372	429	27329
$1\ ^8E_g$	2.417	420	24709	2.370	423	27804
$1\ ^8T_{1g}$	2.419	420	25333	2.373	429	28008
$2\ ^8T_{1g}$	2.419	420	26392	2.373	429	29265
$2\ ^8T_{2g}$	2.418	420	28127	2.372	429	30178
Sextets						
$1\ ^6T_{1g}$	2.420	419	30627	2.372	427	31468
$1\ ^6T_{2g}$	2.418	420	34491	2.370	430	34362
$1\ ^6E_g$	2.416	419	35180	2.366	428	34942
$2\ ^6T_{1g}$	2.418	419	35857	2.370	430	35142
$2\ ^6T_{2g}$	2.417	420	38708	2.369	429	37059
$4f^6(^7F)(5dt_{2g}^1 + ITE_{a_{1g}}^1)$ [a]						
Octets						
$3\ ^8T_{1g}$	2.466	414	44495	2.418	407	47987
$3\ ^8T_{2g}$	2.467	414	43971	2.421	406	48085
$2\ ^8E_g$	2.467	414	43750	2.421	420	48122
$1\ ^8A_{2g}$	2.467	413	48041	2.312	403	48572
$4\ ^8T_{1g}$	2.467	414	46877	2.380	406	49474
$4\ ^8T_{2g}$	2.468	414	48102	2.354	758	50161
$3\ ^8E_g$	2.467	414	47453	2.421	419	51029
$5\ ^8T_{1g}$	2.467	412	48842	2.376	456	51179
$2\ ^8A_{2g}$	2.400	870	51527	2.399	1060	51591
$5\ ^8T_{2g}$	2.400	867	51644	2.394	622	51819
$6\ ^8T_{1g}$	2.401	962	51567	2.397	834	51968
$1\ ^8A_{1g}$	2.467	413	48888	2.421	419	51984
			$4f^7$ excited states			
$4f^7(^6P)$						
$1\ ^6T_{1u}$	2.432	416	33652	2.386	422	30587
$4f^7(^6I)$						
$1\ ^6T_{2u}$	2.432	416	37088	2.386	422	34192
$1\ ^6E_u$	2.432	416	37108	2.386	423	34424

$1\ ^6A_{2u}$	2.432	416	37117	2.386	422	34553
$2\ ^6T_{2u}$	2.432	415	37277	2.386	422	34560
$1\ ^6A_{1u}$	2.432	416	37375	2.386	422	34701
$2\ ^6T_{1u}$	2.433	416	37359	2.386	423	34705
$4f^7(^6D)$						
$2\ ^6E_u$	2.432	416	41048	2.385	423	37164
$3\ ^6T_{2u}$	2.432	416	41198	2.386	422	37294
$4f^7(^6G,^6F)$						
$4\ ^6T_{2u}$	2.429	416	54808	2.383	423	48989
$3\ ^6T_{1u}$	2.429	416	55007	2.383	422	49254
$3\ ^6E_u$	2.432	416	55369	2.386	422	49298
$2\ ^6A_{2u}$	2.431	416	55387	2.385	423	49723
$2\ ^6A_{1u}$	2.433	415	56104	2.387	422	50047
$5\ ^6T_{2u}$	2.432	416	55651	2.386	422	50263
$4\ ^6T_{1u}$	2.433	416	56051	2.387	422	50517
$4f^7(^6H)$						
$5\ ^6T_{1u}$	2.431	416	60996	2.384	423	54720
$4\ ^6E_u$	2.431	416	61118	2.384	422	54796
$6\ ^6T_{1u}$	2.432	416	61532	2.386	423	55261
$6\ ^6T_{2u}$	2.432	416	61626	2.387	423	55411
			Eu^{3+}-doped CaF_2			
$4f^6(^7F)$ [a]						
$1\ ^7A_{2g}$	2.290	488	0	2.257	501	0
$1\ ^7T_{1g}$	2.293	488	1215	2.261	493	1532
$1\ ^7T_{2g}$	2.294	488	1485	2.262	495	1663
$4f^6(^5D)$						
$1\ ^5E_g$	2.292	488	23818	2.260	493	22107
$1\ ^5T_{2g}$	2.292	488	23977	2.260	493	22239
$4f^6(^5L,^5G)$						
$2\ ^5E_g$	2.290	488	27372	2.258	493	26362
$1\ ^5T_{1g}$	2.290	488	27419	2.258	493	26451
$1\ ^5A_{1g}$	2.290	488	27444	2.258	493	26676
$2\ ^5T_{2g}$	2.292	487	28136	2.259	496	26702
$2\ ^5T_{1g}$	2.292	488	28148	2.261	494	27288
$3\ ^5E_g$	2.292	488	28329	2.260	494	27314
$3\ ^5T_{2g}$	2.292	488	28337	2.261	493	27808
$3\ ^5T_{1g}$	2.292	488	28941	2.260	494	27819
$2\ ^5A_{1g}$	2.294	488	29209	2.262	494	27841
$4\ ^5E_g$	2.292	489	28793	2.261	495	28031
$4\ ^5T_{2g}$	2.293	489	28684	2.263	492	28240

[a] Mixings and avoided crossings between states of the $4f^6(^7F)5dt^1_{2g}$ and $4f^6(^7F)ITE^1_{a_{1g}}$ configurations make most energy curves strongly anharmonic. The shape of the energy curves can be seen in Fig. S1. A value of $d_{\mathrm{Eu-F},e}$ for states of the $4f^6(^7F)5dt^1_{2g}$ configuration of about 2.421 Å can be deduced from states in the ^8E_g and $^8A_{1g}$ symmetry blocks where the $4f^6(^7F) \times ITE_{a_{1g}}$ coupling is absent.

[b] The energy difference between the Eu^{3+} $4f^6 - 1^7A_{2g}$ and the Eu^{2+} $4f^7 - 1^8A_{1u}$ minima at MS-RASPT2 level is 17494 cm^{-1}.

TABLE S2: Spectroscopic constants of the ground and excited states of Eu^{2+} and Eu^{3+} -doped SrF_2 cubic defects calculated using the relativistic spin-free second order Douglas-Kroll-Hess Hamiltonian with AIMP SrF_2 embedding. The embedded cluster RASSCF results include basic bonding interactions and $4f$–shell radial correlation; the MS-RASPT2 ones include also dynamic correlation of 79 or 78 valence electrons in the Eu $5s, 5p$, F $2s, 2p$, closed shells and Eu $4f, 5d, 6s$ open shells. Eu–F bond distances ($d_{\mathrm{Eu-F},e}$ in Å), EuF_8 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), and minimum-to-minimum energy differences (T_e in cm^{-1}) are given. See Figs. S1, S2 and text for details.

	RASSCF			MS-RASPT2		
term	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e
			Eu^{2+}-doped SrF_2			
$4f^7(^8F)$						
$1\ ^8A_{1u}$	2.522	363	0	2.470	370	0
			$4f^6(5d + ITE_{a_{1g}})^1$ excited states			
$4f^6(^7F)5de_g^1$						
Octets						
$1\ ^8T_{2g}$	2.506	366	25443	2.451	371	28455
$1\ ^8E_g$	2.503	363	25933	2.448	374	29048
$1\ ^8T_{1g}$	2.506	365	26378	2.451	366	29114
$2\ ^8T_{1g}$	2.506	365	27436	2.451	377	30359
$2\ ^8T_{2g}$	2.505	365	29232	2.450	362	31344
Sextets						
$1\ ^6T_{1g}$	2.506	365	31590	2.451	372	32521
$1\ ^6T_{2g}$	2.504	364	35498	2.448	360	35531
$1\ ^6E_g$	2.502	360	36320	2.444	372	36179
$2\ ^6T_{1g}$	2.505	364	36826	2.449	365	36292
$2\ ^6T_{2g}$	2.502	362	39728	2.448	375	38266
$4f^6(^7F)(5dt_{2g}^1 + ITE_{a_{1g}}^1)$ [a]						
Octets						
$3\ ^8T_{2g}$	2.558	363	41696	2.503	430	45834
$3\ ^8T_{1g}$	2.555	363	42315	2.501	522	45862
$2\ ^8E_g$	2.557	363	41455	2.504	364	45864
$4\ ^8T_{1g}$	2.557	363	44592	2.502	465	47230
$1\ ^8A_{2g}$	2.558	362	45705	2.374	332	47522
$3\ ^8E_g$	2.557	363	45158	2.503	367	48766
$4\ ^8T_{2g}$	2.558	362	45750	2.498	344	48922
$5\ ^8T_{1g}$	2.558	362	46529	2.462	382	48981
$1\ ^8A_{1g}$	2.558	362	46545	2.504	367	49692
$5\ ^8T_{2g}$	2.462	597	49705	2.451	932	50005
$2\ ^8A_{2g}$	2.462	588	49734	2.460	524	50108
$6\ ^8T_{1g}$	2.470	553	49974	2.458	518	50492
			$4f^7$ excited states			
$4f^7(^6P)$						
$1\ ^6T_{1u}$	2.522	362	33747	2.469	369	30725
$4f^7(^6I)$						
$1\ ^6T_{2u}$	2.522	363	37184	2.468	369	34372
$1\ ^6E_u$	2.521	363	37206	2.468	370	34585

$2\ ^6T_{2u}$	2.522	363	37356	2.469	369	34713
$1\ ^6A_{2u}$	2.522	363	37206	2.469	369	34713
$1\ ^6A_{1u}$	2.522	363	37431	2.469	369	34811
$2\ ^6T_{1u}$	2.522	363	37410	2.469	369	34819
$4f^7(^6D)$						
$2\ ^6E_u$	2.521	363	41156	2.468	370	37346
$3\ ^6T_{2u}$	2.522	362	41288	2.469	369	37454
$4f^7(^6G,^6F)$						
$4\ ^6T_{2u}$	2.519	362	55029	2.466	369	49353
$3\ ^6E_u$	2.521	363	55497	2.467	370	49494
$3\ ^6T_{1u}$	2.519	362	55235	2.466	369	49557
$2\ ^6A_{2u}$	2.521	363	55518	2.467	370	49951
$2\ ^6A_{1u}$	2.522	363	56111	2.470	369	50135
$5\ ^6T_{2u}$	2.522	363	55746	2.469	369	50404
$4\ ^6T_{1u}$	2.523	363	56043	2.470	369	50582
$4f^7(^6H)$						
$5\ ^6T_{1u}$	2.520	363	61170	2.467	369	55007
$4\ ^6E_u$	2.520	363	61293	2.467	370	55073
$6\ ^6T_{1u}$	2.522	363	61612	2.469	370	55401
$6\ ^6T_{2u}$	2.522	363	61682	2.469	370	55561
			Eu^{3+}-doped SrF_2			
$4f^6(^7F)$ [b]						
$1\ ^7A_{2g}$	2.346	436	0	2.310	440	0
$1\ ^7T_{1g}$	2.349	432	1037	2.314	447	1265
$1\ ^7T_{2g}$	2.349	431	1281	2.315	445	1387
$4f^6(^5D)$						
$1\ ^5E_g$	2.347	434	23717	2.311	449	21930
$1\ ^5T_{2g}$	2.348	432	23858	2.313	447	22047
$4f^6(^5L,^5G)$						
$2\ ^5E_g$	2.346	436	27364	2.310	448	26282
$1\ ^5T_{1g}$	2.346	436	27400	2.310	448	26362
$1\ ^5A_{1g}$	2.346	435	27413	2.310	449	26577
$2\ ^5T_{2g}$	2.348	432	28021	2.310	448	26615
$2\ ^5T_{1g}$	2.348	433	28010	2.313	448	27059
$3\ ^5E_g$	2.349	432	28171	2.312	449	27133
$2\ ^5A_{1g}$	2.349	431	28999	2.314	450	27539
$3\ ^5T_{2g}$	2.349	431	28174	2.314	445	27540
$3\ ^5T_{1g}$	2.349	432	28788	2.313	447	27604
$4\ ^5E_g$	2.349	432	28639	2.313	448	27759
$4\ ^5T_{2g}$	2.349	433	28521	2.315	450	27843

[a] Mixings and avoided crossings between states of the $4f^6(^7F)5dt^1_{2g}$ and $4f^6(^7F)ITE^1_{a_{1g}}$ configurations make most energy curves strongly anharmonic. The shape of the energy curves can be seen in Fig. S1. A value of $d_{\mathrm{Eu-F},e}$ for states of the $4f^6(^7F)5dt^1_{2g}$ configuration of about 2.504 Å can be deduced from states in the ^8E_g and $^8A_{1g}$ symmetry blocks where the $4f^6(^7F) \times ITE_{a_{1g}}$ coupling is absent.

[b] The energy difference between the Eu^{3+} $4f^6 - 1^7A_{2g}$ and the Eu^{2+} $4f^7 - 1^8A_{1u}$ minima at MS-RASPT2 level is 18459 cm^{-1}.

TABLE S3: Spectroscopic constants of the ground and excited states of Eu^{2+} and Eu^{3+} -doped BaF_2 cubic defects calculated using the relativistic spin-free second order Douglas-Kroll-Hess Hamiltonian with AIMP BaF_2 embedding. The embedded cluster RASSCF results include basic bonding interactions and $4f$–shell radial correlation; the MS-RASPT2 ones include also dynamic correlation of 79 or 78 valence electrons in the Eu $5s, 5p$, F $2s, 2p$, closed shells and Eu $4f, 5d, 6s$ open shells. Eu–F bond distances ($d_{\mathrm{Eu-F},e}$ in Å), EuF_8 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), and minimum-to-minimum energy differences (T_e in cm^{-1}) are given. See Fig. S1, S2 and text for details.

	RASSCF			MS-RASPT2		
term	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e
			Eu^{2+}-doped BaF_2			
$4f^7(^8F)$						
$1\ ^8A_{1u}$	2.621	311	0	2.558	320	0
			$4f^6(5d + ITE_{a_{1g}})^1$ excited states			
$4f^6(^7F)5de_g^1$						
Octets						
$1\ ^8T_{2g}$	2.599	277	26522	2.533	327	29705
$1\ ^8T_{1g}$	2.601	276	27396	2.534	327	30323
$1\ ^8E_g$	2.597	293	27101	2.535	324	30458
$2\ ^8T_{1g}$	2.601	276	28458	2.534	326	31578
$2\ ^8T_{2g}$	2.597	294	30334	2.532	327	32626
Sextets						
$1\ ^6T_{1g}$	2.601	275	32542	2.533	323	33714
$1\ ^6T_{2g}$	2.596	297	36528	2.529	325	36784
$1\ ^6E_g$	2.595	307	37442	2.526	325	37547
$2\ ^6T_{1g}$	2.597	292	37819	2.530	325	37574
$2\ ^6T_{2g}$	2.595	309	40792	2.529	322	39610
$4f^6(^7F)(5dt_{2g}^1 + ITE_{a_{1g}}^1)$ [a]						
Octets						
$3\ ^8T_{2g}$	2.655	319	39787	2.591	317	44164
$2\ ^8E_g$	2.655	319	39537	2.591	316	44166
$3\ ^8T_{1g}$	2.653	325	40503	2.588	317	44315
$4\ ^8T_{1g}$	2.655	319	42698	2.591	315	45569
$3\ ^8E_g$	2.655	319	43245	2.591	316	47066
$1\ ^8A_{2g}$	2.656	318	43739	2.500	812	47092
$4\ ^8T_{2g}$	2.656	319	43772	2.599	416	47222
$5\ ^8T_{1g}$	2.656	318	44577	2.599	475	47679
$1\ ^8A_{1g}$	2.656	318	44577	2.591	315	47969
$5\ ^8T_{2g}$	2.530	467	49334	2.516	480	49419
$2\ ^8A_{2g}$	2.526	486	49362	2.540	455	49457
$6\ ^8T_{1g}$	2.552	345	49428	2.523	466	49529
			$4f^7$ excited states			
$4f^7(^6P)$						
$1\ ^6T_{1u}$	2.620	310	33822	2.556	320	30960
$4f^7(^6I)$						
$1\ ^6T_{2u}$	2.620	310	37264	2.555	321	34626
$1\ ^6E_u$	2.620	310	37287	2.555	321	34834

$2\ ^6T_{2u}$	2.620	310	37419	2.556	320	34956
$1\ ^6A_{2u}$	2.620	310	37281	2.556	320	34960
$1\ ^6A_{1u}$	2.621	310	37476	2.557	320	35019
$2\ ^6T_{1u}$	2.621	310	37455	2.557	320	35027
$4f^7(^6D)$						
$2\ ^6E_u$	2.620	310	41246	2.555	321	37609
$3\ ^6T_{2u}$	2.620	310	41359	2.555	317	37723
$4f^7(^6G,^6F)$						
$4\ ^6T_{2u}$	2.618	309	55213	2.553	353	49754
$3\ ^6E_u$	2.619	310	55606	2.555	320	49781
$3\ ^6T_{1u}$	2.618	309	55424	2.554	323	49939
$2\ ^6A_{2u}$	2.619	310	55627	2.555	320	50251
$2\ ^6A_{1u}$	2.621	310	56112	2.557	320	50311
$5\ ^6T_{2u}$	2.620	310	55825	2.555	320	50644
$4\ ^6T_{1u}$	2.622	310	56034	2.557	321	50741
$4f^7(^6H)$						
$5\ ^6T_{1u}$	2.619	310	61316	2.554	322	55355
$4\ ^6E_u$	2.619	310	61439	2.554	321	55415
$6\ ^6T_{1u}$	2.620	310	61688	2.556	320	55635
$6\ ^6T_{2u}$	2.620	310	61734	2.557	320	55787
			Eu^{3+}-doped BaF_2			
$4f^6(^7F)$ [b]						
$1\ ^7A_{2g}$	2.399	409	0	2.360	401	0
$1\ ^7T_{1g}$	2.401	408	897	2.363	400	1128
$1\ ^7T_{2g}$	2.402	406	1124	2.364	401	1210
$4f^6(^5D)$						
$1\ ^5E_g$	2.400	410	23639	2.361	399	21897
$1\ ^5T_{2g}$	2.400	410	23765	2.362	399	21993
$4f^6(^5L,^5G)$						
$2\ ^5E_g$	2.399	408	27357	2.360	399	26329
$1\ ^5T_{1g}$	2.399	410	27385	2.360	399	26411
$1\ ^5A_{1g}$	2.399	410	27388	2.360	399	26620
$2\ ^5T_{2g}$	2.401	408	27924	2.360	396	26662
$2\ ^5T_{1g}$	2.401	409	27903	2.362	400	26986
$3\ ^5E_g$	2.401	409	28047	2.362	400	27091
$3\ ^5T_{2g}$	2.401	407	28047	2.365	400	27392
$2\ ^5A_{1g}$	2.402	406	28840	2.364	400	27409
$3\ ^5T_{1g}$	2.401	409	28671	2.362	399	27532
$4\ ^5E_g$	2.401	409	28527	2.363	401	27636
$4\ ^5T_{2g}$	2.401	410	28409	2.364	404	27664

[a] Mixings and avoided crossings between states of the $4f^6(^7F)5dt^1_{2g}$ and $4f^6(^7F)ITE^1_{a_{1g}}$ configurations make most energy curves strongly anharmonic. The shape of the energy curves can be seen in Fig. S1. A value of $d_{\mathrm{Eu-F},e}$ for states of the $4f^6(^7F)5dt^1_{2g}$ configuration of about 2.591 Å can be deduced from states in the ^8E_g and $^8A_{1g}$ symmetry blocks where the $4f^6(^7F) \times ITE_{a_{1g}}$ coupling is absent.

[b] The energy difference between the Eu^{3+} $4f^6 - 1^7A_{2g}$ and the Eu^{2+} $4f^7 - 1^8A_{1u}$ minima at MS-RASPT2 level is 17463 cm^{-1}.

TABLE S4: Spectroscopic constants of the ground and excited states of Eu^{2+} and Eu^{3+} -doped CaS octahedral defects calculated using the relativistic spin-free second order Douglas-Kroll-Hess Hamiltonian with AIMP CaS embedding. The embedded cluster RASSCF results include basic bonding interactions and $4f$–shell radial correlation; the MS-RASPT2 ones include also dynamic correlation of 99 or 98 valence electrons in the Eu $5s, 5p$, S $3s, 3p$, Ca $3p$ closed shells and Eu $4f, 5d, 6s$ open shells. Eu–S bond distances ($d_{\mathrm{Eu-S},e}$ in Å), EuS_6 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), and minimum-to-minimum energy differences (T_e in cm^{-1}) are given. See Fig. S1, S2 and text for details.

	RASSCF			MS-RASPT2		
term	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e
			Eu^{2+}-doped CaS			
$4f^7(^8F)$						
$1\ ^8A_{1u}$	2.911	305	0	2.876	284	0
$4f^6(^7F)5dt^1_{2g}$						
Octets						
$1\ ^8E_g$	2.892	303	20437	2.849	292	19952
$1\ ^8T_{2g}$	2.892	303	20504	2.848	279	20278
$1\ ^8T_{1g}$	2.893	303	20938	2.847	276	20492
$2\ ^8T_{1g}$	2.891	303	21914	2.848	282	21014
$2\ ^8E_g$	2.890	302	22710	2.847	283	21603
$1\ ^8A_{2g}$	2.890	302	23435	2.846	281	22004
$2\ ^8T_{2g}$	2.890	303	23428	2.847	280	22664
$1\ ^8A_{1g}$	2.890	302	24309	2.846	281	22750
$3\ ^8T_{1g}$	2.890	303	24324	2.847	281	23292
Sextets						
$1\ ^6T_{1g}$	2.890	303	25290	2.849	283	25656
$2\ ^6T_{1g}$	2.888	302	29115	2.845	284	28318
$1\ ^6E_g$	2.888	302	29049	2.845	284	28363
$1\ ^6T_{2g}$	2.887	302	29211	2.845	284	28543
$1\ ^6A_{2g}$	2.885	302	31345	2.843	284	29071
$2\ ^6T_{2g}$	2.885	302	31799	2.844	284	29805
$2\ ^6E_g$	2.884	301	32148	2.842	284	30267
$3\ ^6T_{1g}$	2.885	301	32565	2.843	283	30551
$1\ ^6A_{1g}$	2.883	301	33701	2.841	284	31007
$4f^6(^7F)(5de^1_g + 6sa^1_{1g})$						
Octets						
$3\ ^8T_{2g}$	2.925	303	40556	2.883	276	41139
$4\ ^8T_{1g}$	2.924	302	42007	2.881	275	42067
$3\ ^8E_g$	2.924	302	41934	2.878	277	42955
$5\ ^8T_{1g}$	2.924	302	42930	2.881	275	43750
$4\ ^8T_{2g}$	2.923	301	44113	2.881	274	43933
$6\ ^8T_{1g}$	2.947	303	56762	2.901	274	50986
$5\ ^8T_{2g}$	2.947	303	57017	2.901	275	51380
$2\ ^8A_{2g}$	2.947	304	57185	2.901	228	51621
Sextets						
$3\ ^6T_{2g}$	2.891	303	45053	2.849	281	45389
$4\ ^6T_{1g}$	2.905	292	45346	2.850	453	45722
$3\ ^6E_g$	2.891	302	45660	2.849	281	45741
$5\ ^6T_{1g}$	2.891	306	45779	2.850	419	45904
$4\ ^6T_{2g}$	2.895	298	46171	2.851	282	46328
$2\ ^6A_{1g}$	2.890	302	47372	2.848	280	46790
$6\ ^6T_{1g}$	2.891	303	48057	2.867	289	48651

5 $^6T_{2g}$	2.891	303	48057	2.854	273	49773
2 $^6A_{2g}$	2.890	303	49514	2.849	279	49881
7 $^6T_{1g}$	2.890	303	48286	2.855	252	49936
3 $^6A_{1g}$	2.890	303	48523	2.849	279	50183
4 ^6E_g	2.891	303	48285	2.852	277	50185
6 $^6T_{2g}$	2.890	303	48733	2.850	335	50219
8 $^6T_{1g}$	2.890	302	48651	2.857	286	50291
7 $^6T_{2g}$	2.890	303	48901	2.850	288	50447
9 $^6T_{1g}$	2.897	293	48941	2.851	265	50504
5 ^6E_g	2.890	303	48901	2.850	281	50535
10 $^6T_{1g}$	2.895	293	49536	2.850	285	50581
4 $^6A_{1g}$	2.891	303	49656	2.849	279	50754
8 $^6T_{2g}$	2.893	298	49367	2.849	271	50829
11 $^6T_{1g}$	2.890	304	49689	2.848	235	50994
9 $^6T_{2g}$	2.891	299	49831	2.849	300	51024
6 ^6E_g	2.890	298	49883	2.849	286	51095
10 $^6T_{2g}$	2.891	305	49899	2.849	282	51112
11 $^6T_{2g}$	2.890	300	50515	2.849	268	51280
3 $^6A_{2g}$	2.890	302	49842	2.849	280	51311
7 ^6E_g	2.893	303	50032	2.853	264	51366
12 $^6T_{2g}$	2.891	303	50685	2.848	277	51460
12 $^6T_{1g}$	2.895	304	49944	2.850	289	51473
8 ^6E_g	2.891	299	51194	2.849	279	51604
13 $^6T_{2g}$	2.892	297	51111	2.849	272	51886
13 $^6T_{1g}$	2.890	303	50558	2.849	279	51925
14 $^6T_{2g}$	2.890	304	51165	2.853	265	52342
14 $^6T_{1g}$	2.890	302	51147	2.853	273	52370
5 $^6A_{1g}$	2.890	302	51114	2.848	280	52373
15 $^6T_{1g}$	2.892	303	52685	2.849	266	52435
4 $^6A_{2g}$	2.890	302	51129	2.848	280	52482
9 ^6E_g	2.891	300	51865	2.857	261	52525
15 $^6T_{2g}$	2.893	302	51787	2.852	243	52581
16 $^6T_{2g}$	2.895	307	52917	2.851	293	52713
16 $^6T_{1g}$	2.901	296	53231	2.861	301	52753
10 ^6E_g	2.900	294	53098	2.860	306	52778
17 $^6T_{2g}$	2.894	298	53638	2.865	249	53831
11 ^6E_g	2.895	305	54308	2.849	276	54406
17 $^6T_{1g}$	2.891	303	54278	2.848	282	54553
6 $^6A_{1g}$	2.890	303	54514	2.849	279	54802
18 $^6T_{2g}$	2.891	302	54677	2.858	270	54820
5 $^6A_{2g}$	2.890	302	54426	2.849	278	54885
19 $^6T_{2g}$	2.902	221	55628	2.848	281	55061
18 $^6T_{1g}$	2.891	303	55098	2.849	265	55216
12 ^6E_g	2.890	302	55202	2.848	275	55332
19 $^6T_{1g}$	2.891	303	55737	2.848	282	55441
20 $^6T_{2g}$	2.900	378	55967	2.848	236	55694
13 ^6E_g	2.893	304	56276	2.848	262	55792
21 $^6T_{2g}$	2.891	307	56681	2.846	309	56063
20 $^6T_{1g}$	2.891	303	56887	2.848	263	56265
6 $^6A_{2g}$	2.890	302	56548	2.848	282	56266

$4f^7$ excited states

$4f^7(^6P)$						
1 $^6T_{1u}$	2.909	304	33449	2.870	280	30009
$4f^7(^6I)$						
1 $^6T_{2u}$	2.909	304	36913	2.869	281	33773
1 $^6A_{1u}$	2.909	304	36931	2.870	281	33887
2 $^6T_{1u}$	2.909	304	36938	2.869	280	33914

$2\ ^6T_{2u}$	2.909	304	36944	2.869	280	33957
$1\ ^6E_u$	2.909	304	36957	2.870	280	33957
$1\ ^6A_{2u}$	2.909	304	36922	2.870	281	34063
$4f^7(^6D)$						
$3\ ^6T_{2u}$	2.909	304	40805	2.869	281	36463
$2\ ^6E_u$	2.908	304	40838	2.869	280	36637
			Eu^{3+}-doped CaS			
$4f^6(^7F)$ [a]						
$1\ ^7T_{1g}$	2.763	320	0	2.728	308	0
$1\ ^7T_{2g}$	2.764	321	563	2.729	308	472
$1\ ^7A_{2g}$	2.764	320	412	2.731	308	793
$4f^6(^5D)$						
$1\ ^5T_{2g}$	2.763	320	23001	2.727	307	21050
$1\ ^5E_g$	2.763	320	23064	2.727	307	21176
$4f^6(^5L,^5G)$						
$1\ ^5T_{1g}$	2.763	320	26932	2.726	307	25573
$2\ ^5E_g$	2.763	320	26867	2.726	307	25617
$1\ ^5A_{1g}$	2.763	320	27262	2.726	307	25619
$2\ ^5T_{2g}$	2.763	320	26830	2.727	307	25994
$3\ ^5T_{2g}$	2.763	320	27068	2.725	307	26111
$3\ ^5E_g$	2.763	320	27251	2.726	307	26238
$4\ ^5T_{2g}$	2.763	320	27871	2.727	308	26253
$2\ ^5T_{1g}$	2.763	320	27246	2.727	307	26322
$3\ ^5T_{1g}$	2.763	320	27760	2.727	308	26552
$4\ ^5E_g$	2.763	320	27731	2.727	307	26621
$2\ ^5A_{1g}$	2.763	320	27651	2.727	307	26751

[a] The energy difference between the Eu^{3+} $4f^6 - 1^7T_{1g}$ and the Eu^{2+} $4f^7 - 1^8A_{1u}$ at MS-RASPT2 level is 25681 cm^{-1}.

TABLE S5: Spectroscopic constants of the ground and excited states of Eu^{2+} and Eu^{3+} -doped SrS octahedral defects calculated using the relativistic spin-free second order Douglas-Kroll-Hess Hamiltonian with AIMP SrS embedding. The embedded cluster RASSCF results include basic bonding interactions and $4f$–shell radial correlation; the MS-RASPT2 ones include also dynamic correlation of 99 or 98 valence electrons in the Eu $5s, 5p$, S $3s, 3p$, Sr $4p$ closed shells and Eu $4f, 5d, 6s$ open shells. Eu–S bond distances ($d_{\mathrm{Eu-S},e}$ in Å), EuS_6 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), and minimum-to-minimum energy differences (T_e in cm^{-1}) are given. See Fig. S1, S2 and text for details.

	RASSCF			MS-RASPT2		
term	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e
			Eu^{2+}-doped SrS			
$4f^7(^8S)$						
$1\ ^8A_{1u}$	2.984	282	0	2.974	267	0
			$4f^6(5d+6s)^1$ excited states			
$4f^6(^7F)5dt^1_{2g}$						
Octets						
$1\ ^8T_{2g}$	2.963	280	21571	2.943	264	21873
$1\ ^8E_g$	2.963	280	21479	2.944	263	21960
$1\ ^8T_{1g}$	2.963	280	21975	2.943	263	22092
$2\ ^8T_{1g}$	2.963	280	22987	2.943	264	22596
$2\ ^8E_g$	2.962	279	23840	2.942	264	23747
$1\ ^8A_{2g}$	2.961	279	24611	2.941	264	24194
$2\ ^8T_{2g}$	2.962	279	24568	2.942	264	24309
$1\ ^8A_{1g}$	2.961	279	25482	2.941	264	24922
$3\ ^8T_{1g}$	2.961	279	25493	2.941	264	24934
Sextets						
$1\ ^6T_{1g}$	2.962	279	26429	2.945	264	27174
$2\ ^6T_{1g}$	2.958	279	30382	2.940	264	30034
$1\ ^6E_g$	2.958	279	30329	2.940	265	30073
$1\ ^6T_{2g}$	2.958	279	30514	2.940	264	30279
$1\ ^6A_{2g}$	2.955	278	32748	2.938	264	30893
$2\ ^6T_{2g}$	2.955	278	33191	2.938	264	31633
$2\ ^6E_g$	2.955	278	33564	2.936	264	32153
$3\ ^6T_{1g}$	2.956	278	33949	2.937	263	32409
$1\ ^6A_{1g}$	2.954	277	35165	2.935	264	32927
$4f^6(^7F)(5de^1_g+6sa^1_{1g})$						
Octets						
$3\ ^8T_{2g}$	3.000	277	39729	2.984	263	40486
$4\ ^8T_{1g}$	2.998	278	41229	2.982	263	41435
$3\ ^8E_g$	2.999	278	41114	2.981	262	42198
$5\ ^8T_{1g}$	2.998	278	42128	2.982	263	43095
$4\ ^8T_{2g}$	2.998	277	43320	2.982	262	43333
$6\ ^8T_{1g}$	3.022	282	55155	2.999	261	49671
$5\ ^8T_{2g}$	3.022	283	55385	3.000	264	50028
$2\ ^8A_{2g}$	3.023	283	55559	3.000	265	50087
Sextets						
$4\ ^6T_{1g}$	2.985	274	45413	2.973	258	46244
$3\ ^6T_{2g}$	2.962	279	46169	2.945	263	46885
$3\ ^6E_g$	2.962	278	46753	2.945	266	47237
$5\ ^6T_{1g}$	2.963	278	46857	2.946	263	47409
$4\ ^6T_{2g}$	2.972	272	46891	2.953	250	47576

2 $^6A_{1g}$	2.961	279	48528	2.943	264	48382
6 $^6T_{1g}$	2.963	280	49135	2.951	379	49378
7 $^6T_{1g}$	2.962	277	49407	2.971	266	50347
5 $^6T_{2g}$	2.962	280	49137	2.957	286	50372
4 ^6E_g	2.962	279	49401	2.978	254	50945
2 $^6A_{2g}$	2.962	279	50632	2.945	264	51398
6 $^6T_{2g}$	2.961	278	49888	2.946	268	51558
3 $^6A_{1g}$	2.962	279	49644	2.945	264	51680
8 $^6T_{1g}$	2.969	274	49666	2.941	267	51701
7 $^6T_{2g}$	2.961	273	50068	2.946	256	51897
9 $^6T_{1g}$	2.961	283	49798	2.945	270	51954
5 ^6E_g	2.961	279	50068	2.945	265	52016
8 $^6T_{2g}$	2.969	286	50179	2.954	242	52047
10 $^6T_{1g}$	2.975	285	50124	2.945	264	52059
9 $^6T_{2g}$	2.963	280	50866	2.952	295	52226
4 $^6A_{1g}$	2.962	279	50773	2.945	264	52266
6 ^6E_g	2.973	267	50724	2.950	306	52390
11 $^6T_{1g}$	2.961	278	50851	2.941	261	52479
10 $^6T_{2g}$	2.961	280	51017	2.945	257	52629
7 ^6E_g	2.961	281	51071	2.944	266	52665
11 $^6T_{2g}$	2.966	273	51524	2.942	266	52700
3 $^6A_{2g}$	2.962	279	50983	2.944	263	52853
12 $^6T_{1g}$	2.963	283	50885	2.962	229	52990
12 $^6T_{2g}$	2.962	280	51777	2.945	262	53014
8 ^6E_g	2.966	277	52157	2.942	265	53135
13 $^6T_{1g}$	2.961	279	51710	2.954	208	53381
13 $^6T_{2g}$	2.966	278	52033	2.944	262	53418
14 $^6T_{1g}$	2.961	279	52315	2.946	255	53440
9 ^6E_g	2.964	279	52876	2.946	276	53528
14 $^6T_{2g}$	2.961	279	52321	2.958	239	53731
15 $^6T_{1g}$	2.967	270	53682	2.967	253	53792
4 $^6A_{2g}$	2.961	279	52290	2.989	286	53820
15 $^6T_{2g}$	2.963	280	52795	2.962	264	53826
5 $^6A_{1g}$	2.961	279	52286	2.942	264	53991
16 $^6T_{1g}$	2.966	292	53777	2.959	238	54072
10 ^6E_g	2.967	286	53723	2.943	268	54102
16 $^6T_{2g}$	2.963	282	53832	2.959	241	54109
17 $^6T_{2g}$	2.972	271	54385	2.955	245	54366
17 $^6T_{1g}$	2.962	280	55351	2.992	368	54662
5 $^6A_{2g}$	2.962	279	55555	2.992	376	54687
18 $^6T_{2g}$	2.966	267	55752	2.988	348	54907
11 ^6E_g	2.963	280	55266	2.943	264	55993
19 $^6T_{2g}$	2.969	298	55878	2.954	363	56141
18 $^6T_{1g}$	2.963	279	56159	2.952	470	56175
6 $^6A_{1g}$	2.962	279	55652	2.945	264	56331
6 $^6A_{2g}$	2.959	250	57701	2.958	373	56456
20 $^6T_{2g}$	2.961	274	56965	2.952	519	56530
19 $^6T_{1g}$	2.962	275	56801	2.950	354	56809
12 ^6E_g	2.961	279	56370	2.943	263	56926
20 $^6T_{1g}$	2.959	246	57966	2.954	376	57039
21 $^6T_{2g}$	2.959	259	57774	2.952	436	57341
13 ^6E_g	2.962	280	57289	2.943	263	57378
21 $^6T_{1g}$	3.000	684	58336	2.950	1149	57916
22 $^6T_{2g}$	3.000	624	58487	2.954	723	58008
7 $^6A_{2g}$	3.000	552	58587	2.951	919	58135

$4f^7$ excited states

$4f^7(^6P)$

1 $^6T_{1u}$	2.982	281	33535	2.969	267	30266

$4f^7(^6I)$						
$1\ ^6T_{2u}$	2.982	281	37010	2.968	265	34034
$1\ ^6A_{1u}$	2.982	281	37031	2.969	267	34135
$2\ ^6T_{1u}$	2.982	281	37036	2.969	265	34178
$1\ ^6E_u$	2.982	281	37052	2.969	266	34215
$2\ ^6T_{2u}$	2.982	281	37040	2.969	264	34228
$1\ ^6A_{2u}$	2.982	281	37014	2.969	267	34308
$4f^7(^6D)$						
$3\ ^6T_{2u}$	2.981	281	40916	2.968	265	36773
$2\ ^6E_u$	2.981	281	40948	2.968	267	36908
			Eu^{3+}-doped SrS			
$4f^6(^7F)$ [a]						
$1\ ^7T_{1g}$	2.812	300	0	2.799	286	0
$1\ ^7T_{2g}$	2.813	300	531	2.800	285	425
$1\ ^7A_{2g}$	2.813	300	366	2.801	295	654
$4f^6(^5D)$						
$1\ ^5T_{2g}$	2.812	300	23014	2.797	285	21111
$1\ ^5E_g$	2.812	300	23069	2.798	284	21228
$4f^6(^5L,^5G)$						
$1\ ^5T_{1g}$	2.811	300	26960	2.797	285	25657
$2\ ^5E_g$	2.811	300	26901	2.797	283	25702
$1\ ^5A_{1g}$	2.812	300	27254	2.797	285	25710
$2\ ^5T_{2g}$	2.811	299	26866	2.798	284	26033
$3\ ^5T_{2g}$	2.812	300	27084	2.797	285	26210
$3\ ^5E_g$	2.812	300	27248	2.797	284	26320
$4\ ^5T_{2g}$	2.812	300	27873	2.797	285	26328
$2\ ^5T_{1g}$	2.812	300	27241	2.797	285	26385
$3\ ^5T_{1g}$	2.811	300	27780	2.798	284	26599
$4\ ^5E_g$	2.812	300	27749	2.798	285	26665
$2\ ^5A_{1g}$	2.811	300	27675	2.798	284	26785

[a] The energy difference between the Eu^{3+} $4f^6 - 1^7T_{1g}$ and the Eu^{2+} $4f^7 - 1^8A_{1u}$ at MS-RASPT2 level is 19903 cm^{-1}.

TABLE S6: Spectroscopic constants of the ground and excited states of Eu^{2+} and Eu^{3+} -doped BaS octahedral defects calculated using the relativistic spin-free second order Douglas-Kroll-Hess Hamiltonian with AIMP BaS embedding. The embedded cluster RASSCF results include basic bonding interactions and $4f$–shell radial correlation; the MS-RASPT2 ones include also dynamic correlation of 99 or 98 valence electrons in the Eu $5s, 5p$, S $3s, 3p$, Ba $5p$ closed shells and Eu $4f, 5d, 6s$ open shells. Eu–S bond distances ($d_{\mathrm{Eu-S},e}$ in Å), EuS_6 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), and minimum-to-minimum energy differences (T_e in cm^{-1}) are given. See Fig. S1, S2 and text for details.

	RASSCF			MS-RASPT2		
term	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e
			Eu^{2+}-doped BaS			
$4f^7(^8S)$						
$1\ ^8A_{1u}$	3.135	227	0	3.087	204	0
			$4f^6 5d^1$ excited states			
$4f^6(^7F)5dt^1_{2g}$						
Octets						
$1\ ^8T_{2g}$	3.112	226	23409	3.034	196	22371
$1\ ^8T_{1g}$	3.113	226	23722	3.033	195	22555
$1\ ^8E_g$	3.112	226	23268	3.038	197	22742
$2\ ^8T_{1g}$	3.112	226	24713	3.034	197	23036
$2\ ^8E_g$	3.109	225	25617	3.034	196	24531
$2\ ^8T_{2g}$	3.109	225	26344	3.030	194	24667
$1\ ^8A_{2g}$	3.107	225	26440	3.032	196	25014
$3\ ^8T_{1g}$	3.107	225	27273	3.030	195	25323
$1\ ^8A_{1g}$	3.107	224	27275	3.032	196	25703
Sextets						
$1\ ^6T_{1g}$	3.109	225	28108	3.034	194	28268
$2\ ^6T_{1g}$	3.104	223	32046	3.025	192	31068
$1\ ^6E_g$	3.104	223	32006	3.025	191	31108
$1\ ^6T_{2g}$	3.103	222	32239	3.024	192	31345
$1\ ^6A_{2g}$	3.099	219	34467	3.022	191	31968
$2\ ^6T_{2g}$	3.099	219	34883	3.021	191	32662
$2\ ^6E_g$	3.099	219	35243	3.018	190	33167
$3\ ^6T_{1g}$	3.100	218	35547	3.019	191	33410
$1\ ^6A_{1g}$	3.096	220	36846	3.016	189	33907
$4f^6(^7F)5de^1_g$						
Octets						
$3\ ^8T_{2g}$	3.145	221	37477	3.056	162	37539
$4\ ^8T_{1g}$	3.142	219	39025	3.051	163	38254
$3\ ^8E_g$	3.143	219	38842	3.059	188	39554
$5\ ^8T_{1g}$	3.142	218	39846	3.050	161	40091
$4\ ^8T_{2g}$	3.141	217	41019	3.044	153	40265
			$4f^7$ excited states			
$4f^7(^6P)$						
$1\ ^6T_{1u}$	3.134	227	33666	3.080	158	30453
$4f^7(^6I)$						
$1\ ^6T_{2u}$	3.134	227	37150	3.075	254	34195

$2\ ^6T_{1u}$	3.134	227	37186	3.080	202	34350
$1\ ^6A_{1u}$	3.134	227	37183	3.080	202	34353
$1\ ^6E_u$	3.134	227	37187	3.081	204	34416
$2\ ^6T_{2u}$	3.134	227	37187	3.080	188	34422
$1\ ^6A_{2u}$	3.134	227	37153	3.080	202	34517
$4f^7(^6D)$						
$3\ ^6T_{2u}$	3.133	227	41086	3.079	176	37006
$2\ ^6E_u$	3.133	227	41109	3.079	171	37138
			Eu^{3+}-doped BaS			
$4f^6(^7F)$ [a]						
$1\ ^7T_{1g}$	2.893	259	0	2.828	249	0
$1\ ^7T_{2g}$	2.893	259	464	2.829	249	363
$1\ ^7A_{2g}$	2.940	374	-218	2.831	249	592
$4f^6(^5D)$						
$1\ ^5T_{2g}$	2.892	259	23028	2.826	249	21123
$1\ ^5E_g$	2.892	259	23064	2.827	249	21227
$4f^6(^5L,^5G)$						
$1\ ^5T_{1g}$	2.892	258	27001	2.826	249	25692
$2\ ^5E_g$	2.891	259	26955	2.826	248	25738
$1\ ^5A_{1g}$	2.892	259	27220	2.826	248	25746
$2\ ^5T_{2g}$	2.891	259	26924	2.827	248	26008
$3\ ^5T_{2g}$	2.892	259	27098	2.826	249	26265
$3\ ^5E_g$	2.892	259	27223	2.826	248	26354
$4\ ^5T_{2g}$	2.892	259	27859	2.826	248	26357
$2\ ^5T_{1g}$	2.892	259	27214	2.826	248	26393
$3\ ^5T_{1g}$	2.892	259	27806	2.827	249	26589
$4\ ^5E_g$	2.892	259	27770	2.827	248	26647
$2\ ^5A_{1g}$	2.892	259	27708	2.827	248	26753

[a] The energy difference between the Eu^{3+} $4f^6 - 1^7T_{1g}$ and the Eu^{2+} $4f^7 - 1^8A_{1u}$ at MS-RASPT2 level is 24089 cm^{-1}.

TABLE S7. O_h Γ_{6u}, Γ_{7u}, and Γ_{8u} states derived from the lowest energy multiplets of the $4f^7$ configuration.

	2J								Γ_{6u}	Γ_{7u}	Γ_{8u}
$4f^7(^8S_J)$			7						1	1	1
$4f^7(^6P_J)$		3	5	7					1	2	3
$4f^7(^6D_J)$	1	3	5	7	9				3	2	5
$4f^7(^6F_J)$	1	3	5	7	9	11			4	3	7
$4f^7(^6G_J)$		3	5	7	9	11	13		4	5	9
$4f^7(^6H_J)$			5	7	9	11	13	15	5	6	11
$4f^7(^6I_J)$				7	9	11	13	15	17	7	6	13

TABLE S8. O_h Γ_{6g}, Γ_{7g}, and Γ_{8g} states derived from the ${}^7F_J \times ({}^2E_g +^2 T_{2g} +^2 A_{1g})$ coupling.

		Total			High spin			Low spin		
	J	Γ_{6g}	Γ_{7g}	Γ_{8g}	Γ_{6g}	Γ_{7g}	Γ_{8g}	Γ_{6g}	Γ_{7g}	Γ_{8g}
$4f^6({}^7F_J) \times^2 E_g$										
	0	0	0	1	0	0	1	0	0	0
	1	1	1	2	1	1	1	0	0	1
	2	2	2	3	1	1	2	1	1	1
	3	2	2	5	1	1	3	1	1	2
	4	3	3	6	2	2	3	1	1	3
	5	4	4	7	2	2	4	2	2	3
	6	4	4	9	2	2	5	2	2	4
	${}^7F_{0,1,2,3,4,5,6}$	16	16	33	9	9	19	7	7	14
$4f^6({}^7F_J) \times^2 T_{2g}$										
	0	0	1	1	0	1	1	0	0	0
	1	1	2	3	1	1	2	0	1	1
	2	3	2	5	2	1	3	1	1	2
	3	4	3	7	2	2	4	2	1	3
	4	4	5	9	2	3	5	2	2	4
	5	5	6	11	3	3	6	2	3	5
	6	7	6	13	4	3	7	3	3	6
	${}^7F_{0,1,2,3,4,5,6}$	24	25	49	14	14	28	10	11	21
$4f^6({}^7F_J) \times^2 A_{1g}$										
	0	1	0	0	1	0	0	0	0	0
	1	1	0	1	0	0	1	1	0	0
	2	0	1	2	0	1	1	0	0	1
	3	1	2	2	1	1	1	0	1	1
	4	2	1	3	1	0	2	1	1	1
	5	2	1	4	1	1	2	1	0	2
	6	2	3	4	1	2	2	1	1	2
	${}^7F_{0,1,2,3,4,5,6}$	9	8	16	5	5	9	4	3	7

TABLE S9: Spectroscopic constants and analyses of the spin-orbit wave functions of the ground and lowest lying excited states of Eu^{2+} and Eu^{3+} -doped CaF_2 cubic defects. Eu–F bond distances ($d_{\mathrm{Eu-F},e}$ in Å), EuF_8 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), minimum-to-minimum energy differences (T_e in cm^{-1}), and relative absorption and emission oscillator strengths (f_i^{abs}/f_{ref} and f_i^{emi}/f_{ref}) are given. Calculated radiative emission lifetime for the $4f^6(^7F_J)5de_g^1$ – 1 Γ_{8g} excited state is 0.553 μs. Local distortion around the Eu^{2+}impurity, relative to experimental crystal structure d_{Ca-F}= 2.366 Å, is $d_{\mathrm{Eu-F},e}(1\Gamma_{6u}) - d_{\mathrm{Ca-F}} = +0.022$; ionic radii mismatch is +0.13 Å[31]. See Fig. 3, S3 and text for details.

State	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e	f_i^{abs}/f_{ref} [a]	f_i^{emi}/f_{ref} [a]	weights of terms larger than 10% [b]							
						Eu^{2+}-doped CaF_2							
$4f^7(^8S_{7/2})$ [c]													
1 Γ_{6u}	2.388	423	0		1.00	97.76	1 $^8A_{1u}$						
1 Γ_{8u}	2.388	423	0		0.86	97.76	1 $^8A_{1u}$						
1 Γ_{7u}	2.388	423	0		0.04	97.76	1 $^8A_{1u}$						
						$4f^6(5d + ITE_{a_{1g}})^1$ excited states							
$4f^6(^7F_J)5de_g^1$ High-Spin coupling [d]													
1 Γ_{8g}	2.373	428	25720	1.00		51.00	1 $^8T_{2g}$	31.49	1 $^8T_{1g}$	11.47	1 ^8E_g		
1 Γ_{7g}	2.373	428	25897	0.54		55.32	1 $^8T_{2g}$	34.13	1 $^8T_{1g}$				
2 Γ_{8g}	2.372	428	25984	0.09		68.21	1 $^8T_{2g}$	20.76	1 ^8E_g				
2 Γ_{7g}	2.372	428	26407	0.74		41.59	1 $^8T_{1g}$	41.14	1 $^8T_{2g}$	13.55	1 ^8E_g		
3 Γ_{8g}	2.372	427	26676	0.99		34.12	1 $^8T_{2g}$	29.75	1 ^8E_g	26.23	1 $^8T_{1g}$		
1 Γ_{6g}	2.372	427	26797	0.38		32.70	1 ^8E_g	27.51	1 $^8T_{2g}$	20.68	1 $^8T_{1g}$	14.25	2 $^8T_{1g}$
4 Γ_{8g}	2.373	428	27326	2.10		57.24	1 $^8T_{1g}$	17.05	1 $^8T_{2g}$	13.08	2 $^8T_{1g}$		
2 Γ_{6g}	2.372	428	27376	0.26		36.28	1 $^8T_{2g}$	19.85	2 $^8T_{1g}$	19.21	1 ^8E_g	18.83	1 $^8T_{1g}$
5 Γ_{8g}	2.372	426	27511	0.25		49.00	1 ^8E_g	27.02	2 $^8T_{1g}$	17.52	1 $^8T_{2g}$		
3 Γ_{7g}	2.372	428	27602	0.87		46.62	1 $^8T_{1g}$	28.71	1 ^8E_g	19.55	1 $^8T_{2g}$		
6 Γ_{8g}	2.372	427	27779	0.44		36.07	1 ^8E_g	34.16	1 $^8T_{2g}$	12.48	1 $^8T_{1g}$	10.57	2 $^8T_{2g}$
7 Γ_{8g}	2.372	429	28219	0.72		40.15	2 $^8T_{1g}$	22.52	1 $^8T_{1g}$	17.94	1 $^8T_{2g}$	17.64	2 $^8T_{2g}$
3 Γ_{6g}	2.372	429	28221	0.74		48.24	1 $^8T_{1g}$	19.50	2 $^8T_{1g}$	18.55	2 $^8T_{2g}$		
8 Γ_{8g}	2.372	428	28738	1.79		50.76	1 $^8T_{1g}$	24.95	2 $^8T_{1g}$	11.50	1 $^8T_{2g}$		
9 Γ_{8g}	2.372	428	28823	0.48		26.68	1 $^8T_{2g}$	23.99	1 ^8E_g	18.32	2 $^8T_{1g}$	16.50	1 $^8T_{1g}$
						14.01	2 $^8T_{2g}$						
4 Γ_{7g}	2.372	428	28870	0.60		31.19	1 $^8T_{2g}$	25.68	1 $^8T_{1g}$	22.02	1 ^8E_g	10.58	2 $^8T_{1g}$
						10.18	2 $^8T_{2g}$						
4 Γ_{6g}	2.372	429	28916	0.31		29.84	2 $^8T_{1g}$	24.84	1 $^8T_{2g}$	24.10	2 $^8T_{2g}$	15.49	1 $^8T_{1g}$
5 Γ_{7g}	2.372	430	29006	0.99		39.81	1 $^8T_{1g}$	30.80	1 $^8T_{2g}$	23.62	2 $^8T_{1g}$		
10 Γ_{8g}	2.372	428	29256	0.01		55.51	2 $^8T_{2g}$	22.40	1 ^8E_g	16.32	1 $^8T_{2g}$		
5 Γ_{6g}	2.372	429	29259	0.07		52.76	2 $^8T_{2g}$	23.28	1 $^8T_{2g}$	12.29	2 $^8T_{1g}$	10.12	1 ^8E_g
11 Γ_{8g}	2.372	428	29545	0.98		34.42	1 $^8T_{2g}$	26.81	1 $^8T_{1g}$	18.48	1 ^8E_g	15.65	2 $^8T_{1g}$
6 Γ_{6g}	2.372	429	29549	0.57		41.65	1 $^8T_{2g}$	19.23	1 $^8T_{1g}$	18.74	2 $^8T_{2g}$	14.56	2 $^8T_{1g}$
6 Γ_{7g}	2.372	429	30023	0.01		54.67	2 $^8T_{1g}$	18.58	2 $^8T_{2g}$	13.20	1 $^8T_{2g}$		
14 Γ_{8g}	2.372	429	30260	1.37		41.50	2 $^8T_{1g}$	26.42	1 $^8T_{1g}$	16.03	2 $^8T_{2g}$	10.30	1 $^8T_{2g}$
7 Γ_{7g}	2.372	428	30685			72.69	2 $^8T_{2g}$	13.28	1 ^8E_g				
15 Γ_{8g}	2.372	429	30738	3.19		65.59	1 $^8T_{1g}$	23.35	1 $^8T_{2g}$				
7 Γ_{6g}	2.372	429	30758	1.71		70.89	1 $^8T_{1g}$	23.27	1 $^8T_{2g}$				
16 Γ_{8g}	2.372	429	30867	0.87		55.89	2 $^8T_{2g}$	20.59	2 $^8T_{1g}$	13.81	1 $^8T_{1g}$		
8 Γ_{6g}	2.372	429	30998	0.14		54.15	2 $^8T_{2g}$	30.54	2 $^8T_{1g}$				
18 Γ_{8g}	2.372	428	31238	1.27		42.66	2 $^8T_{1g}$	20.62	1 $^8T_{1g}$	16.96	1 ^8E_g		
9 Γ_{6g}	2.372	428	31295	0.05		55.46	2 $^8T_{1g}$	17.91	2 $^8T_{2g}$	12.84	1 ^8E_g	10.56	1 $^8T_{2g}$
19 Γ_{8g}	2.372	429	31600	0.16		67.44	2 $^8T_{1g}$	11.14	1 ^8E_g				
9 Γ_{7g}	2.372	429	31753			76.40	2 $^8T_{1g}$						
20 Γ_{8g}	2.372	429	32531	0.02		87.68	2 $^8T_{2g}$						
21 Γ_{8g}	2.372	429	32707	0.01		78.56	2 $^8T_{2g}$	18.93	2 $^8T_{1g}$				
10 Γ_{7g}	2.372	429	32742			80.31	2 $^8T_{2g}$	18.12	2 $^8T_{1g}$				
$4f^6(^7F_J)5de_g^1$ Mixed-Spin coupling [d]													

12 Γ_{8g}	2.373	427	29855	0.24	50.18	1 $^6T_{1g}$	13.53	1 $^8T_{2g}$	12.57	2 $^8T_{1g}$	10.93	2 $^8T_{2g}$
13 Γ_{8g}	2.372	428	29950	0.38	42.22	1 $^6T_{1g}$	15.14	1 ^8E_g	12.74	2 $^8T_{2g}$	12.61	2 $^8T_{1g}$
					10.38	1 $^8T_{2g}$						
$4f^6(^7F_J)5de_g^1$ Low-Spin coupling [d]												
8 Γ_{7g}	2.372	427	31106	0.01	83.67	1 $^6T_{1g}$	12.47	1 $^6T_{2g}$				
17 Γ_{8g}	2.372	427	31202	0.17	81.84	1 $^6T_{1g}$						
10 Γ_{6g}	2.370	428	32743	0.02	49.43	1 $^6T_{1g}$	34.31	1 $^6T_{2g}$	13.51	2 $^6T_{1g}$		
22 Γ_{8g}	2.371	428	32877	0.04	54.33	1 $^6T_{1g}$	31.95	1 $^6T_{2g}$	11.23	2 $^6T_{1g}$		
11 Γ_{7g}	2.371	428	33177	0.03	75.35	1 $^6T_{1g}$	11.53	1 $^6T_{2g}$				
11 Γ_{6g}	2.369	428	33390	0.01	55.12	1 $^6T_{2g}$	26.34	1 ^6E_g	16.16	1 $^6T_{1g}$		
23 Γ_{8g}	2.370	428	33632	0.02	27.98	1 ^6E_g	26.93	1 $^6T_{1g}$	19.86	1 $^6T_{2g}$	18.97	2 $^6T_{1g}$
12 Γ_{7g}	2.370	429	33723		48.88	2 $^6T_{1g}$	23.30	1 ^6E_g	19.13	1 $^6T_{2g}$		
24 Γ_{8g}	2.369	428	34252	0.01	30.17	1 ^6E_g	29.69	2 $^6T_{1g}$	25.51	1 $^6T_{2g}$		
13 Γ_{7g}	2.370	430	34392		39.51	1 $^6T_{2g}$	31.62	2 $^6T_{1g}$	22.37	1 $^6T_{1g}$		
12 Γ_{6g}	2.372	429	34401	0.01	62.39	2 $^6T_{1g}$	17.50	1 $^6T_{1g}$				
25 Γ_{8g}	2.369	428	34962	0.02	39.13	2 $^6T_{1g}$	23.79	1 $^6T_{2g}$	22.94	1 ^6E_g	11.11	2 $^6T_{2g}$
26 Γ_{8g}	2.370	430	35076	0.01	50.56	1 $^6T_{2g}$	18.41	2 $^6T_{1g}$	13.40	1 $^6T_{1g}$	11.72	1 ^6E_g
27 Γ_{8g}	2.369	428	35778	0.02	32.90	1 ^6E_g	30.68	1 $^6T_{2g}$	23.64	2 $^6T_{1g}$		
13 Γ_{6g}	2.369	428	35820	0.01	41.06	1 $^6T_{2g}$	38.67	1 ^6E_g	11.84	1 $^6T_{1g}$		
14 Γ_{7g}	2.370	429	35994		63.69	2 $^6T_{1g}$	12.53	1 $^6T_{2g}$	12.35	1 ^6E_g		
28 Γ_{8g}	2.370	430	36086	0.01	82.38	2 $^6T_{2g}$	11.17	2 $^6T_{1g}$				
14 Γ_{6g}	2.369	430	36332	0.03	56.75	1 $^6T_{2g}$	23.93	1 ^6E_g				
29 Γ_{8g}	2.370	430	36530	0.04	68.38	1 $^6T_{2g}$	20.43	2 $^6T_{1g}$				
15 Γ_{7g}	2.369	428	37046		47.03	1 ^6E_g	42.56	2 $^6T_{1g}$				
30 Γ_{8g}	2.369	429	37415	0.04	36.06	2 $^6T_{1g}$	33.80	1 ^6E_g	25.74	1 $^6T_{2g}$		
31 Γ_{8g}	2.369	429	37553	0.02	64.56	2 $^6T_{2g}$	15.31	1 ^6E_g	15.21	2 $^6T_{1g}$		
15 Γ_{6g}	2.370	430	37558	0.01	84.80	2 $^6T_{2g}$	11.26	2 $^6T_{1g}$				
32 Γ_{8g}	2.370	429	37605	0.01	66.14	2 $^6T_{1g}$	17.54	2 $^6T_{2g}$				
16 Γ_{6g}	2.369	428	39325		91.44	2 $^6T_{2g}$						
33 Γ_{8g}	2.369	429	39343		90.53	2 $^6T_{2g}$						
16 Γ_{7g}	2.370	429	39354		90.02	2 $^6T_{2g}$						
$4f^6(^7F_J)(5dt_{2g}^1 + ITE_{a_{1g}}^1)$ High-Spin coupling [d,e]												
34 Γ_{8g}	2.419	401	46209	0.47	39.85	3 $^8T_{2g}$	32.64	3 $^8T_{1g}$				
35 Γ_{8g}	2.419	407	46403	0.24	49.49	4 $^8T_{1g}$	25.18	2 ^8E_g	16.72	4 $^8T_{2g}$		
17 Γ_{6g}	2.417	324	46948	0.19	39.83	3 $^8T_{2g}$	36.67	3 $^8T_{1g}$				
17 Γ_{7g}	2.420	372	46979	0.58	41.85	3 $^8T_{2g}$						
36 Γ_{8g}	2.420	377	47043	0.69	39.85	4 $^8T_{1g}$	31.81	4 $^8T_{2g}$	20.65	2 ^8E_g		
18 Γ_{7g}	2.420	384	47529	1.23	62.43	4 $^8T_{2g}$	13.53	5 $^8T_{1g}$	12.78	2 ^8E_g		
18 Γ_{6g}	2.419	376	47531	0.49	63.21	4 $^8T_{1g}$	15.45	2 ^8E_g				
37 Γ_{8g}	2.418	338	47694	0.80	59.15	3 $^8T_{1g}$	33.76	3 $^8T_{2g}$				
38 Γ_{8g}	2.419	345	48144	3.21	44.03	4 $^8T_{2g}$	31.51	2 ^8E_g	17.64	4 $^8T_{1g}$		
39 Γ_{8g}	2.418	338	48284	2.11	55.87	3 $^8T_{1g}$	20.48	3 $^8T_{2g}$				
40 Γ_{8g}	2.419	353	48627	4.16	46.28	4 $^8T_{2g}$	35.05	4 $^8T_{1g}$				
19 Γ_{7g}	2.418	311	48749	3.45	47.65	3 $^8T_{1g}$	45.41	3 $^8T_{2g}$				
20 Γ_{7g}	2.418	320	48940	1.59	39.82	4 $^8T_{2g}$	27.82	2 ^8E_g	18.85	5 $^8T_{1g}$	11.24	4 $^8T_{1g}$
19 Γ_{6g}	2.418	283	48992	0.69	39.06	3 $^8T_{1g}$	37.92	3 $^8T_{2g}$				
41 Γ_{8g}	2.420	349	49130	2.73	29.06	4 $^8T_{2g}$	25.75	4 $^8T_{1g}$	17.31	5 $^8T_{1g}$	13.86	2 ^8E_g
20 Γ_{6g}	2.376	289	49355	0.01	52.07	4 $^8T_{1g}$	33.90	2 ^8E_g				
21 Γ_{6g}	2.388	318	49508	0.29	40.35	3 $^8T_{1g}$	25.22	3 $^8T_{2g}$				
21 Γ_{7g}	2.419	358	49558	1.03	47.34	4 $^8T_{1g}$	33.40	5 $^8T_{1g}$				
42 Γ_{8g}	2.419	312	49617	0.15	59.70	3 $^8T_{1g}$	19.30	3 $^8T_{2g}$				
43 Γ_{8g}	2.409	297	49740	0.02	47.39	4 $^8T_{1g}$	11.49	4 $^8T_{2g}$	10.95	3 $^8T_{2g}$	10.57	2 ^8E_g
22 Γ_{6g}	2.407	380	49843	0.35	52.76	4 $^8T_{2g}$	21.08	4 $^8T_{1g}$	19.27	5 $^8T_{1g}$		
22 Γ_{7g}	2.421	348	49844	0.17	48.77	4 $^8T_{1g}$	28.51	4 $^8T_{2g}$	10.95	5 $^8T_{1g}$		
44 Γ_{8g}	2.385	318	49937	1.00	57.68	3 $^8T_{2g}$	25.40	3 $^8T_{1g}$				
45 Γ_{8g}	2.412	295	50150	3.28	42.95	4 $^8T_{2g}$	24.08	4 $^8T_{1g}$	20.55	5 $^8T_{1g}$		
23 Γ_{7g}	2.413	350	50162	0.01	40.48	3 $^8T_{1g}$	24.08	3 $^8T_{2g}$				
23 Γ_{6g}	2.405	393	50202	4.00	45.21	3 $^8T_{1g}$	30.11	3 $^8T_{2g}$				
46 Γ_{8g}	2.413	343	50216	0.11	37.24	2 ^8E_g	25.27	5 $^8T_{1g}$	18.77	4 $^8T_{2g}$	11.85	4 $^8T_{1g}$
47 Γ_{8g}	2.409	356	50336	2.65	57.28	3 $^8T_{2g}$	24.35	3 $^8T_{1g}$				

24 Γ_{7g}	2.400	602	50362	1.30	29.65	5 $^8T_{1g}$	24.48	4 $^8T_{1g}$	17.05	2 ^8E_g	12.58	4 $^8T_{2g}$		
48 Γ_{8g}	2.407	366	50433	0.40	63.73	3 $^8T_{2g}$	32.80	3 $^8T_{1g}$						
49 Γ_{8g}	2.397	434	50664	0.67	23.27	6 $^8T_{1g}$	15.18	5 $^8T_{1g}$	14.50	3 ^8E_g	11.68	5 $^8T_{2g}$		
					10.19	4 $^8T_{1g}$								
24 Γ_{6g}	2.391	413	50669	0.20	19.07	4 $^8T_{2g}$	16.21	6 $^8T_{1g}$	14.37	3 $^8T_{1g}$	10.69	4 $^8T_{1g}$		
50 Γ_{8g}	2.400	500	50774	1.66	29.22	4 $^8T_{2g}$	27.72	2 ^8E_g	10.93	5 $^8T_{1g}$				
25 Γ_{7g}	2.405	350	50964	0.13	22.06	3 ^8E_g	21.67	6 $^8T_{1g}$	20.31	5 $^8T_{2g}$	13.08	4 $^8T_{2g}$		
51 Γ_{8g}	2.401	382	50972	0.20	24.42	4 $^8T_{1g}$	21.13	5 $^8T_{1g}$	19.61	2 ^8E_g	12.57	6 $^8T_{1g}$		
25 Γ_{6g}	2.392	394	51032	0.16	40.21	4 $^8T_{2g}$	19.87	3 ^8E_g	13.86	6 $^8T_{1g}$				
26 Γ_{7g}	2.405	373	51281	0.84	43.31	5 $^8T_{1g}$	12.64	6 $^8T_{1g}$	11.90	4 $^8T_{2g}$	11.04	5 $^8T_{2g}$		
52 Γ_{8g}	2.410	335	51415	0.98	29.09	5 $^8T_{1g}$	18.71	3 ^8E_g	15.85	6 $^8T_{1g}$	11.32	5 $^8T_{2g}$		
26 Γ_{6g}	2.389	395	51430	0.12	59.10	5 $^8T_{1g}$	16.88	2 ^8E_g	12.11	4 $^8T_{1g}$				
27 Γ_{7g}	2.398	693	51430	0.61	45.78	3 $^8T_{1g}$	38.48	3 $^8T_{2g}$						
53 Γ_{8g}	2.396	317	51471	0.28	32.13	4 $^8T_{2g}$	18.88	5 $^8T_{2g}$	16.15	2 ^8E_g	14.18	3 ^8E_g		
54 Γ_{8g}	2.405	356	51604	1.55	19.68	5 $^8T_{2g}$	17.84	3 ^8E_g	15.97	4 $^8T_{2g}$	13.33	2 ^8E_g		
27 Γ_{6g}	2.396	440	51612	0.01	32.46	3 $^8T_{2g}$	14.82	5 $^8T_{2g}$	13.32	3 $^8T_{1g}$				
55 Γ_{8g}	2.395	428	51672	3.57	49.71	3 $^8T_{2g}$	30.23	3 $^8T_{1g}$						
28 Γ_{7g}	2.394	489	51712	0.16	47.66	3 $^8T_{1g}$	46.21	3 $^8T_{2g}$						
28 Γ_{6g}	2.392	437	51722	1.05	32.39	5 $^8T_{2g}$	17.56	3 $^8T_{2g}$						
56 Γ_{8g}	2.389	437	51919	5.37	29.81	3 $^8T_{1g}$	18.59	3 $^8T_{2g}$	10.82	3 ^8E_g	10.13	5 $^8T_{1g}$		
57 Γ_{8g}	2.390	441	51938	1.41	30.23	3 $^8T_{1g}$	20.51	3 $^8T_{2g}$	17.97	5 $^8T_{1g}$				
29 Γ_{6g}	2.405	448	52069	2.94	38.33	4 $^8T_{2g}$	19.72	2 ^8E_g						
58 Γ_{8g}	2.399	522	52082	3.81	17.24	4 $^8T_{2g}$	16.62	5 $^8T_{2g}$	16.04	5 $^8T_{1g}$	15.63	4 $^8T_{1g}$		
					12.11	2 ^8E_g								
59 Γ_{8g}	2.397	518	52192	2.22	25.48	6 $^8T_{1g}$	12.36	3 ^8E_g	10.76	5 $^8T_{1g}$				
60 Γ_{8g}	2.393	475	52499	0.80	32.95	3 ^8E_g	30.70	5 $^8T_{2g}$	19.87	5 $^8T_{1g}$				
30 Γ_{6g}	2.391	494	52534	0.37	49.30	5 $^8T_{2g}$								
29 Γ_{7g}	2.377	454	52712	0.02	31.64	6 $^8T_{1g}$	15.26	5 $^8T_{1g}$						
30 Γ_{7g}	2.380	469	52782	0.03	17.63	6 $^8T_{1g}$	17.58	4 $^8T_{1g}$	16.60	5 $^8T_{1g}$	10.67	4 $^8T_{2g}$		
31 Γ_{6g}	2.394	483	52815	0.39	71.42	5 $^8T_{1g}$	13.58	4 $^8T_{2g}$						
61 Γ_{8g}	2.387	466	52819	0.24	45.72	5 $^8T_{1g}$	12.80	4 $^8T_{2g}$	10.81	3 ^8E_g	10.51	4 $^8T_{1g}$		
62 Γ_{8g}	2.390	456	52994	0.17	41.25	5 $^8T_{1g}$	17.96	6 $^8T_{1g}$						
31 Γ_{7g}	2.380	462	53160	0.33	31.61	3 ^8E_g	14.76	4 $^8T_{1g}$	11.81	4 $^8T_{2g}$	10.99	2 ^8E_g		
63 Γ_{8g}	2.389	461	53163	0.30	41.91	5 $^8T_{1g}$	25.90	5 $^8T_{2g}$	12.82	6 $^8T_{1g}$				
32 Γ_{6g}	2.396	542	53209	0.25	35.96	6 $^8T_{1g}$	22.16	5 $^8T_{2g}$	17.87	3 ^8E_g				
64 Γ_{8g}	2.393	508	53305	0.58	43.46	5 $^8T_{2g}$	42.40	6 $^8T_{1g}$						
65 Γ_{8g}	2.393	480	53752	0.07	46.27	5 $^8T_{2g}$	14.36	3 ^8E_g						
32 Γ_{7g}	2.394	435	53885		74.23	5 $^8T_{2g}$								
33 Γ_{6g}	2.387	446	54020	0.09	28.56	6 $^8T_{1g}$	21.91	3 ^8E_g						
66 Γ_{8g}	2.392	455	54085	0.33	50.13	6 $^8T_{1g}$	29.38	5 $^8T_{2g}$	11.34	3 ^8E_g				
67 Γ_{8g}	2.396	577	54338	0.41	45.18	5 $^8T_{2g}$	23.09	3 ^8E_g						
33 Γ_{7g}	2.386	496	54401	0.11	55.55	6 $^8T_{1g}$	19.53	3 ^8E_g						
34 Γ_{6g}	2.398	662	54510	0.07	42.67	5 $^8T_{2g}$	20.19	6 $^8T_{1g}$						
68 Γ_{8g}	2.398	671	54520	0.19	32.67	5 $^8T_{2g}$	31.05	6 $^8T_{1g}$	16.71	3 ^8E_g				
34 Γ_{7g}	2.392	607	54527	0.10	42.06	5 $^8T_{2g}$	16.80	3 ^8E_g						
69 Γ_{8g}	2.396	760	54573	0.37	47.31	6 $^8T_{1g}$	27.41	3 ^8E_g	14.82	5 $^8T_{2g}$				
35 Γ_{7g}	2.398	1031	54764	0.24	42.11	6 $^8T_{1g}$								
70 Γ_{8g}	2.399	1033	54978	0.41	48.50	6 $^8T_{1g}$	15.35	3 ^8E_g						
35 Γ_{6g}	2.400	1074	55022	0.20	48.20	6 $^8T_{1g}$	14.55	3 ^8E_g						

$4f^7$ excited states

$4f^7(^6P_{3/2,5/2,7/2})$ [c]														
2 Γ_{8u}	2.386	422	30442		89.24	1 $^6T_{1u}$								
2 Γ_{7u}	2.386	422	30453		89.74	1 $^6T_{1u}$								
3 Γ_{8u}	2.386	422	30826		94.06	1 $^6T_{1u}$								
2 Γ_{6u}	2.386	422	31053		85.07	1 $^6T_{1u}$	12.15	3 $^6T_{2u}$						
4 Γ_{8u}	2.386	422	31065		85.15	1 $^6T_{1u}$								
3 Γ_{7u}	2.386	422	31087		85.28	1 $^6T_{1u}$	10.76	2 ^6E_u						
$4f^7(^6I_{7/2,9/2,11/2,13/2,15/2,17/2})$ [c]														
3 Γ_{6u}	2.385	422	34758		77.14	1 $^6T_{2u}$	19.36	1 ^6E_u						

5 Γ_{8u}	2.385	422	34766	83.92	1 $^6T_{2u}$	12.38	1 ^6E_u				
4 Γ_{7u}	2.385	422	34776	93.85	1 $^6T_{2u}$						
6 Γ_{8u}	2.386	422	34798	80.83	1 $^6T_{2u}$	12.57	1 ^6E_u				
7 Γ_{8u}	2.386	422	34807	87.86	1 $^6T_{2u}$						
4 Γ_{6u}	2.386	422	34808	87.58	1 $^6T_{2u}$						
5 Γ_{6u}	2.386	427	35026	84.72	1 ^6E_u	12.34	2 $^6T_{1u}$				
8 Γ_{8u}	2.386	422	35033	43.59	1 ^6E_u	29.81	2 $^6T_{2u}$	23.21	1 $^6A_{2u}$		
9 Γ_{8u}	2.386	423	35085	67.87	1 ^6E_u	14.20	2 $^6T_{2u}$	10.28	1 $^6T_{2u}$		
6 Γ_{6u}	2.385	426	35092	46.77	2 $^6T_{2u}$	27.81	1 $^6A_{2u}$	12.68	1 ^6E_u		
10 Γ_{8u}	2.386	422	35172	75.34	2 $^6T_{2u}$	19.01	2 $^6T_{1u}$				
5 Γ_{7u}	2.386	412	35182	80.51	2 $^6T_{2u}$	17.75	2 $^6T_{1u}$				
7 Γ_{6u}	2.389	429	35191	69.23	2 $^6T_{2u}$	11.14	2 $^6T_{1u}$	10.06	1 $^6T_{2u}$		
11 Γ_{8u}	2.386	422	35202	29.51	2 $^6T_{1u}$	27.29	2 $^6T_{2u}$	23.73	1 ^6E_u		
6 Γ_{7u}	2.385	418	35210	49.46	1 ^6E_u	37.09	2 $^6T_{2u}$				
12 Γ_{8u}	2.386	422	35213	41.38	2 $^6T_{2u}$	37.57	2 $^6T_{1u}$				
7 Γ_{7u}	2.385	422	35242	50.70	2 $^6T_{1u}$	39.35	1 $^6A_{1u}$				
13 Γ_{8u}	2.386	423	35264	26.71	1 $^6A_{2u}$	22.33	2 $^6T_{1u}$	21.71	1 $^6A_{1u}$	13.61	1 ^6E_u
8 Γ_{6u}	2.386	422	35265	48.38	1 $^6A_{2u}$	28.30	2 $^6T_{1u}$				
8 Γ_{7u}	2.386	422	35307	58.40	2 $^6T_{1u}$	27.07	1 $^6A_{1u}$				
14 Γ_{8u}	2.386	422	35315	29.81	2 $^6T_{2u}$	29.36	1 $^6A_{2u}$	25.51	1 $^6A_{1u}$		
15 Γ_{8u}	2.386	422	35376	71.42	2 $^6T_{1u}$	17.80	2 $^6T_{2u}$				
16 Γ_{8u}	2.386	423	35401	52.04	2 $^6T_{1u}$	32.48	2 $^6T_{2u}$				
9 Γ_{6u}	2.386	422	35451	49.56	2 $^6T_{1u}$	33.66	2 $^6T_{2u}$	13.82	1 $^6A_{2u}$		
17 Γ_{8u}	2.386	422	35496	48.82	2 $^6T_{1u}$	32.68	1 $^6A_{1u}$	13.06	2 $^6T_{2u}$		
9 Γ_{7u}	2.386	422	35510	56.03	2 $^6T_{1u}$	32.90	1 $^6A_{1u}$				
$4f^7(^6D_{1/2,3/2,5/2,7/2})$ [c]											
18 Γ_{8u}	2.385	422	37485	78.62	3 $^6T_{2u}$	17.76	2 ^6E_u				
10 Γ_{6u}	2.385	423	37633	93.85	2 ^6E_u						
19 Γ_{8u}	2.386	422	37672	51.78	2 ^6E_u	44.68	3 $^6T_{2u}$				
11 Γ_{6u}	2.386	422	37925	97.37	3 $^6T_{2u}$						
20 Γ_{8u}	2.385	422	38099	51.12	3 $^6T_{2u}$	39.73	2 ^6E_u				
21 Γ_{8u}	2.385	423	38311	65.23	2 ^6E_u	19.54	3 $^6T_{2u}$	10.59	1 $^6T_{1u}$		
10 Γ_{7u}	2.386	422	38393	80.40	2 ^6E_u	11.50	1 $^6T_{1u}$				
12 Γ_{6u}	2.386	422	38515	80.47	3 $^6T_{2u}$	11.98	1 $^6T_{1u}$				
22 Γ_{8u}	2.386	422	38609	79.70	3 $^6T_{2u}$	10.91	1 $^6T_{1u}$				
11 Γ_{7u}	2.386	422	38679	84.08	3 $^6T_{2u}$	10.50	1 $^6T_{1u}$				
$4f^7(^6G_{3/2,5/2,7/2,9/2,11/2,13/2})$ [c]											
23 Γ_{8u}	2.384	422	47769	62.96	4 $^6T_{2u}$	21.55	2 $^6A_{2u}$				
13 Γ_{6u}	2.384	422	47790	64.33	4 $^6T_{2u}$	22.71	2 $^6A_{2u}$				
24 Γ_{8u}	2.385	422	47926	49.13	4 $^6T_{2u}$	20.04	3 ^6E_u	17.18	3 $^6T_{1u}$		
12 Γ_{7u}	2.384	422	48119	65.05	3 $^6T_{1u}$	26.79	3 ^6E_u				
14 Γ_{6u}	2.385	422	48143	46.95	3 ^6E_u	38.82	5 $^6T_{2u}$				
15 Γ_{6u}	2.384	422	48226	81.85	3 $^6T_{1u}$						
25 Γ_{8u}	2.384	421	48227	59.57	3 $^6T_{1u}$	17.92	5 $^6T_{2u}$	16.50	4 $^6T_{2u}$		
26 Γ_{8u}	2.385	422	48329	42.11	3 ^6E_u	16.82	5 $^6T_{2u}$	11.71	2 $^6A_{1u}$		
13 Γ_{7u}	2.385	422	48351	28.71	5 $^6T_{2u}$	28.03	3 $^6T_{1u}$	15.27	4 $^6T_{2u}$	15.00	2 $^6A_{1u}$
27 Γ_{8u}	2.385	423	48448	29.89	4 $^6T_{2u}$	24.77	3 ^6E_u	16.53	5 $^6T_{2u}$	10.56	3 $^6T_{1u}$
28 Γ_{8u}	2.386	422	48915	80.24	4 $^6T_{1u}$						
14 Γ_{7u}	2.387	422	49170	41.78	4 $^6T_{1u}$	30.90	2 $^6A_{1u}$	18.98	5 $^6T_{2u}$		
29 Γ_{8u}	2.386	422	49502	30.61	2 $^6A_{1u}$	25.55	4 $^6T_{1u}$	18.01	5 $^6T_{2u}$	12.15	3 ^6E_u
16 Γ_{6u}	2.384	422	49648	68.78	4 $^6T_{2u}$	13.91	3 ^6E_u				
30 Γ_{8u}	2.384	422	49731	56.83	4 $^6T_{2u}$	14.64	3 ^6E_u	13.97	3 $^6T_{1u}$		
15 Γ_{7u}	2.384	422	49771	52.44	4 $^6T_{2u}$	21.37	3 $^6T_{1u}$				
16 Γ_{7u}	2.385	422	50048	43.17	3 ^6E_u	33.68	3 $^6T_{1u}$	11.14	4 $^6T_{1u}$		
31 Γ_{8u}	2.385	422	50076	41.99	3 $^6T_{1u}$	22.15	3 ^6E_u	21.60	4 $^6T_{1u}$		
$4f^7(^6F_{1/2,3/2,5/2,7/2,9/2,11/2})$ [c]											
17 Γ_{6u}	2.386	422	50640	44.37	5 $^6T_{2u}$	24.72	2 $^6A_{2u}$	18.88	4 $^6T_{1u}$		
32 Γ_{8u}	2.385	422	51421	23.11	2 $^6A_{2u}$	21.94	5 $^6T_{2u}$	15.65	4 $^6T_{2u}$	15.12	3 $^6T_{1u}$
33 Γ_{8u}	2.384	422	51754	71.22	3 $^6T_{1u}$						

17 Γ_{7u}	2.384	422	51799	43.56	5 $^6T_{2u}$	21.88	3 $^6T_{1u}$	15.68	4 $^6T_{2u}$		
34 Γ_{8u}	2.385	422	51978	24.18	2 $^6A_{2u}$	21.24	5 $^6T_{2u}$	20.26	4 $^6T_{2u}$	10.60	3 ^6E_u
18 Γ_{6u}	2.385	422	52123	41.74	2 $^6A_{2u}$	31.24	5 $^6T_{2u}$	15.08	4 $^6T_{2u}$		
35 Γ_{8u}	2.385	422	52384	55.99	5 $^6T_{2u}$	12.07	3 ^6E_u	11.77	2 $^6A_{2u}$		
18 Γ_{7u}	2.386	422	52387	39.11	4 $^6T_{1u}$	26.12	2 $^6A_{1u}$	16.23	3 $^6T_{1u}$		
19 Γ_{6u}	2.385	422	52499	51.87	5 $^6T_{2u}$	24.18	3 ^6E_u	14.49	4 $^6T_{2u}$		
36 Γ_{8u}	2.385	422	52530	28.21	4 $^6T_{1u}$	24.85	5 $^6T_{2u}$	14.83	3 $^6T_{1u}$	14.02	2 $^6A_{1u}$
37 Γ_{8u}	2.386	423	52616	46.37	4 $^6T_{1u}$	21.53	5 $^6T_{2u}$				
19 Γ_{7u}	2.386	422	52744	77.81	4 $^6T_{1u}$						
20 Γ_{6u}	2.387	422	52793	67.34	4 $^6T_{1u}$						
38 Γ_{8u}	2.386	422	52909	47.86	5 $^6T_{2u}$	31.75	4 $^6T_{1u}$				
$4f^7(^6H_{5/2,7/2,9/2,11/2,13/2,15/2})$ [c]											
20 Γ_{7u}	2.385	423	55493	57.10	5 $^6T_{1u}$	27.00	4 ^6E_u				
39 Γ_{8u}	2.385	422	55617	45.16	5 $^6T_{1u}$	23.05	4 ^6E_u	14.81	6 $^6T_{2u}$	10.19	6 $^6T_{1u}$
40 Γ_{8u}	2.384	423	55790	81.51	5 $^6T_{1u}$	11.96	4 ^6E_u				
21 Γ_{6u}	2.384	423	55869	64.47	5 $^6T_{1u}$	11.93	4 ^6E_u				
41 Γ_{8u}	2.384	423	55871	68.06	5 $^6T_{1u}$	20.53	4 ^6E_u				
21 Γ_{7u}	2.384	423	55892	46.06	4 ^6E_u	41.02	5 $^6T_{1u}$	11.35	6 $^6T_{1u}$		
42 Γ_{8u}	2.385	422	55909	72.67	4 ^6E_u	12.74	6 $^6T_{1u}$				
43 Γ_{8u}	2.384	423	56039	66.90	5 $^6T_{1u}$	20.83	4 ^6E_u				
22 Γ_{7u}	2.384	421	56049	64.26	5 $^6T_{1u}$	13.82	4 ^6E_u				
22 Γ_{6u}	2.384	422	56065	72.86	4 ^6E_u	17.27	5 $^6T_{1u}$				
23 Γ_{7u}	2.386	424	56116	38.82	6 $^6T_{2u}$	29.98	6 $^6T_{1u}$	18.94	5 $^6T_{1u}$		
44 Γ_{8u}	2.385	423	56211	42.19	6 $^6T_{1u}$	22.47	6 $^6T_{2u}$	21.19	4 ^6E_u		
23 Γ_{6u}	2.386	422	56242	86.06	6 $^6T_{1u}$						
45 Γ_{8u}	2.386	423	56335	72.83	6 $^6T_{1u}$	12.49	6 $^6T_{2u}$				
24 Γ_{7u}	2.386	423	56435	82.48	6 $^6T_{1u}$						
24 Γ_{6u}	2.386	423	56453	83.33	6 $^6T_{2u}$						
46 Γ_{8u}	2.386	423	56485	49.73	6 $^6T_{1u}$	36.26	6 $^6T_{2u}$				
47 Γ_{8u}	2.387	423	56707	86.53	6 $^6T_{2u}$						
48 Γ_{8u}	2.387	423	56768	49.35	6 $^6T_{2u}$	37.79	6 $^6T_{1u}$				
25 Γ_{6u}	2.387	423	56774	84.93	6 $^6T_{2u}$						
49 Γ_{8u}	2.387	423	56837	47.30	6 $^6T_{2u}$	41.15	6 $^6T_{1u}$				
25 Γ_{7u}	2.387	423	56875	50.14	6 $^6T_{1u}$	39.91	6 $^6T_{2u}$				

Eu^{3+}-doped CaF_2

$4f^6(^7F_{0-6})$											
1 A_{1g}	2.261	495	0	35.10	1 $^7T_{2g}$	30.28	1 $^7A_{2g}$	28.94	1 $^7T_{1g}$		
1 T_{1g}	2.260	495	345	35.77	1 $^7A_{2g}$	34.53	1 $^7T_{2g}$	24.93	1 $^7T_{1g}$		
1 T_{2g}	2.259	497	803	55.37	1 $^7A_{2g}$	32.46	1 $^7T_{2g}$				
1 E_g	2.261	494	1406	63.62	1 $^7T_{1g}$	32.67	1 $^7T_{2g}$				
2 T_{1g}	2.260	496	1971	44.05	1 $^7T_{1g}$	28.35	1 $^7A_{2g}$	24.96	1 $^7T_{2g}$		
2 T_{2g}	2.261	495	2111	63.47	1 $^7T_{1g}$	23.97	1 $^7T_{2g}$				
1 A_{2g}	2.261	494	2352	50.50	1 $^7T_{1g}$	46.93	1 $^7T_{2g}$				
2 A_{1g}	2.259	498	2501	53.64	1 $^7A_{2g}$	43.69	1 $^7T_{1g}$				
3 T_{1g}	2.261	495	3114	47.23	1 $^7T_{2g}$	36.02	1 $^7T_{1g}$	14.61	1 $^7A_{2g}$		
3 T_{2g}	2.261	494	3361	78.93	1 $^7T_{1g}$	16.24	1 $^7T_{2g}$				
2 E_g	2.262	494	3472	79.22	1 $^7T_{2g}$	18.74	1 $^7T_{1g}$				
4 T_{2g}	2.261	496	4132	41.46	1 $^7T_{2g}$	34.92	1 $^7T_{1g}$	21.25	1 $^7A_{2g}$		
4 T_{1g}	2.261	495	4404	75.39	1 $^7T_{2g}$	13.52	1 $^7T_{1g}$				
3 E_g	2.261	494	4600	49.48	1 $^7T_{2g}$	48.17	1 $^7T_{1g}$				
5 T_{1g}	2.261	494	4602	54.94	1 $^7T_{2g}$	42.53	1 $^7T_{1g}$				
3 A_{1g}	2.261	495	5524	60.12	1 $^7T_{2g}$	23.43	1 $^7T_{1g}$	13.19	1 $^7A_{2g}$		
6 T_{1g}	2.261	495	5580	54.28	1 $^7T_{2g}$	32.88	1 $^7T_{1g}$				
5 T_{2g}	2.261	495	5603	48.97	1 $^7T_{1g}$	39.90	1 $^7T_{2g}$				
4 E_g	2.261	494	5806	63.29	1 $^7T_{1g}$	33.36	1 $^7T_{2g}$				
6 T_{2g}	2.261	494	5813	56.81	1 $^7T_{1g}$	39.80	1 $^7T_{2g}$				
2 A_{2g}	2.261	494	5827	50.05	1 $^7T_{2g}$	46.56	1 $^7T_{1g}$				

$4f^6(^5D_{0-3})$

4 A_{1g}	2.260	494	20023	55.09	1 $^5T_{2g}$	38.95	1 ^5E_g				
7 T_{1g}	2.260	494	20828	55.07	1 $^5T_{2g}$	39.56	1 ^5E_g				
5 E_g	2.260	494	22414	54.59	1 ^5E_g	40.93	1 $^5T_{2g}$				
7 T_{2g}	2.260	494	22566	64.36	1 $^5T_{2g}$	31.00	1 ^5E_g				
3 A_{2g}	2.260	493	25074	95.53	1 ^5E_g						
8 T_{2g}	2.260	493	25175	52.00	1 $^5T_{2g}$	43.69	1 ^5E_g				
8 T_{1g}	2.260	494	25180	87.42	1 $^5T_{2g}$						
$4f^6(^5D_4,^5L_{6-10},^5G_{2-6})$											
9 T_{2g}	2.258	492	27978	36.81	1 $^5T_{1g}$	29.22	2 ^5E_g				
6 E_g	2.258	493	27981	39.28	1 $^5T_{1g}$	26.45	2 ^5E_g	13.01	1 $^5A_{1g}$		
4 A_{2g}	2.259	493	28021	43.58	1 $^5T_{1g}$	38.58	2 ^5E_g				
10 T_{2g}	2.258	495	28166	48.22	2 $^5T_{2g}$	12.53	1 $^5T_{2g}$	11.81	1 $^5T_{1g}$		
9 T_{1g}	2.257	494	28189	34.82	2 ^5E_g	23.82	1 $^5T_{1g}$	22.73	2 $^5T_{2g}$		
7 E_g	2.258	495	28304	38.22	2 $^5T_{2g}$	13.39	1 $^5T_{2g}$	11.24	1 $^5A_{1g}$	10.66	1 ^5E_g
5 A_{1g}	2.258	494	28360	60.12	2 ^5E_g	17.62	2 $^5T_{2g}$				
10 T_{1g}	2.259	494	28403	38.55	1 $^5T_{1g}$	25.57	2 $^5T_{2g}$				
11 T_{2g}	2.259	493	28550	42.34	1 $^5T_{1g}$	18.85	1 $^5A_{1g}$	13.89	2 $^5T_{2g}$	13.07	2 ^5E_g
12 T_{2g}	2.260	494	28647	29.75	3 ^5E_g	26.11	2 $^5T_{1g}$				
5 A_{2g}	2.260	494	28653	38.00	3 ^5E_g	32.86	2 $^5T_{1g}$	11.18	2 ^5E_g		
11 T_{1g}	2.259	492	28852	34.99	1 $^5T_{1g}$	15.63	3 ^5E_g	14.01	2 $^5T_{2g}$		
8 E_g	2.260	493	28856	35.68	2 $^5T_{1g}$	23.92	3 ^5E_g				
12 T_{1g}	2.259	494	28905	21.60	1 $^5T_{1g}$	20.58	2 ^5E_g	18.30	2 $^5T_{1g}$	10.43	2 $^5T_{2g}$
13 T_{2g}	2.260	491	28960	20.18	2 $^5T_{2g}$	17.41	2 $^5T_{1g}$	12.62	1 $^5A_{1g}$		
14 T_{2g}	2.261	495	29028	34.21	1 $^5T_{2g}$	10.06	1 ^5E_g				
6 A_{1g}	2.260	493	29047	53.91	1 ^5E_g	37.44	1 $^5T_{2g}$				
13 T_{1g}	2.261	492	29094	20.63	1 $^5T_{2g}$	19.47	1 ^5E_g	15.70	3 $^5T_{2g}$	13.40	3 $^5T_{1g}$
9 E_g	2.259	493	29096	34.75	2 ^5E_g	30.61	1 $^5A_{1g}$				
14 T_{1g}	2.260	496	29161	22.12	2 $^5T_{2g}$	18.96	1 $^5T_{1g}$	18.69	2 $^5T_{1g}$	12.60	3 ^5E_g
10 E_g	2.261	495	29199	31.94	1 $^5T_{2g}$	26.17	2 $^5T_{2g}$	23.26	1 ^5E_g		
15 T_{2g}	2.260	495	29263	26.36	2 $^5T_{1g}$	18.79	2 $^5A_{1g}$	14.66	3 $^5T_{2g}$		
15 T_{1g}	2.261	494	29269	15.86	3 $^5T_{1g}$	13.59	3 $^5T_{2g}$	10.38	2 $^5T_{1g}$	10.26	1 $^5T_{2g}$
7 A_{1g}	2.261	493	29311	37.69	4 $^5T_{2g}$	36.08	4 ^5E_g	14.51	3 $^5T_{2g}$		
16 T_{2g}	2.261	494	29324	27.60	3 $^5T_{1g}$	15.34	2 $^5T_{2g}$	10.96	1 $^5T_{2g}$		
6 A_{2g}	2.260	493	29396	55.88	3 $^5T_{1g}$	23.90	4 ^5E_g	11.83	2 $^5T_{1g}$		
17 T_{2g}	2.261	491	29615	43.99	3 $^5T_{2g}$	24.91	4 $^5T_{2g}$				
16 T_{1g}	2.261	493	29630	54.81	2 $^5T_{1g}$						
8 A_{1g}	2.260	495	29713	60.20	3 ^5E_g	15.11	2 $^5T_{2g}$				
11 E_g	2.261	487	29766	34.95	4 ^5E_g	20.10	4 $^5T_{2g}$	17.98	3 $^5T_{1g}$		
17 T_{1g}	2.261	494	29777	25.01	3 $^5T_{1g}$	23.27	3 $^5T_{2g}$	20.02	4 $^5T_{2g}$	15.29	4 ^5E_g
12 E_g	2.260	495	29831	21.32	3 ^5E_g	19.94	1 $^5A_{1g}$	18.57	1 $^5T_{1g}$		
18 T_{2g}	2.259	493	29973	26.02	1 $^5T_{1g}$	15.63	2 ^5E_g	15.26	1 $^5A_{1g}$		
13 E_g	2.260	497	30016	32.96	2 $^5A_{1g}$	22.99	3 $^5T_{2g}$	10.81	1 $^5T_{1g}$		
7 A_{2g}	2.259	493	30018	36.38	1 $^5T_{1g}$	34.35	2 ^5E_g				
19 T_{2g}	2.259	492	30074	30.09	2 $^5T_{2g}$	17.50	1 $^5T_{1g}$	11.13	1 $^5A_{1g}$		
18 T_{1g}	2.259	493	30098	36.29	2 $^5T_{2g}$	12.56	1 $^5T_{1g}$	12.11	2 $^5T_{1g}$	10.50	2 ^5E_g
9 A_{1g}	2.259	495	30104	43.00	2 $^5T_{2g}$	22.96	3 ^5E_g	12.37	5 ^5E_g		
20 T_{2g}	2.260	497	30185	26.91	3 $^5T_{1g}$	19.79	3 $^5T_{2g}$	18.45	4 ^5E_g		
19 T_{1g}	2.261	494	30363	36.68	4 $^5T_{2g}$	24.76	3 $^5T_{2g}$	14.23	4 ^5E_g		
14 E_g	2.261	494	30380	44.85	3 $^5T_{2g}$	19.71	4 ^5E_g				
21 T_{2g}	2.261	493	30521	31.72	3 $^5T_{1g}$	27.00	4 $^5T_{2g}$	18.30	4 ^5E_g		
20 T_{1g}	2.260	494	30551	41.63	3 ^5E_g	37.58	2 $^5T_{1g}$				
22 T_{2g}	2.261	495	30655	29.09	2 $^5A_{1g}$	25.97	2 $^5T_{1g}$	15.48	3 ^5E_g		
21 T_{1g}	2.261	493	31025	39.70	3 $^5T_{2g}$	26.33	3 $^5T_{1g}$	11.17	4 ^5E_g		
15 E_g	2.261	493	31099	40.57	3 $^5T_{1g}$	31.23	4 $^5T_{2g}$				
10 A_{1g}	2.261	494	31149	58.62	3 $^5T_{2g}$	27.10	4 ^5E_g				
22 T_{1g}	2.261	493	31303	49.13	4 $^5T_{2g}$	22.61	3 $^5T_{2g}$	21.00	3 $^5T_{1g}$		
8 A_{2g}	2.261	494	31313	66.85	4 ^5E_g	26.75	3 $^5T_{1g}$				
23 T_{2g}	2.261	493	31340	35.76	4 $^5T_{2g}$	29.94	3 $^5T_{1g}$	18.95	4 ^5E_g		
9 A_{2g}	2.260	495	31586	43.44	3 ^5E_g	36.43	2 $^5T_{1g}$				
24 T_{2g}	2.260	495	31626	33.62	2 $^5T_{1g}$	27.30	3 ^5E_g	15.77	2 $^5A_{1g}$		
16 E_g	2.260	495	31645	33.34	2 $^5T_{1g}$	22.55	2 $^5A_{1g}$	19.52	3 ^5E_g		

23 T_{1g}	2.261	493	32115	52.58	3 $^5T_{1g}$	24.51	3 $^5T_{2g}$						
25 T_{2g}	2.261	493	32165	38.90	3 $^5T_{2g}$	22.62	4 $^5T_{2g}$	20.64	3 $^5T_{1g}$				
17 E_g	2.261	494	32402	33.48	4 ^5E_g	26.82	4 $^5T_{2g}$	21.15	3 $^5T_{1g}$	15.72	3 $^5T_{2g}$		
24 T_{1g}	2.261	494	32429	41.42	4 $^5T_{2g}$	32.73	4 ^5E_g	11.02	3 $^5T_{2g}$				
26 T_{2g}	2.261	494	32452	41.88	4 $^5T_{2g}$	28.97	3 $^5T_{2g}$	18.88	4 ^5E_g				
11 A_{1g}	2.262	493	32458	52.98	4 $^5T_{2g}$	32.54	4 ^5E_g						

[a] Absorption oscillator strengths for 1 $\Gamma_{6u,8u,7u} \rightarrow i$ transitions are calculated at $d_{\mathrm{Eu-F}}$= 2.400 Å; the reference value is f_{ref} = 1.704×10^{-2}. Emission oscillator strengths for 1 $\Gamma_{8g} \rightarrow$1 Γ_{6u},1 Γ_{8u},1 Γ_{7u} and radiative emission lifetime are calculated at $d_{\mathrm{Eu-F}}$= 2.350 Å; the reference value is f_{ref} = 2.233×10^{-3}.

[b] The analyses of the wave functions have been done at $d_{\mathrm{Eu-F}}$= 2.400 Å ($4f^7$), 2.350 Å ($4f^6(5d^1 + ITE^1_{a_{1g}})$), 2.250 Å ($4f^6$).

[c] C.f. Table S7.

[d] C.f. Table S8.

[e] Low-spin ($S = 5/2$) wave functions of the $4f^6(^7F_J)(5dt^1_{2g} + ITE^1_{a_{1g}})$ configurations have not been included in the spin-orbit calculations.

TABLE S10: Spectroscopic constants and analyses of the spin-orbit wave functions of the ground and lowest lying excited states of Eu^{2+} and Eu^{3+} -doped SrF_2 cubic defects. Eu–F bond distances ($d_{\mathrm{Eu-F},e}$ in Å), EuF_8 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), minimum-to-minimum energy differences (T_e in cm^{-1}), and relative absorption and emission oscillator strengths (f_i^{abs}/f_{ref} and f_i^{emi}/f_{ref}) are given. Calculated radiative emission lifetime for the $4f^6(^7F_J)5de_g^1$ – 1 Γ_{8g} excited state is 0.498 μs. Local distortion around the Eu^{2+}impurity, relative to experimental crystal structure d_{Sr-F}= 2.510 Å, is $d_{\mathrm{Eu-F},e}(1\Gamma_{6u}) - d_{\mathrm{Ca-F}} = -0.040$; ionic radii mismatch is –0.01 Å[31]. See Fig. 3, S3 and text for details.

State	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e	f_i^{abs}/f_{ref} [a]	f_i^{emi}/f_{ref} [a]	weights of terms larger than 10% [b]							
$4f^7(^8S_{7/2})$ [c]													
1 Γ_{6u}	2.470	370	0	1.00	1.00	97.78	1 $^8A_{1u}$						
1 Γ_{8u}	2.470	370	0	0.86	0.86	97.77	1 $^8A_{1u}$						
1 Γ_{7u}	2.470	370	0	0.03	0.03	97.77	1 $^8A_{1u}$						
$4f^6(5d + ITE_{a_{1g}})^1$ excited states													
$4f^6(^7F_J)5de_g^1$ High-Spin coupling [d]													
1 Γ_{8g}	2.451	370	26828	1.00		50.73	1 $^8T_{2g}$	33.29	1 $^8T_{1g}$	10.05	1 ^8E_g		
1 Γ_{7g}	2.451	370	27002	0.53		55.50	1 $^8T_{2g}$	35.36	1 $^8T_{1g}$				
2 Γ_{8g}	2.451	371	27118	0.10		69.49	1 $^8T_{2g}$	18.65	1 ^8E_g				
2 Γ_{7g}	2.451	369	27523	0.75		45.07	1 $^8T_{1g}$	39.44	1 $^8T_{2g}$	11.79	1 ^8E_g		
3 Γ_{8g}	2.451	370	27814	1.01		35.29	1 $^8T_{2g}$	29.06	1 $^8T_{1g}$	26.15	1 ^8E_g		
1 Γ_{6g}	2.451	371	27939	0.38		30.40	1 $^8T_{2g}$	27.31	1 ^8E_g	22.73	1 $^8T_{1g}$	15.16	2 $^8T_{1g}$
4 Γ_{8g}	2.451	369	28437	2.01		54.31	1 $^8T_{1g}$	20.24	1 $^8T_{2g}$	13.31	2 $^8T_{1g}$		
2 Γ_{6g}	2.451	370	28515	0.27		33.46	1 $^8T_{2g}$	20.97	1 ^8E_g	19.98	2 $^8T_{1g}$	19.61	1 $^8T_{1g}$
5 Γ_{8g}	2.450	374	28670	0.23		47.41	1 ^8E_g	30.90	2 $^8T_{1g}$	15.87	1 $^8T_{2g}$		
3 Γ_{7g}	2.451	369	28745	0.83		42.89	1 $^8T_{1g}$	28.29	1 ^8E_g	23.69	1 $^8T_{2g}$		
6 Γ_{8g}	2.450	370	28944	0.45		35.40	1 ^8E_g	32.83	1 $^8T_{2g}$	12.78	1 $^8T_{1g}$	11.33	2 $^8T_{2g}$
7 Γ_{8g}	2.451	371	29333	0.72		41.26	2 $^8T_{1g}$	22.86	1 $^8T_{1g}$	17.94	1 $^8T_{2g}$	16.34	2 $^8T_{2g}$
3 Γ_{6g}	2.451	367	29343	0.70		46.69	1 $^8T_{1g}$	20.47	2 $^8T_{1g}$	18.55	2 $^8T_{2g}$		
8 Γ_{8g}	2.451	370	29858	1.70		47.14	1 $^8T_{1g}$	26.11	2 $^8T_{1g}$	14.79	1 $^8T_{2g}$		
9 Γ_{8g}	2.450	369	29974	0.54		24.00	1 ^8E_g	23.47	1 $^8T_{2g}$	19.35	1 $^8T_{1g}$	17.83	2 $^8T_{1g}$
						14.81	2 $^8T_{2g}$						
4 Γ_{7g}	2.450	368	30017	0.76		37.84	1 $^8T_{1g}$	24.01	1 $^8T_{2g}$	20.17	1 ^8E_g		
4 Γ_{6g}	2.451	373	30038	0.31		31.70	2 $^8T_{1g}$	25.22	1 $^8T_{2g}$	22.35	2 $^8T_{2g}$	15.36	1 $^8T_{1g}$
5 Γ_{7g}	2.451	371	30127	0.82		34.85	1 $^8T_{2g}$	27.01	2 $^8T_{1g}$	26.83	1 $^8T_{1g}$		
5 Γ_{6g}	2.450	372	30395	0.08		47.46	2 $^8T_{2g}$	27.99	1 $^8T_{2g}$	13.20	2 $^8T_{1g}$		
10 Γ_{8g}	2.450	371	30414	0.03		56.07	2 $^8T_{2g}$	22.77	1 ^8E_g	14.36	1 $^8T_{2g}$		
11 Γ_{8g}	2.451	367	30688	0.96		32.93	1 $^8T_{2g}$	26.47	1 $^8T_{1g}$	20.06	1 ^8E_g	14.18	2 $^8T_{1g}$
6 Γ_{6g}	2.451	368	30689	0.55		36.39	1 $^8T_{2g}$	24.47	2 $^8T_{2g}$	18.20	1 $^8T_{1g}$	12.98	2 $^8T_{1g}$
13 Γ_{8g}	2.450	381	31077	0.51		21.92	2 $^8T_{1g}$	21.81	1 ^8E_g	20.95	1 $^8T_{2g}$	20.75	2 $^8T_{2g}$
6 Γ_{7g}	2.451	372	31147	0.01		55.97	2 $^8T_{1g}$	16.98	2 $^8T_{2g}$	13.35	1 $^8T_{2g}$		
14 Γ_{8g}	2.451	371	31388	1.39		41.83	2 $^8T_{1g}$	27.20	1 $^8T_{1g}$	15.09	2 $^8T_{2g}$		
7 Γ_{7g}	2.450	366	31839			72.69	2 $^8T_{2g}$	14.43	1 ^8E_g				
15 Γ_{8g}	2.451	366	31865	3.21		67.43	1 $^8T_{1g}$	23.73	1 $^8T_{2g}$				
7 Γ_{6g}	2.451	366	31882	1.73		71.87	1 $^8T_{1g}$	22.50	1 $^8T_{2g}$				
16 Γ_{8g}	2.450	368	32006	0.77		59.23	2 $^8T_{2g}$	18.93	2 $^8T_{1g}$	10.34	1 $^8T_{1g}$		
8 Γ_{6g}	2.450	367	32137	0.11		56.55	2 $^8T_{2g}$	27.99	2 $^8T_{1g}$				
18 Γ_{8g}	2.451	374	32371	1.36		43.64	2 $^8T_{1g}$	21.54	1 $^8T_{1g}$	19.36	1 ^8E_g		
9 Γ_{6g}	2.451	373	32430	0.05		53.86	2 $^8T_{1g}$	17.53	2 $^8T_{2g}$	14.28	1 ^8E_g	10.93	1 $^8T_{2g}$
19 Γ_{8g}	2.451	378	32721	0.17		68.10	2 $^8T_{1g}$	12.15	1 ^8E_g				
9 Γ_{7g}	2.451	378	32869			76.07	2 $^8T_{1g}$						
20 Γ_{8g}	2.450	362	33686	0.02		87.94	2 $^8T_{2g}$						
21 Γ_{8g}	2.450	365	33854	0.01		79.78	2 $^8T_{2g}$	17.93	2 $^8T_{1g}$				
10 Γ_{7g}	2.450	366	33887			80.82	2 $^8T_{2g}$	17.32	2 $^8T_{1g}$				
$4f^6(^7F_J)5de_g^1$ Low-Spin coupling [d]													
12 Γ_{8g}	2.452	370	30901	0.11		85.87	1 $^6T_{1g}$						
8 Γ_{7g}	2.451	367	32158	0.02		85.15	1 $^6T_{1g}$	11.55	1 $^6T_{2g}$				
17 Γ_{8g}	2.451	367	32252	0.06		88.33	1 $^6T_{1g}$						

10 Γ_{6g}	2.450	368	33832	0.03	54.30	1 $^6T_{1g}$	31.21	1 $^6T_{2g}$	12.44	2 $^6T_{1g}$			
22 Γ_{8g}	2.450	371	33961	0.05	58.37	1 $^6T_{1g}$	29.62	1 $^6T_{2g}$	10.08	2 $^6T_{1g}$			
11 Γ_{7g}	2.450	370	34259	0.03	77.91	1 $^6T_{1g}$	11.15	1 $^6T_{2g}$					
11 Γ_{6g}	2.447	357	34534	0.01	57.84	1 $^6T_{2g}$	24.77	1 ^6E_g	13.90	1 $^6T_{1g}$			
23 Γ_{8g}	2.448	356	34767	0.02	24.97	1 ^6E_g	24.79	1 $^6T_{1g}$	22.25	1 $^6T_{2g}$	21.24	2 $^6T_{1g}$	
12 Γ_{7g}	2.448	361	34870	0.01	48.86	2 $^6T_{1g}$	22.09	1 ^6E_g	20.11	1 $^6T_{2g}$			
24 Γ_{8g}	2.448	358	35399	0.01	31.41	2 $^6T_{1g}$	27.99	1 $^6T_{2g}$	26.34	1 ^6E_g			
13 Γ_{7g}	2.450	368	35513		39.40	1 $^6T_{2g}$	34.02	2 $^6T_{1g}$	18.70	1 $^6T_{1g}$			
12 Γ_{6g}	2.450	364	35519	0.01	63.14	2 $^6T_{1g}$	15.72	1 $^6T_{1g}$	10.57	1 $^6T_{2g}$			
25 Γ_{8g}	2.448	362	36109	0.03	43.09	2 $^6T_{1g}$	21.93	1 ^6E_g	20.42	1 $^6T_{2g}$	11.12	2 $^6T_{2g}$	
26 Γ_{8g}	2.449	355	36219	0.01	52.99	1 $^6T_{2g}$	14.67	2 $^6T_{1g}$	14.14	1 ^6E_g	11.94	1 $^6T_{1g}$	
27 Γ_{8g}	2.448	355	36935	0.03	32.35	1 ^6E_g	30.17	1 $^6T_{2g}$	24.65	2 $^6T_{1g}$			
13 Γ_{6g}	2.448	363	36971	0.02	44.55	1 $^6T_{2g}$	33.82	1 ^6E_g	12.07	1 $^6T_{1g}$			
14 Γ_{7g}	2.449	362	37123		64.14	2 $^6T_{1g}$	13.19	1 $^6T_{2g}$	11.34	1 ^6E_g			
28 Γ_{8g}	2.449	374	37266	0.01	82.32	2 $^6T_{2g}$	10.01	2 $^6T_{1g}$					
14 Γ_{6g}	2.448	362	37481	0.04	52.17	1 $^6T_{2g}$	29.96	1 ^6E_g					
29 Γ_{8g}	2.448	351	37667	0.06	68.12	1 $^6T_{2g}$	20.72	2 $^6T_{1g}$					
15 Γ_{7g}	2.447	365	38213		50.54	1 ^6E_g	39.33	2 $^6T_{1g}$					
30 Γ_{8g}	2.448	364	38568	0.06	36.43	2 $^6T_{1g}$	35.51	1 ^6E_g	25.00	1 $^6T_{2g}$			
31 Γ_{8g}	2.448	367	38720	0.04	36.34	2 $^6T_{1g}$	28.66	2 $^6T_{2g}$	24.75	1 ^6E_g			
15 Γ_{6g}	2.449	376	38746		84.66	2 $^6T_{2g}$	10.90	2 $^6T_{1g}$					
32 Γ_{8g}	2.450	372	38763		54.76	2 $^6T_{2g}$	40.04	2 $^6T_{1g}$					
16 Γ_{6g}	2.448	376	40510	0.01	90.84	2 $^6T_{2g}$							
33 Γ_{8g}	2.448	373	40526		90.22	2 $^6T_{2g}$							
16 Γ_{7g}	2.448	371	40535		89.83	2 $^6T_{2g}$							
$4f^6(^7F_J)(5dt^1_{2g} + ITE^1_{a_{1g}})$ High-Spin coupling [d,e]													
34 Γ_{8g}	2.502	504	44056	0.50	46.30	3 $^8T_{1g}$	25.83	2 ^8E_g	19.33	3 $^8T_{2g}$			
35 Γ_{8g}	2.502	469	44243	0.24	35.64	3 $^8T_{2g}$	35.14	3 $^8T_{1g}$	22.01	2 ^8E_g			
17 Γ_{7g}	2.502	494	44740	0.58	63.92	3 $^8T_{2g}$	13.63	4 $^8T_{1g}$	12.39	2 ^8E_g			
17 Γ_{6g}	2.501	620	44760	0.21	59.34	3 $^8T_{1g}$	19.02	2 ^8E_g	10.64	3 $^8T_{2g}$			
36 Γ_{8g}	2.502	466	44823	0.71	42.38	3 $^8T_{2g}$	32.71	2 ^8E_g	18.44	3 $^8T_{1g}$			
18 Γ_{7g}	2.502	469	45306	1.20	40.42	3 $^8T_{2g}$	29.59	2 ^8E_g	18.80	4 $^8T_{1g}$			
18 Γ_{6g}	2.502	507	45358	0.47	51.12	3 $^8T_{1g}$	33.12	2 ^8E_g					
37 Γ_{8g}	2.502	514	45468	0.78	46.01	3 $^8T_{2g}$	34.49	3 $^8T_{1g}$					
38 Γ_{8g}	2.502	540	45919	3.22	30.02	3 $^8T_{2g}$	29.83	3 $^8T_{1g}$	21.73	4 $^8T_{1g}$	15.52	2 ^8E_g	
39 Γ_{8g}	2.502	499	46076	1.99	49.78	3 $^8T_{1g}$	16.96	3 $^8T_{2g}$	13.67	4 $^8T_{1g}$	13.64	2 ^8E_g	
40 Γ_{8g}	2.502	511	46401	3.42	30.20	3 $^8T_{2g}$	21.67	4 $^8T_{1g}$	21.01	3 $^8T_{1g}$			
19 Γ_{7g}	2.502	546	46507	3.64	47.41	4 $^8T_{1g}$	32.28	3 $^8T_{1g}$	11.55	2 ^8E_g			
19 Γ_{6g}	2.489	290	46689	0.03	39.30	4 $^8T_{2g}$	36.48	5 $^8T_{1g}$					
20 Γ_{7g}	2.501	529	46734	1.49	59.27	3 $^8T_{1g}$	25.89	3 $^8T_{2g}$					
41 Γ_{8g}	2.496	304	46873	0.94	31.91	4 $^8T_{2g}$	27.69	5 $^8T_{1g}$					
20 Γ_{6g}	2.498	357	47181	0.69	53.99	3 $^8T_{2g}$	21.73	3 $^8T_{1g}$	19.61	4 $^8T_{1g}$			
21 Γ_{7g}	2.490	317	47312	0.02	44.19	4 $^8T_{2g}$							
42 Γ_{8g}	2.493	302	47316	2.22	25.58	2 ^8E_g	24.29	4 $^8T_{1g}$	13.41	5 $^8T_{1g}$	13.39	3 $^8T_{2g}$	
					11.97	3 $^8T_{1g}$							
21 Γ_{6g}	2.500	490	47446	0.30	23.18	3 $^8T_{2g}$	14.91	3 $^8T_{1g}$	13.57	6 $^8T_{1g}$	11.50	4 $^8T_{1g}$	
					10.06	3 ^8E_g							
22 Γ_{7g}	2.501	365	47534	1.01	27.13	3 $^8T_{1g}$	25.72	4 $^8T_{1g}$	16.95	2 ^8E_g	14.34	3 $^8T_{2g}$	
43 Γ_{8g}	2.489	300	47567	0.70	42.84	5 $^8T_{1g}$	26.33	4 $^8T_{2g}$					
44 Γ_{8g}	2.491	299	47857	0.18	19.29	4 $^8T_{1g}$	13.34	6 $^8T_{1g}$	12.96	3 $^8T_{1g}$	11.35	3 ^8E_g	
22 Γ_{6g}	2.498	320	47894	0.35	40.07	3 $^8T_{2g}$	19.56	3 ^8E_g	10.31	6 $^8T_{1g}$			
45 Γ_{8g}	2.498	313	47944	0.13	27.81	5 $^8T_{1g}$	15.59	4 $^8T_{2g}$					
23 Γ_{7g}	2.491	314	47992	0.07	24.29	5 $^8T_{1g}$	14.04	4 $^8T_{2g}$	11.78	3 ^8E_g	11.01	5 $^8T_{2g}$	
46 Γ_{8g}	2.499	342	48025	1.64	22.28	2 ^8E_g	21.24	3 $^8T_{2g}$	14.92	5 $^8T_{1g}$	11.56	4 $^8T_{1g}$	
23 Γ_{6g}	2.488	307	48222	0.34	40.41	4 $^8T_{2g}$	33.64	5 $^8T_{1g}$					
47 Γ_{8g}	2.500	372	48273	4.35	30.24	4 $^8T_{1g}$	23.48	2 ^8E_g	20.24	3 $^8T_{1g}$			
48 Γ_{8g}	2.494	310	48408	1.87	23.98	3 ^8E_g	21.79	4 $^8T_{1g}$	15.25	6 $^8T_{1g}$	13.27	5 $^8T_{2g}$	
24 Γ_{7g}	2.470	370	48510	0.15	24.20	4 $^8T_{2g}$	24.20	5 $^8T_{1g}$	13.72	5 $^8T_{2g}$	11.70	3 ^8E_g	
24 Γ_{6g}	2.464	391	48696	3.37	46.82	4 $^8T_{1g}$	18.86	2 ^8E_g	15.75	3 $^8T_{1g}$			
25 Γ_{7g}	2.470	367	48804	1.31	36.91	4 $^8T_{1g}$	14.00	3 $^8T_{2g}$	11.13	6 $^8T_{1g}$	10.72	4 $^8T_{2g}$	
49 Γ_{8g}	2.470	355	48834	0.54	32.60	3 $^8T_{2g}$	16.89	2 ^8E_g	12.86	5 $^8T_{2g}$			

50 Γ_{8g}	2.479	319	48993	0.55	19.97	5 $^8T_{2g}$	17.92	3 ^8E_g	16.16	3 $^8T_{2g}$			
25 Γ_{6g}	2.471	349	49010	0.17	22.80	4 $^8T_{2g}$	20.29	5 $^8T_{1g}$	18.77	5 $^8T_{2g}$			
51 Γ_{8g}	2.479	318	49091	2.25	24.14	4 $^8T_{1g}$	17.55	3 ^8E_g	13.87	3 $^8T_{2g}$	12.52	3 $^8T_{1g}$	
					11.33	2 ^8E_g							
26 Γ_{6g}	2.483	335	49179	0.11	22.92	5 $^8T_{2g}$	16.08	5 $^8T_{1g}$					
52 Γ_{8g}	2.486	306	49246	0.10	40.80	4 $^8T_{2g}$	25.11	5 $^8T_{1g}$					
26 Γ_{7g}	2.494	305	49294	1.20	31.15	6 $^8T_{1g}$	14.51	4 $^8T_{1g}$					
53 Γ_{8g}	2.478	323	49409	0.05	43.62	5 $^8T_{1g}$	37.04	4 $^8T_{2g}$	10.73	6 $^8T_{1g}$			
27 Γ_{6g}	2.489	363	49554	0.16	42.52	3 $^8T_{2g}$	20.70	2 ^8E_g	11.48	3 $^8T_{1g}$			
54 Γ_{8g}	2.493	314	49576	0.71	21.99	3 $^8T_{2g}$	19.08	3 $^8T_{1g}$	17.70	2 ^8E_g	13.91	4 $^8T_{1g}$	
55 Γ_{8g}	2.489	354	49643	0.26	18.38	6 $^8T_{1g}$	18.31	5 $^8T_{2g}$	13.28	3 ^8E_g			
27 Γ_{7g}	2.471	331	49821	0.13	22.62	3 $^8T_{1g}$	12.52	4 $^8T_{1g}$	10.89	5 $^8T_{2g}$			
56 Γ_{8g}	2.474	350	49930	1.76	30.89	3 ^8E_g	21.75	5 $^8T_{2g}$	18.47	4 $^8T_{1g}$	10.59	4 $^8T_{2g}$	
57 Γ_{8g}	2.475	363	49992	4.94	47.03	4 $^8T_{1g}$							
28 Γ_{6g}	2.475	335	50026	0.26	46.06	5 $^8T_{2g}$							
28 Γ_{7g}	2.462	346	50187	0.13	29.98	3 ^8E_g	14.76	3 $^8T_{1g}$	10.78	3 $^8T_{2g}$	10.37	2 ^8E_g	
58 Γ_{8g}	2.474	409	50202	5.92	43.29	4 $^8T_{1g}$	11.18	6 $^8T_{1g}$					
29 Γ_{6g}	2.476	415	50202	3.68	67.91	4 $^8T_{1g}$	12.96	3 $^8T_{2g}$					
59 Γ_{8g}	2.471	410	50408	4.77	35.24	4 $^8T_{1g}$	14.99	5 $^8T_{2g}$	12.28	6 $^8T_{1g}$	10.38	4 $^8T_{2g}$	
29 Γ_{7g}	2.466	392	50446	0.07	39.25	5 $^8T_{1g}$	20.64	4 $^8T_{2g}$					
60 Γ_{8g}	2.470	413	50496	0.26	42.35	4 $^8T_{2g}$	26.68	5 $^8T_{1g}$					
30 Γ_{6g}	2.471	400	50581	0.13	53.84	5 $^8T_{1g}$	31.26	4 $^8T_{2g}$					
61 Γ_{8g}	2.458	460	50718	0.06	40.64	4 $^8T_{2g}$	27.35	5 $^8T_{2g}$	23.21	5 $^8T_{1g}$			
30 Γ_{7g}	2.493	453	50854	0.04	54.71	5 $^8T_{2g}$							
31 Γ_{6g}	2.462	438	51068	0.15	26.85	3 ^8E_g	24.31	5 $^8T_{2g}$	17.83	6 $^8T_{1g}$			
62 Γ_{8g}	2.459	438	51118	0.42	33.58	5 $^8T_{2g}$	33.38	6 $^8T_{1g}$					
32 Γ_{6g}	2.466	458	51232	0.35	27.51	6 $^8T_{1g}$	11.92	3 ^8E_g					
63 Γ_{8g}	2.462	410	51345	0.24	33.62	5 $^8T_{2g}$	13.25	3 ^8E_g					
31 Γ_{7g}	2.484	358	51431	0.23	24.97	6 $^8T_{1g}$	21.43	5 $^8T_{1g}$	19.29	3 ^8E_g	10.32	4 $^8T_{2g}$	
64 Γ_{8g}	2.470	414	51529	0.33	43.48	5 $^8T_{2g}$	28.36	6 $^8T_{1g}$	11.90	5 $^8T_{1g}$			
65 Γ_{8g}	2.477	462	51676	0.06	40.14	4 $^8T_{2g}$	22.86	5 $^8T_{1g}$	14.04	5 $^8T_{2g}$			
32 Γ_{7g}	2.467	411	51937	0.03	34.82	4 $^8T_{2g}$	28.18	5 $^8T_{1g}$	11.97	5 $^8T_{2g}$	11.86	6 $^8T_{1g}$	
33 Γ_{6g}	2.462	436	52018	0.01	43.12	4 $^8T_{2g}$	16.08	6 $^8T_{1g}$	12.84	5 $^8T_{1g}$			
66 Γ_{8g}	2.468	439	52089	0.01	36.48	5 $^8T_{1g}$	33.13	6 $^8T_{1g}$	27.20	4 $^8T_{2g}$			
33 Γ_{7g}	2.462	486	52121	0.01	31.91	5 $^8T_{1g}$	28.61	6 $^8T_{1g}$	26.12	4 $^8T_{2g}$			
67 Γ_{8g}	2.465	500	52261	0.07	40.86	5 $^8T_{2g}$	17.69	3 ^8E_g	10.98	6 $^8T_{1g}$			
34 Γ_{6g}	2.470	489	52499	0.05	39.88	5 $^8T_{2g}$	23.20	6 $^8T_{1g}$					
68 Γ_{8g}	2.470	490	52509	0.19	34.49	6 $^8T_{1g}$	29.95	5 $^8T_{2g}$	15.31	3 ^8E_g			
34 Γ_{7g}	2.450	1067	52544	0.01	42.12	5 $^8T_{2g}$	14.21	3 ^8E_g					
69 Γ_{8g}	2.453	756	52933	0.29	49.19	6 $^8T_{1g}$	24.61	3 ^8E_g	13.51	5 $^8T_{2g}$			
35 Γ_{7g}	2.457	544	53291	0.10	46.47	6 $^8T_{1g}$							
70 Γ_{8g}	2.460	525	53468	0.24	50.13	6 $^8T_{1g}$	14.58	3 ^8E_g					
35 Γ_{6g}	2.462	514	53482	0.12	49.73	6 $^8T_{1g}$	14.01	3 ^8E_g					

$4f^7$ excited states

$4f^7(^6P_{3/2,5/2,7/2})$ [c]													
2 Γ_{8u}	2.469	369	30577		89.30	1 $^6T_{1u}$							
2 Γ_{7u}	2.469	369	30585		89.71	1 $^6T_{1u}$							
3 Γ_{8u}	2.469	369	30962		94.09	1 $^6T_{1u}$							
2 Γ_{6u}	2.469	369	31194		85.07	1 $^6T_{1u}$	12.14	3 $^6T_{2u}$					
4 Γ_{8u}	2.469	369	31205		85.15	1 $^6T_{1u}$							
3 Γ_{7u}	2.469	369	31222		85.28	1 $^6T_{1u}$	10.77	2 ^6E_u					
$4f^7(^6I_{7/2,9/2,11/2,13/2,15/2,17/2})$ [c]													
3 Γ_{6u}	2.468	369	34938		76.60	1 $^6T_{2u}$	20.28	1 ^6E_u					
5 Γ_{8u}	2.468	369	34945		83.29	1 $^6T_{2u}$	13.36	1 ^6E_u					
4 Γ_{7u}	2.468	369	34957		93.96	1 $^6T_{2u}$							
6 Γ_{8u}	2.468	370	34977		79.77	1 $^6T_{2u}$	13.87	1 ^6E_u					
4 Γ_{6u}	2.468	370	34989		87.62	1 $^6T_{2u}$							
7 Γ_{8u}	2.468	370	34992		86.85	1 $^6T_{2u}$							
5 Γ_{7u}	2.468	370	35191		84.88	1 ^6E_u	12.40	2 $^6T_{1u}$					

8 Γ_{8u}	2.468	370	35205	42.57	1 ^6E_u	29.43	2 $^6T_{2u}$	23.88	1 $^6A_{2u}$		
9 Γ_{8u}	2.468	370	35253	65.97	1 ^6E_u	14.31	2 $^6T_{2u}$	11.10	1 $^6T_{2u}$		
5 Γ_{6u}	2.468	369	35261	49.64	2 $^6T_{2u}$	26.00	1 $^6A_{2u}$				
10 Γ_{8u}	2.469	369	35310	72.77	2 $^6T_{2u}$	23.19	2 $^6T_{1u}$				
6 Γ_{7u}	2.469	369	35315	74.83	2 $^6T_{2u}$	23.02	2 $^6T_{1u}$				
6 Γ_{6u}	2.469	369	35317	72.55	2 $^6T_{2u}$	12.43	2 $^6T_{1u}$				
11 Γ_{8u}	2.469	369	35339	37.42	2 $^6T_{1u}$	22.25	2 $^6T_{2u}$	16.47	1 $^6A_{1u}$	15.86	1 ^6E_u
12 Γ_{8u}	2.469	369	35356	37.63	2 $^6T_{2u}$	36.79	2 $^6T_{1u}$	11.34	1 ^6E_u		
7 Γ_{6u}	2.469	369	35362	50.11	1 ^6E_u	30.90	2 $^6T_{2u}$				
7 Γ_{7u}	2.469	369	35382	51.60	1 $^6A_{1u}$	37.42	2 $^6T_{1u}$				
13 Γ_{8u}	2.469	370	35405	26.57	1 $^6A_{1u}$	17.32	1 ^6E_u	16.60	2 $^6T_{2u}$	14.93	2 $^6T_{1u}$
				14.86	1 $^6A_{2u}$						
8 Γ_{6u}	2.469	370	35414	48.77	1 $^6A_{2u}$	25.38	2 $^6T_{1u}$	12.30	1 ^6E_u		
8 Γ_{7u}	2.469	370	35442	66.68	2 $^6T_{1u}$	16.51	1 $^6A_{1u}$				
14 Γ_{8u}	2.469	369	35456	34.49	1 $^6A_{2u}$	24.06	2 $^6T_{2u}$	17.08	1 $^6A_{1u}$	15.05	2 $^6T_{1u}$
15 Γ_{8u}	2.469	369	35499	65.34	2 $^6T_{1u}$	20.75	2 $^6T_{2u}$	10.18	1 $^6A_{2u}$		
16 Γ_{8u}	2.469	369	35543	47.58	2 $^6T_{1u}$	36.48	2 $^6T_{2u}$				
9 Γ_{6u}	2.469	370	35590	45.95	2 $^6T_{1u}$	36.19	2 $^6T_{2u}$	15.29	1 $^6A_{2u}$		
17 Γ_{8u}	2.469	369	35624	49.66	2 $^6T_{1u}$	28.93	1 $^6A_{1u}$	15.41	2 $^6T_{2u}$		
9 Γ_{7u}	2.469	369	35633	56.70	2 $^6T_{1u}$	30.46	1 $^6A_{1u}$	10.94	2 $^6T_{2u}$		
$4f^7(^6D_{1/2,3/2,5/2,7/2})$ [c]											
18 Γ_{8u}	2.468	369	37679	77.72	3 $^6T_{2u}$	18.79	2 ^6E_u				
10 Γ_{6u}	2.468	370	37811	93.23	2 ^6E_u						
19 Γ_{8u}	2.469	369	37829	51.18	2 ^6E_u	45.39	3 $^6T_{2u}$				
11 Γ_{6u}	2.469	369	38062	97.04	3 $^6T_{2u}$						
20 Γ_{8u}	2.468	369	38276	51.08	3 $^6T_{2u}$	40.14	2 ^6E_u				
21 Γ_{8u}	2.468	370	38489	64.56	2 ^6E_u	20.60	3 $^6T_{2u}$	10.67	1 $^6T_{1u}$		
10 Γ_{7u}	2.469	370	38557	80.77	2 ^6E_u	11.61	1 $^6T_{1u}$				
12 Γ_{6u}	2.469	369	38667	80.48	3 $^6T_{2u}$	12.16	1 $^6T_{1u}$				
22 Γ_{8u}	2.469	369	38737	79.18	3 $^6T_{2u}$	11.13	1 $^6T_{1u}$				
11 Γ_{7u}	2.469	369	38798	84.06	3 $^6T_{2u}$	10.59	1 $^6T_{1u}$				
$4f^7(^6G_{3/2,5/2,7/2,9/2,11/2,13/2})$ [c]											
23 Γ_{8u}	2.466	369	48083	60.50	4 $^6T_{2u}$	21.28	2 $^6A_{2u}$				
13 Γ_{6u}	2.466	369	48106	59.69	4 $^6T_{2u}$	21.71	2 $^6A_{2u}$				
24 Γ_{8u}	2.467	369	48191	40.69	4 $^6T_{2u}$	23.19	3 ^6E_u	20.98	3 $^6T_{1u}$		
14 Γ_{6u}	2.467	370	48350	43.03	3 ^6E_u	36.43	5 $^6T_{2u}$	10.70	4 $^6T_{2u}$		
12 Γ_{7u}	2.467	369	48371	62.84	3 $^6T_{1u}$	28.22	3 ^6E_u				
15 Γ_{6u}	2.467	369	48468	81.00	3 $^6T_{1u}$	10.45	5 $^6T_{2u}$				
25 Γ_{8u}	2.467	368	48473	54.96	3 $^6T_{1u}$	21.61	5 $^6T_{2u}$	12.63	4 $^6T_{2u}$		
26 Γ_{8u}	2.468	370	48511	39.03	3 ^6E_u	18.21	5 $^6T_{2u}$	11.12	2 $^6A_{1u}$		
13 Γ_{7u}	2.467	369	48553	28.90	5 $^6T_{2u}$	27.93	3 $^6T_{1u}$	16.01	2 $^6A_{1u}$	14.60	4 $^6T_{2u}$
27 Γ_{8u}	2.467	369	48689	37.40	4 $^6T_{2u}$	20.31	3 ^6E_u	11.14	5 $^6T_{2u}$	10.43	3 $^6T_{1u}$
28 Γ_{8u}	2.469	369	49042	79.28	4 $^6T_{1u}$	10.21	3 $^6T_{1u}$				
14 Γ_{7u}	2.470	369	49255	41.34	4 $^6T_{1u}$	30.65	2 $^6A_{1u}$	19.17	5 $^6T_{2u}$		
29 Γ_{8u}	2.469	370	49618	27.90	2 $^6A_{1u}$	25.62	4 $^6T_{1u}$	18.35	5 $^6T_{2u}$	12.65	3 ^6E_u
16 Γ_{6u}	2.466	369	49946	67.52	4 $^6T_{2u}$	14.54	3 ^6E_u				
30 Γ_{8u}	2.467	369	50015	56.51	4 $^6T_{2u}$	15.05	3 ^6E_u	13.89	3 $^6T_{1u}$		
15 Γ_{7u}	2.466	369	50064	51.40	4 $^6T_{2u}$	20.87	3 $^6T_{1u}$				
16 Γ_{7u}	2.468	369	50236	39.44	3 ^6E_u	34.75	3 $^6T_{1u}$	11.92	4 $^6T_{1u}$		
31 Γ_{8u}	2.468	369	50270	41.76	3 $^6T_{1u}$	21.48	3 ^6E_u	20.42	4 $^6T_{1u}$		
$4f^7(^6F_{1/2,3/2,5/2,7/2,9/2,11/2})$ [c]											
17 Γ_{6u}	2.468	369	50811	44.61	5 $^6T_{2u}$	22.67	2 $^6A_{2u}$	20.41	4 $^6T_{1u}$		
32 Γ_{8u}	2.467	369	51645	23.31	5 $^6T_{2u}$	20.69	2 $^6A_{2u}$	15.73	3 $^6T_{1u}$	15.48	4 $^6T_{2u}$
33 Γ_{8u}	2.466	369	52036	71.52	3 $^6T_{1u}$	10.67	4 $^6T_{1u}$				
17 Γ_{7u}	2.467	369	52060	42.62	5 $^6T_{2u}$	22.50	3 $^6T_{1u}$	16.16	4 $^6T_{2u}$		
34 Γ_{8u}	2.467	369	52219	23.44	2 $^6A_{2u}$	21.23	4 $^6T_{2u}$	21.13	5 $^6T_{2u}$	10.51	3 ^6E_u
18 Γ_{6u}	2.467	369	52360	42.45	2 $^6A_{2u}$	30.03	5 $^6T_{2u}$	15.59	4 $^6T_{2u}$		
18 Γ_{7u}	2.469	369	52547	39.91	4 $^6T_{1u}$	25.21	2 $^6A_{1u}$	15.75	3 $^6T_{1u}$		
35 Γ_{8u}	2.468	369	52570	56.91	5 $^6T_{2u}$	12.60	2 $^6A_{2u}$	12.35	3 ^6E_u		

36 Γ_{8u}	2.469	369	52686	34.60	5 $^6T_{2u}$	29.39	4 $^6T_{1u}$	10.54	3 $^6T_{1u}$		
19 Γ_{6u}	2.467	369	52708	51.31	5 $^6T_{2u}$	23.73	3 ^6E_u	15.59	4 $^6T_{2u}$		
37 Γ_{8u}	2.469	371	52748	43.86	4 $^6T_{1u}$	12.17	2 $^6A_{1u}$				
19 Γ_{7u}	2.469	370	52867	76.14	4 $^6T_{1u}$						
20 Γ_{6u}	2.470	369	52885	66.23	4 $^6T_{1u}$	10.02	5 $^6T_{2u}$				
38 Γ_{8u}	2.469	369	53052	49.51	5 $^6T_{2u}$	29.97	4 $^6T_{1u}$				
$4f^7(^6H_{5/2,7/2,9/2,11/2,13/2,15/2})$ [c]											
20 Γ_{7u}	2.467	370	55742	56.35	5 $^6T_{1u}$	27.78	4 ^6E_u				
39 Γ_{8u}	2.467	369	55864	41.52	5 $^6T_{1u}$	22.97	4 ^6E_u	16.15	6 $^6T_{2u}$	13.13	6 $^6T_{1u}$
40 Γ_{8u}	2.467	369	56075	80.52	5 $^6T_{1u}$	11.90	4 ^6E_u				
41 Γ_{8u}	2.467	369	56139	66.73	5 $^6T_{1u}$	15.24	4 ^6E_u				
21 Γ_{6u}	2.467	369	56146	59.31	5 $^6T_{1u}$	14.53	4 ^6E_u	11.44	6 $^6T_{2u}$		
21 Γ_{7u}	2.467	369	56154	44.16	4 ^6E_u	39.99	5 $^6T_{1u}$	14.46	6 $^6T_{1u}$		
42 Γ_{8u}	2.467	370	56161	73.73	4 ^6E_u	13.55	6 $^6T_{1u}$				
22 Γ_{7u}	2.468	367	56301	36.42	6 $^6T_{2u}$	35.41	6 $^6T_{1u}$	13.29	4 ^6E_u		
43 Γ_{8u}	2.467	369	56324	70.94	5 $^6T_{1u}$	14.42	4 ^6E_u				
22 Γ_{6u}	2.467	369	56343	64.74	4 ^6E_u	22.88	5 $^6T_{1u}$				
23 Γ_{7u}	2.466	372	56356	79.51	5 $^6T_{1u}$						
23 Γ_{6u}	2.468	369	56437	85.21	6 $^6T_{1u}$						
44 Γ_{8u}	2.467	369	56442	42.83	6 $^6T_{1u}$	25.37	4 ^6E_u	19.12	6 $^6T_{2u}$		
45 Γ_{8u}	2.468	370	56513	67.81	6 $^6T_{1u}$	10.99	6 $^6T_{2u}$	10.09	4 ^6E_u		
24 Γ_{7u}	2.467	370	56629	80.44	6 $^6T_{1u}$						
24 Γ_{6u}	2.469	370	56636	81.71	6 $^6T_{2u}$						
46 Γ_{8u}	2.469	370	56645	51.77	6 $^6T_{1u}$	32.07	6 $^6T_{2u}$				
47 Γ_{8u}	2.469	370	56837	84.24	6 $^6T_{2u}$						
48 Γ_{8u}	2.469	370	56896	52.48	6 $^6T_{2u}$	33.88	6 $^6T_{1u}$				
25 Γ_{6u}	2.469	370	56902	84.22	6 $^6T_{2u}$						
49 Γ_{8u}	2.470	370	56940	52.35	6 $^6T_{2u}$	35.45	6 $^6T_{1u}$				
25 Γ_{7u}	2.470	370	56972	47.80	6 $^6T_{1u}$	41.88	6 $^6T_{2u}$				

Eu^{3+}-doped SrF_2

$4f^6(^7F_{0-6})$											
1 A_{1g}	2.313	445	0	36.42	1 $^7T_{2g}$	31.64	1 $^7T_{1g}$	26.18	1 $^7A_{2g}$		
1 T_{1g}	2.313	445	359	36.24	1 $^7T_{2g}$	30.33	1 $^7A_{2g}$	28.55	1 $^7T_{1g}$		
1 T_{2g}	2.313	443	873	49.66	1 $^7A_{2g}$	35.60	1 $^7T_{2g}$	11.22	1 $^7T_{1g}$		
1 E_g	2.314	447	1327	63.49	1 $^7T_{1g}$	32.80	1 $^7T_{2g}$				
2 T_{1g}	2.313	445	1974	41.13	1 $^7T_{1g}$	28.23	1 $^7A_{2g}$	28.07	1 $^7T_{2g}$		
2 T_{2g}	2.313	447	2065	61.66	1 $^7T_{1g}$	24.20	1 $^7T_{2g}$	11.50	1 $^7A_{2g}$		
1 A_{2g}	2.314	447	2274	50.36	1 $^7T_{1g}$	47.09	1 $^7T_{2g}$				
2 A_{1g}	2.312	443	2581	55.76	1 $^7A_{2g}$	42.06	1 $^7T_{1g}$				
3 T_{1g}	2.313	446	3082	45.64	1 $^7T_{2g}$	35.23	1 $^7T_{1g}$	17.03	1 $^7A_{2g}$		
3 T_{2g}	2.313	447	3293	78.32	1 $^7T_{1g}$	16.92	1 $^7T_{2g}$				
2 E_g	2.314	447	3393	79.35	1 $^7T_{2g}$	18.61	1 $^7T_{1g}$				
4 T_{2g}	2.313	446	4121	37.15	1 $^7T_{2g}$	36.62	1 $^7T_{1g}$	23.87	1 $^7A_{2g}$		
4 T_{1g}	2.313	447	4353	72.25	1 $^7T_{2g}$	15.33	1 $^7T_{1g}$	10.04	1 $^7A_{2g}$		
3 E_g	2.314	447	4525	49.42	1 $^7T_{2g}$	48.23	1 $^7T_{1g}$				
5 T_{1g}	2.314	447	4527	55.24	1 $^7T_{2g}$	42.20	1 $^7T_{1g}$				
3 A_{1g}	2.313	446	5490	59.20	1 $^7T_{2g}$	22.37	1 $^7T_{1g}$	15.17	1 $^7A_{2g}$		
6 T_{1g}	2.313	447	5536	53.90	1 $^7T_{2g}$	31.51	1 $^7T_{1g}$	11.32	1 $^7A_{2g}$		
5 T_{2g}	2.313	447	5555	47.01	1 $^7T_{1g}$	40.35	1 $^7T_{2g}$				
4 E_g	2.314	447	5734	63.51	1 $^7T_{1g}$	33.15	1 $^7T_{2g}$				
6 T_{2g}	2.314	447	5741	56.99	1 $^7T_{1g}$	39.63	1 $^7T_{2g}$				
2 A_{2g}	2.314	447	5753	49.93	1 $^7T_{2g}$	46.69	1 $^7T_{1g}$				
$4f^6(^5D_{0-3})$											
4 A_{1g}	2.313	448	20028	55.32	1 $^5T_{2g}$	38.81	1 ^5E_g				
7 T_{1g}	2.313	448	20835	55.33	1 $^5T_{2g}$	39.38	1 ^5E_g				
5 E_g	2.312	448	22439	54.68	1 ^5E_g	40.89	1 $^5T_{2g}$				
7 T_{2g}	2.313	448	22570	64.91	1 $^5T_{2g}$	30.53	1 ^5E_g				
3 A_{2g}	2.311	449	25110	95.59	1 ^5E_g						

8 T_{2g}	2.312	448	25195	51.40	1 $^5T_{2g}$	44.32	1 ^5E_g				
8 T_{1g}	2.312	447	25204	87.26	1 $^5T_{2g}$						
$4f^6(^5D_4,^5L_{6-10},^5G_{2-6})$											
9 T_{2g}	2.310	448	28095	38.32	1 $^5T_{1g}$	28.24	2 ^5E_g				
6 E_g	2.310	448	28096	38.42	1 $^5T_{1g}$	23.43	2 ^5E_g	14.46	1 $^5A_{1g}$		
4 A_{2g}	2.310	448	28121	42.36	1 $^5T_{1g}$	36.21	2 ^5E_g				
10 T_{2g}	2.310	448	28311	52.37	2 $^5T_{2g}$	12.59	1 $^5T_{2g}$				
9 T_{1g}	2.310	447	28323	34.05	2 ^5E_g	25.08	1 $^5T_{1g}$	22.24	2 $^5T_{2g}$		
7 E_g	2.310	448	28439	39.85	2 $^5T_{2g}$	13.57	1 $^5T_{2g}$	11.00	1 ^5E_g		
5 A_{1g}	2.310	447	28480	59.05	2 ^5E_g	16.65	2 $^5T_{2g}$				
10 T_{1g}	2.311	447	28490	37.29	1 $^5T_{1g}$	24.15	2 $^5T_{2g}$				
11 T_{2g}	2.311	447	28633	31.89	1 $^5T_{1g}$	16.68	2 $^5T_{2g}$	16.39	1 $^5A_{1g}$	15.95	2 ^5E_g
5 A_{2g}	2.312	448	28670	36.27	3 ^5E_g	32.56	2 $^5T_{1g}$	12.52	2 ^5E_g		
12 T_{2g}	2.311	449	28692	27.18	3 ^5E_g	24.33	2 $^5T_{1g}$	15.58	1 $^5T_{1g}$		
8 E_g	2.312	447	28875	35.89	2 $^5T_{1g}$	20.48	3 ^5E_g				
11 T_{1g}	2.311	445	28925	22.30	3 ^5E_g	21.76	1 $^5T_{1g}$	18.10	2 $^5T_{1g}$		
13 T_{2g}	2.313	445	28960	20.22	3 $^5T_{2g}$	12.90	3 $^5T_{1g}$	11.66	4 $^5T_{2g}$	11.43	1 $^5T_{2g}$
				10.99	2 $^5T_{1g}$						
12 T_{1g}	2.311	446	28988	25.60	1 $^5T_{1g}$	20.87	2 ^5E_g	13.28	2 $^5T_{2g}$	12.19	2 $^5T_{1g}$
14 T_{2g}	2.313	449	29027	23.69	1 $^5T_{2g}$	20.77	2 $^5T_{1g}$	15.83	2 $^5T_{2g}$		
13 T_{1g}	2.313	449	29061	18.81	3 $^5T_{2g}$	18.04	1 $^5T_{2g}$	16.97	1 ^5E_g	16.94	3 $^5T_{1g}$
				13.15	4 $^5T_{2g}$						
6 A_{1g}	2.312	446	29071	55.04	1 ^5E_g	37.70	1 $^5T_{2g}$				
9 E_g	2.311	447	29156	32.88	2 ^5E_g	29.06	1 $^5A_{1g}$				
10 E_g	2.313	450	29194	32.07	1 $^5T_{2g}$	28.04	2 $^5T_{2g}$	23.33	1 ^5E_g		
14 T_{1g}	2.312	446	29202	35.24	2 $^5T_{2g}$	15.96	1 $^5T_{1g}$				
7 A_{1g}	2.314	449	29208	44.64	4 $^5T_{2g}$	34.23	4 ^5E_g				
15 T_{1g}	2.313	451	29244	15.43	1 $^5T_{1g}$	12.52	3 ^5E_g	11.80	1 $^5T_{2g}$	10.90	1 ^5E_g
				10.68	2 $^5T_{1g}$	10.55	3 $^5T_{1g}$				
15 T_{2g}	2.313	446	29265	23.37	2 $^5A_{1g}$	22.73	2 $^5T_{1g}$				
16 T_{2g}	2.313	450	29292	21.89	3 $^5T_{1g}$	21.14	2 $^5T_{2g}$	11.37	1 $^5T_{2g}$	10.01	3 $^5T_{2g}$
6 A_{2g}	2.313	447	29385	55.50	3 $^5T_{1g}$	25.95	4 ^5E_g	11.67	2 $^5T_{1g}$		
17 T_{2g}	2.315	448	29518	46.14	3 $^5T_{2g}$	26.40	4 $^5T_{2g}$				
16 T_{1g}	2.313	447	29610	50.71	2 $^5T_{1g}$	11.03	4 ^5E_g	10.09	4 $^5T_{2g}$		
11 E_g	2.314	447	29669	34.27	4 ^5E_g	25.18	4 $^5T_{2g}$	15.06	3 $^5T_{1g}$		
17 T_{1g}	2.313	450	29719	29.04	3 $^5T_{1g}$	17.16	4 $^5T_{2g}$	14.72	3 $^5T_{2g}$	13.30	2 $^5T_{1g}$
8 A_{1g}	2.312	449	29745	64.34	3 ^5E_g	12.27	2 $^5T_{2g}$				
12 E_g	2.313	448	29843	30.47	3 ^5E_g	21.02	2 $^5A_{1g}$	12.98	1 $^5A_{1g}$		
18 T_{2g}	2.312	445	30018	21.96	1 $^5T_{1g}$	14.66	2 ^5E_g	11.61	2 $^5T_{1g}$		
13 E_g	2.312	449	30024	27.38	3 $^5T_{2g}$	20.58	2 $^5A_{1g}$	18.85	1 $^5T_{1g}$		
7 A_{2g}	2.311	447	30097	35.84	1 $^5T_{1g}$	34.41	2 ^5E_g				
19 T_{2g}	2.312	447	30116	16.97	3 $^5T_{1g}$	16.06	4 ^5E_g	16.04	2 $^5T_{2g}$	15.65	1 $^5A_{1g}$
18 T_{1g}	2.313	444	30137	31.98	2 $^5T_{2g}$	12.80	1 $^5T_{1g}$				
9 A_{1g}	2.311	448	30167	46.34	2 $^5T_{2g}$	18.70	3 ^5E_g	13.50	5 ^5E_g		
20 T_{2g}	2.311	451	30207	19.95	2 $^5T_{2g}$	19.15	1 $^5T_{1g}$	15.34	3 $^5T_{1g}$	10.85	2 ^5E_g
19 T_{1g}	2.313	452	30279	33.24	4 $^5T_{2g}$	22.11	3 $^5T_{2g}$				
14 E_g	2.313	448	30355	36.18	3 $^5T_{2g}$	16.62	4 ^5E_g				
21 T_{2g}	2.313	448	30440	30.44	4 $^5T_{2g}$	27.41	3 $^5T_{1g}$	18.02	4 ^5E_g		
20 T_{1g}	2.312	449	30569	42.10	3 ^5E_g	37.01	2 $^5T_{1g}$				
22 T_{2g}	2.313	450	30642	28.37	2 $^5A_{1g}$	25.82	2 $^5T_{1g}$	15.92	3 ^5E_g		
21 T_{1g}	2.313	448	30989	36.92	3 $^5T_{2g}$	26.25	3 $^5T_{1g}$	14.03	4 ^5E_g		
15 E_g	2.313	449	31036	39.86	3 $^5T_{1g}$	27.01	4 $^5T_{2g}$				
10 A_{1g}	2.313	448	31088	60.70	3 $^5T_{2g}$	23.96	4 ^5E_g				
22 T_{1g}	2.314	448	31209	49.22	4 $^5T_{2g}$	25.49	3 $^5T_{2g}$	18.74	3 $^5T_{1g}$		
23 T_{2g}	2.313	448	31256	38.66	4 $^5T_{2g}$	28.19	3 $^5T_{1g}$	19.58	4 ^5E_g		
8 A_{2g}	2.313	448	31263	66.19	4 ^5E_g	28.38	3 $^5T_{1g}$				
9 A_{2g}	2.312	449	31614	44.09	3 ^5E_g	37.11	2 $^5T_{1g}$				
24 T_{2g}	2.312	450	31643	34.28	2 $^5T_{1g}$	28.30	3 ^5E_g	14.47	2 $^5A_{1g}$		
16 E_g	2.312	450	31659	34.10	2 $^5T_{1g}$	21.10	2 $^5A_{1g}$	20.49	3 ^5E_g		
23 T_{1g}	2.313	448	32085	51.94	3 $^5T_{1g}$	27.78	3 $^5T_{2g}$				
25 T_{2g}	2.313	449	32093	44.82	3 $^5T_{2g}$	23.52	3 $^5T_{1g}$	12.71	4 $^5T_{2g}$		

11 A_{1g}	2.315	449	32335	46.68	4 $^5T_{2g}$	35.65	4 ^5E_g	10.72	3 $^5T_{2g}$			
24 T_{1g}	2.313	449	32341	36.97	4 $^5T_{2g}$	34.92	4 ^5E_g	13.59	3 $^5T_{1g}$	10.21	3 $^5T_{2g}$	
17 E_g	2.313	448	32345	33.19	4 ^5E_g	29.05	4 $^5T_{2g}$	23.01	3 $^5T_{1g}$	12.12	3 $^5T_{2g}$	
26 T_{2g}	2.313	448	32380	47.08	4 $^5T_{2g}$	22.77	3 $^5T_{2g}$	19.43	4 ^5E_g			

[a] Absorption oscillator strengths for 1 $\Gamma_{6u,8u,7u} \rightarrow i$ transitions are calculated at $d_{\mathrm{Eu-F}}$= 2.450 Å; the reference value is f_{ref} = 1.690×10^{-2}. Emission oscillator strengths for 1 $\Gamma_{8g} \rightarrow$1 Γ_{6u},1 Γ_{8u},1 Γ_{7u} and radiative emission lifetime are calculated at $d_{\mathrm{Eu-F}}$= 2.450 Å; the reference value is f_{ref} = 2.231×10^{-3}.

[b] The analysis of the wave function has been done at $d_{\mathrm{Eu-F}}$= 2.450 Å ($4f^7$), 2.450 Å ($4f^6(5d^1 + ITE^1_{a_{1g}})$), 2.300 Å ($4f^6$).

[c] C.f. Table S8

TABLE S11: Spectroscopic constants and analyses of the spin-orbit wave functions of the ground and lowest lying excited states of Eu^{2+} and Eu^{3+} -doped BaF_2 cubic defects. Eu–F bond distances ($d_{\mathrm{Eu-F},e}$ in Å), EuF_8 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), minimum-to-minimum energy differences (T_e in cm^{-1}), and relative absorption and emission oscillator strengths (f_i^{abs}/f_{ref} and f_i^{emi}/f_{ref}) are given. Calculated radiative emission lifetime for the $4f^6(^7F_J)5de_g^1$ – 1 Γ_{8g} excited state is 0.451 μs. Local distortion around the Eu^{2+}impurity, relative to experimental crystal structure d_{Ba-F}= 2.685 Å, is $d_{\mathrm{Eu-F},e}(1\Gamma_{6u}) - d_{\mathrm{Ba-F}} = -0.127$; ionic radii mismatch is +0.17 Å[31]. See Fig. 3, S3 and text for details.

State	$d_{\mathrm{Eu-F},e}$	$\omega_{a_{1g}}$	T_e	f_i^{abs}/f_{ref} [a]	f_i^{emi}/f_{ref} [a]	weights of terms larger than 10% [b]							
$4f^7(^8S_{7/2})$ [c]													
1 Γ_{6u}	2.558	321	0.000		1.00	97.79	1 $^8A_{1u}$						
1 Γ_{8u}	2.558	321	0.026		0.86	97.79	1 $^8A_{1u}$						
1 Γ_{7u}	2.558	321	0.069		0.03	97.79	1 $^8A_{1u}$						
$4f^6(5d + ITE_{a_{1g}})^1$ excited states													
$4f^6(^7F_J)5de_g^1$ High-Spin coupling [d]													
1 Γ_{8g}	2.535	328	28044	1.00		49.84	1 $^8T_{2g}$	35.40	1 $^8T_{1g}$				
1 Γ_{7g}	2.535	328	28216	0.52		54.74	1 $^8T_{2g}$	37.06	1 $^8T_{1g}$				
2 Γ_{8g}	2.535	328	28369	0.10		70.12	1 $^8T_{2g}$	16.91	1 ^8E_g				
2 Γ_{7g}	2.535	328	28747	0.77		48.37	1 $^8T_{1g}$	37.99	1 $^8T_{2g}$				
3 Γ_{8g}	2.535	328	29066	1.06		35.81	1 $^8T_{2g}$	32.01	1 $^8T_{1g}$	22.86	1 ^8E_g		
1 Γ_{6g}	2.535	328	29198	0.37		32.70	1 $^8T_{2g}$	24.78	1 $^8T_{1g}$	22.58	1 ^8E_g	16.02	2 $^8T_{1g}$
4 Γ_{8g}	2.535	328	29660	1.80		50.95	1 $^8T_{1g}$	23.20	1 $^8T_{2g}$	13.59	2 $^8T_{1g}$		
2 Γ_{6g}	2.535	328	29776	0.31		30.74	1 $^8T_{2g}$	21.95	1 ^8E_g	21.40	1 $^8T_{1g}$	20.03	2 $^8T_{1g}$
5 Γ_{8g}	2.535	328	29952	0.22		45.02	1 ^8E_g	34.65	2 $^8T_{1g}$	14.65	1 $^8T_{2g}$		
3 Γ_{7g}	2.535	329	30009	0.74		39.16	1 $^8T_{1g}$	27.82	1 ^8E_g	27.80	1 $^8T_{2g}$		
6 Γ_{8g}	2.534	329	30238	0.48		34.40	1 ^8E_g	31.67	1 $^8T_{2g}$	13.89	1 $^8T_{1g}$	11.28	2 $^8T_{2g}$
7 Γ_{8g}	2.534	327	30561	0.71		41.88	2 $^8T_{1g}$	23.03	1 $^8T_{1g}$	18.01	1 $^8T_{2g}$	15.44	2 $^8T_{2g}$
3 Γ_{6g}	2.534	328	30578	0.63		44.79	1 $^8T_{1g}$	21.53	2 $^8T_{1g}$	18.33	2 $^8T_{2g}$		
8 Γ_{8g}	2.535	328	31093	1.60		45.56	1 $^8T_{1g}$	25.02	2 $^8T_{1g}$	17.26	1 $^8T_{2g}$		
9 Γ_{8g}	2.534	328	31249	0.52		23.12	1 ^8E_g	21.58	1 $^8T_{2g}$	19.73	1 $^8T_{1g}$	19.35	2 $^8T_{1g}$
						15.43	2 $^8T_{2g}$						
4 Γ_{7g}	2.535	328	31272	1.16		55.17	1 $^8T_{1g}$	18.42	1 $^8T_{2g}$	13.31	1 ^8E_g		
4 Γ_{6g}	2.534	328	31286	0.30		33.65	2 $^8T_{1g}$	25.63	1 $^8T_{2g}$	21.00	2 $^8T_{2g}$	14.78	1 $^8T_{1g}$
5 Γ_{7g}	2.534	328	31375	0.34		37.92	1 $^8T_{2g}$	30.02	2 $^8T_{1g}$	12.74	1 ^8E_g	10.38	2 $^8T_{2g}$
5 Γ_{6g}	2.534	328	31655	0.10		42.63	2 $^8T_{2g}$	32.24	1 $^8T_{2g}$	14.54	2 $^8T_{1g}$		
10 Γ_{8g}	2.534	328	31702	0.05		56.90	2 $^8T_{2g}$	21.90	1 ^8E_g	12.69	1 $^8T_{2g}$		
11 Γ_{8g}	2.535	328	31940	0.74		28.36	1 $^8T_{2g}$	21.18	1 $^8T_{1g}$	20.05	1 $^6T_{1g}$	15.74	1 ^8E_g
						10.29	2 $^8T_{1g}$						
6 Γ_{6g}	2.534	328	31947	0.51		31.78	1 $^8T_{2g}$	30.23	2 $^8T_{2g}$	16.86	1 $^8T_{1g}$	11.37	2 $^8T_{1g}$
13 Γ_{8g}	2.534	327	32366	0.45		26.80	1 ^8E_g	21.65	1 $^8T_{2g}$	20.22	2 $^8T_{1g}$	18.55	2 $^8T_{2g}$
6 Γ_{7g}	2.534	328	32392	0.01		57.19	2 $^8T_{1g}$	15.61	2 $^8T_{2g}$	13.51	1 $^8T_{2g}$		
14 Γ_{8g}	2.534	328	32631	1.40		42.23	2 $^8T_{1g}$	27.52	1 $^8T_{1g}$	14.10	2 $^8T_{2g}$		
15 Γ_{8g}	2.534	328	33097	3.20		67.64	1 $^8T_{1g}$	24.19	1 $^8T_{2g}$				
7 Γ_{6g}	2.534	329	33109	1.72		71.72	1 $^8T_{1g}$	22.29	1 $^8T_{2g}$				
7 Γ_{7g}	2.533	328	33119			72.99	2 $^8T_{2g}$	15.57	1 ^8E_g				
16 Γ_{8g}	2.533	328	33267	0.59		61.65	2 $^8T_{2g}$	17.12	2 $^8T_{1g}$	10.31	1 ^8E_g		
8 Γ_{6g}	2.534	328	33394	0.07		59.12	2 $^8T_{2g}$	25.14	2 $^8T_{1g}$				
18 Γ_{8g}	2.535	328	33632	1.32		42.78	2 $^8T_{1g}$	21.24	1 ^8E_g	20.69	1 $^8T_{1g}$		
9 Γ_{6g}	2.534	328	33691	0.06		52.37	2 $^8T_{1g}$	16.25	1 ^8E_g	16.24	2 $^8T_{2g}$	11.58	1 $^8T_{2g}$
19 Γ_{8g}	2.534	326	33978	0.16		66.84	2 $^8T_{1g}$	13.49	1 ^8E_g				
9 Γ_{7g}	2.534	326	34118			74.63	2 $^8T_{1g}$						
20 Γ_{8g}	2.533	327	34955	0.02		87.51	2 $^8T_{2g}$						
21 Γ_{8g}	2.533	327	35114	0.01		78.75	2 $^8T_{2g}$	16.41	2 $^8T_{1g}$				
10 Γ_{7g}	2.533	327	35149			81.71	2 $^8T_{2g}$	16.44	2 $^8T_{1g}$				
$4f^6(^7F_J)5de_g^1$ Low-Spin coupling [d]													
12 Γ_{8g}	2.534	323	32066	0.36		67.94	1 $^6T_{1g}$						
8 Γ_{7g}	2.533	323	33327	0.02		85.17	1 $^6T_{1g}$	10.69	1 $^6T_{2g}$				

17 Γ_{8g}	2.534	323	33416	0.07	87.95	1 $^6T_{1g}$							
10 Γ_{6g}	2.531	323	35050	0.04	56.42	1 $^6T_{1g}$	30.15	1 $^6T_{2g}$	11.28	2 $^6T_{1g}$			
22 Γ_{8g}	2.531	323	35174	0.07	58.76	1 $^6T_{1g}$	27.41	1 $^6T_{2g}$					
11 Γ_{7g}	2.533	322	35457	0.04	78.77	1 $^6T_{1g}$	10.79	1 $^6T_{2g}$					
11 Γ_{6g}	2.530	304	35760	0.01	58.53	1 $^6T_{2g}$	23.21	1 ^6E_g	13.04	1 $^6T_{1g}$			
23 Γ_{8g}	2.531	324	35994	0.02	24.75	1 $^6T_{2g}$	23.41	1 $^6T_{1g}$	22.47	1 ^6E_g	21.55	2 $^6T_{1g}$	
12 Γ_{7g}	2.531	324	36127	0.01	45.45	2 $^6T_{1g}$	24.51	1 $^6T_{2g}$	19.20	1 ^6E_g			
24 Γ_{8g}	2.530	323	36652	0.02	32.75	2 $^6T_{1g}$	28.62	1 $^6T_{2g}$	23.45	1 ^6E_g			
12 Γ_{6g}	2.533	323	36737	0.01	62.48	2 $^6T_{1g}$	14.54	1 $^6T_{1g}$	11.49	1 $^6T_{2g}$			
13 Γ_{7g}	2.531	323	36746		38.67	2 $^6T_{1g}$	35.03	1 $^6T_{2g}$	15.84	1 $^6T_{1g}$			
25 Γ_{8g}	2.531	323	37360	0.05	46.61	2 $^6T_{1g}$	18.99	1 $^6T_{2g}$	18.75	1 ^6E_g	10.83	2 $^6T_{2g}$	
26 Γ_{8g}	2.531	325	37444	0.02	53.20	1 $^6T_{2g}$	17.28	1 ^6E_g	10.93	2 $^6T_{1g}$	10.85	1 $^6T_{1g}$	
27 Γ_{8g}	2.530	325	38181	0.05	31.36	1 ^6E_g	29.60	1 $^6T_{2g}$	24.83	2 $^6T_{1g}$			
13 Γ_{6g}	2.530	322	38215	0.03	46.04	1 $^6T_{2g}$	30.21	1 ^6E_g	12.06	1 $^6T_{1g}$			
14 Γ_{7g}	2.531	322	38366		64.08	2 $^6T_{1g}$	13.58	1 $^6T_{2g}$	10.50	1 ^6E_g			
28 Γ_{8g}	2.531	321	38550	0.02	80.26	2 $^6T_{2g}$	10.11	2 $^6T_{1g}$					
14 Γ_{6g}	2.530	322	38728	0.06	48.40	1 $^6T_{2g}$	33.12	1 ^6E_g					
29 Γ_{8g}	2.531	323	38890	0.09	67.08	1 $^6T_{2g}$	21.18	2 $^6T_{1g}$					
15 Γ_{7g}	2.530	311	39490	0.01	52.44	1 ^6E_g	36.80	2 $^6T_{1g}$					
30 Γ_{8g}	2.530	323	39823	0.09	36.71	2 $^6T_{1g}$	36.15	1 ^6E_g	23.76	1 $^6T_{2g}$			
31 Γ_{8g}	2.531	322	39959	0.06	61.62	2 $^6T_{1g}$	23.00	1 ^6E_g	11.26	1 $^6T_{2g}$			
15 Γ_{6g}	2.531	322	40038		83.36	2 $^6T_{2g}$	10.89	2 $^6T_{1g}$					
32 Γ_{8g}	2.531	323	40041	0.01	82.19	2 $^6T_{2g}$	10.29	2 $^6T_{1g}$					
16 Γ_{6g}	2.530	518	41803	0.01	89.49	2 $^6T_{2g}$							
16 Γ_{7g}	2.530	344	41807		88.74	2 $^6T_{2g}$							
33 Γ_{8g}	2.531	297	41839	0.01	89.06	2 $^6T_{2g}$							
$4f^6(^7F_J)(5dt^1_{2g} + ITE^1_{a_{1g}})$ High-Spin coupling [d,e]													
34 Γ_{8g}	2.575	835	42590	0.53	41.77	3 $^8T_{1g}$	26.04	2 ^8E_g	22.72	3 $^8T_{2g}$			
35 Γ_{8g}	2.575	473	42750	0.22	39.83	3 $^8T_{2g}$	29.57	3 $^8T_{1g}$	23.08	2 ^8E_g			
17 Γ_{7g}	2.585	403	43066	0.58	65.14	3 $^8T_{2g}$	13.67	4 $^8T_{1g}$	11.60	2 ^8E_g			
36 Γ_{8g}	2.584	418	43160	0.71	39.35	3 $^8T_{2g}$	33.57	2 ^8E_g	19.55	3 $^8T_{1g}$			
17 Γ_{6g}	2.583	403	43182	0.22	53.53	3 $^8T_{1g}$	23.37	2 ^8E_g	11.37	3 $^8T_{2g}$			
18 Γ_{7g}	2.583	484	43559	1.14	40.10	3 $^8T_{2g}$	31.09	2 ^8E_g	18.26	4 $^8T_{1g}$			
18 Γ_{6g}	2.581	491	43666	0.38	49.53	3 $^8T_{1g}$	30.76	2 ^8E_g					
37 Γ_{8g}	2.588	318	43902	0.68	45.68	3 $^8T_{2g}$	32.41	3 $^8T_{1g}$					
38 Γ_{8g}	2.625	1046	44349	3.07	31.32	3 $^8T_{1g}$	27.83	3 $^8T_{2g}$	22.66	4 $^8T_{1g}$	13.94	2 ^8E_g	
39 Γ_{8g}	2.593	274	44540	1.45	43.98	3 $^8T_{1g}$	20.78	3 $^8T_{2g}$	16.63	2 ^8E_g	12.00	4 $^8T_{1g}$	
40 Γ_{8g}	2.599	252	44844	4.66	33.29	3 $^8T_{2g}$	29.59	4 $^8T_{1g}$	24.95	3 $^8T_{1g}$			
19 Γ_{7g}	2.586	371	44883	3.71	57.63	4 $^8T_{1g}$	21.42	3 $^8T_{1g}$	12.04	2 ^8E_g			
19 Γ_{6g}	2.587	380	45085	0.71	53.75	3 $^8T_{2g}$	22.44	3 $^8T_{1g}$	18.82	4 $^8T_{1g}$			
20 Γ_{7g}	2.584	402	45137	1.12	61.97	3 $^8T_{1g}$	26.02	3 $^8T_{2g}$					
41 Γ_{8g}	2.625	939	45234	2.60	32.13	2 ^8E_g	26.74	4 $^8T_{1g}$	18.42	3 $^8T_{2g}$	17.20	3 $^8T_{1g}$	
20 Γ_{6g}	2.588	355	45535	0.13	24.29	5 $^8T_{1g}$	15.01	4 $^8T_{2g}$	14.93	3 ^8E_g	13.91	3 $^8T_{2g}$	
42 Γ_{8g}	2.625	905	45659	0.18	24.17	5 $^8T_{1g}$	17.94	4 $^8T_{2g}$	16.21	3 ^8E_g	14.29	4 $^8T_{1g}$	
21 Γ_{7g}	2.590	330	45734	1.20	32.24	3 $^8T_{1g}$	23.84	4 $^8T_{1g}$	13.15	2 ^8E_g	12.75	3 $^8T_{2g}$	
					10.94	4 $^8T_{2g}$							
21 Γ_{6g}	2.586	401	45735	0.40	46.60	3 $^8T_{2g}$	14.70	3 $^8T_{1g}$	14.52	3 ^8E_g			
22 Γ_{7g}	2.586	403	45810	0.20	22.05	3 ^8E_g	22.03	4 $^8T_{2g}$	19.75	5 $^8T_{1g}$	10.14	3 $^8T_{2g}$	
43 Γ_{8g}	2.602	265	45963	0.84	32.18	2 ^8E_g	26.86	3 $^8T_{2g}$	11.25	4 $^8T_{1g}$	10.80	3 $^8T_{1g}$	
22 Γ_{6g}	2.591	326	46276	4.03	54.77	4 $^8T_{1g}$	15.64	2 ^8E_g	15.29	3 $^8T_{1g}$			
44 Γ_{8g}	2.604	253	46296	3.73	25.72	3 $^8T_{1g}$	25.14	4 $^8T_{1g}$	18.37	2 ^8E_g	14.21	5 $^8T_{1g}$	
45 Γ_{8g}	2.593	311	46298	1.89	24.76	3 ^8E_g	21.20	4 $^8T_{2g}$	18.17	5 $^8T_{1g}$	16.58	4 $^8T_{1g}$	
46 Γ_{8g}	2.594	301	46371	0.79	19.49	4 $^8T_{2g}$	18.11	3 $^8T_{2g}$	17.12	3 ^8E_g	13.94	2 ^8E_g	
23 Γ_{7g}	2.593	312	46372	1.06	34.96	4 $^8T_{1g}$	13.88	3 $^8T_{2g}$	13.68	4 $^8T_{2g}$	12.30	5 $^8T_{1g}$	
23 Γ_{6g}	2.595	314	46574	0.28	42.24	4 $^8T_{2g}$							
47 Γ_{8g}	2.592	313	46630	0.60	29.18	3 $^8T_{2g}$	14.65	4 $^8T_{2g}$	14.16	2 ^8E_g	12.31	3 $^8T_{1g}$	
					10.15	3 ^8E_g							
48 Γ_{8g}	2.592	313	46770	2.05	25.86	4 $^8T_{1g}$	16.31	3 $^8T_{2g}$	16.07	3 ^8E_g	15.21	3 $^8T_{1g}$	
					10.89	2 ^8E_g							
24 Γ_{7g}	2.595	316	47069	1.28	34.54	5 $^8T_{1g}$	17.92	4 $^8T_{1g}$					
24 Γ_{6g}	2.594	307	47363		40.88	5 $^8T_{2g}$	39.11	6 $^8T_{1g}$					

25 Γ_{7g}	2.594	313	47373	0.19	21.72	5 $^8T_{1g}$	14.76	3 $^8T_{1g}$	10.65	4 $^8T_{2g}$			
49 Γ_{8g}	2.595	314	47385	0.25	21.65	5 $^8T_{1g}$	19.35	3 ^8E_g	13.63	4 $^8T_{2g}$			
50 Γ_{8g}	2.593	313	47451	0.70	21.83	3 $^8T_{1g}$	20.69	3 $^8T_{2g}$	15.39	2 ^8E_g	13.41	4 $^8T_{1g}$	
					11.80	5 $^8T_{1g}$							
51 Γ_{8g}	2.593	311	47516	1.27	31.04	4 $^8T_{2g}$	26.34	3 ^8E_g	15.79	4 $^8T_{1g}$			
25 Γ_{6g}	2.588	279	47521	0.12	23.91	3 $^8T_{2g}$	14.56	4 $^8T_{2g}$	14.10	2 ^8E_g	10.14	5 $^8T_{1g}$	
52 Γ_{8g}	2.593	312	47636	2.70	31.91	4 $^8T_{1g}$	13.01	3 $^8T_{1g}$	11.89	3 ^8E_g			
26 Γ_{7g}	2.593	313	47640	0.08	28.84	3 $^8T_{1g}$	20.89	3 ^8E_g	15.29	3 $^8T_{2g}$	14.25	2 ^8E_g	
26 Γ_{6g}	2.573	555	47805	0.07	37.76	4 $^8T_{2g}$	14.42	3 $^8T_{2g}$					
53 Γ_{8g}	2.583	271	47848	0.55	31.52	5 $^8T_{2g}$	28.15	6 $^8T_{1g}$					
54 Γ_{8g}	2.588	292	47980	6.27	49.71	4 $^8T_{1g}$	13.80	5 $^8T_{1g}$	10.35	3 $^8T_{1g}$			
27 Γ_{6g}	2.565	351	48245	3.55	73.50	4 $^8T_{1g}$	12.95	3 $^8T_{2g}$					
55 Γ_{8g}	2.569	326	48284	4.76	48.86	4 $^8T_{1g}$	19.28	4 $^8T_{2g}$					
27 Γ_{7g}	2.558	336	48456	0.02	47.62	5 $^8T_{2g}$	10.74	6 $^8T_{1g}$					
56 Γ_{8g}	2.565	302	48545	0.85	52.88	6 $^8T_{1g}$	33.94	5 $^8T_{2g}$					
28 Γ_{6g}	2.586	266	48712	0.26	26.52	5 $^8T_{1g}$	24.21	3 ^8E_g	22.73	4 $^8T_{2g}$			
57 Γ_{8g}	2.564	288	48809	0.88	43.27	4 $^8T_{2g}$	36.77	5 $^8T_{1g}$					
28 Γ_{7g}	2.583	245	49062	0.04	63.23	4 $^8T_{2g}$							
29 Γ_{6g}	2.558	320	49105	0.42	32.47	5 $^8T_{1g}$	16.56	3 ^8E_g					
58 Γ_{8g}	2.547	351	49138	0.28	42.10	4 $^8T_{2g}$	14.23	3 ^8E_g					
59 Γ_{8g}	2.546	329	49254	0.20	50.63	6 $^8T_{1g}$	25.55	5 $^8T_{2g}$					
30 Γ_{6g}	2.550	393	49304	0.08	50.30	5 $^8T_{2g}$	35.43	6 $^8T_{1g}$					
60 Γ_{8g}	2.545	359	49393	0.33	50.40	5 $^8T_{1g}$	29.41	4 $^8T_{2g}$	11.94	3 ^8E_g			
30 Γ_{7g}	2.555	454	49477	0.19	55.74	5 $^8T_{1g}$	20.75	3 ^8E_g					
62 Γ_{8g}	2.575	965	50122	0.13	53.69	6 $^8T_{1g}$	32.25	5 $^8T_{2g}$					
31 Γ_{7g}	2.560	331	50207	0.01	42.42	4 $^8T_{2g}$	17.30	3 ^8E_g					
29 Γ_{7g}	2.546	334	49317	0.03	42.86	5 $^8T_{2g}$	38.60	6 $^8T_{1g}$					
61 Γ_{8g}	2.525	984	49989	0.09	45.00	4 $^8T_{2g}$	23.25	3 ^8E_g					
31 Γ_{6g}	2.541	371	50076	0.05	38.52	6 $^8T_{1g}$	17.59	5 $^8T_{2g}$					
63 Γ_{8g}	2.546	301	50282	0.10	61.13	5 $^8T_{2g}$	36.60	6 $^8T_{1g}$					
32 Γ_{6g}	2.525	906	50413	0.09	40.06	4 $^8T_{2g}$	24.51	5 $^8T_{1g}$					
64 Γ_{8g}	2.546	299	50431	0.26	33.40	5 $^8T_{1g}$	30.39	4 $^8T_{2g}$	16.44	3 ^8E_g			
65 Γ_{8g}	2.538	434	50590	0.36	48.11	5 $^8T_{1g}$	25.52	3 ^8E_g	15.65	4 $^8T_{2g}$			
32 Γ_{7g}	2.575	1253	50799	0.11	43.53	5 $^8T_{1g}$							
33 Γ_{6g}	2.521	1281	50894	0.10	48.10	5 $^8T_{1g}$	14.27	3 ^8E_g					
33 Γ_{7g}	2.531	469	51124	0.05	46.76	6 $^8T_{1g}$	19.23	5 $^8T_{2g}$					
66 Γ_{8g}	2.540	335	51191	0.25	48.95	5 $^8T_{1g}$	15.35	3 ^8E_g					
67 Γ_{8g}	2.536	489	51249	0.07	52.25	5 $^8T_{2g}$	26.72	6 $^8T_{1g}$					
68 Γ_{8g}	2.540	512	51380	0.10	60.65	5 $^8T_{2g}$	38.79	6 $^8T_{1g}$					
34 Γ_{6g}	2.542	527	51385	0.10	62.23	6 $^8T_{1g}$	34.15	5 $^8T_{2g}$					
34 Γ_{7g}	2.517	521	52120	0.04	44.44	6 $^8T_{1g}$	38.65	5 $^8T_{2g}$					
69 Γ_{8g}	2.519	532	52194	0.06	49.94	5 $^8T_{2g}$	30.69	6 $^8T_{1g}$					
35 Γ_{7g}	2.523	916	52400	0.05	53.93	6 $^8T_{1g}$	45.91	5 $^8T_{2g}$					
35 Γ_{6g}	2.525	696	52483	0.02	54.38	5 $^8T_{2g}$	21.25	6 $^8T_{1g}$					
70 Γ_{8g}	2.525	792	52496	0.13	63.59	6 $^8T_{1g}$	36.31	5 $^8T_{2g}$					

$4f^7$ excited states

$4f^7(^6P_{3/2,5/2,7/2})$ [c]													
2 Γ_{8u}	2.556	321	30809		89.37	1 $^6T_{1u}$							
2 Γ_{7u}	2.556	320	30815		89.68	1 $^6T_{1u}$							
3 Γ_{8u}	2.556	321	31194		94.10	1 $^6T_{1u}$							
2 Γ_{6u}	2.556	320	31428		85.14	1 $^6T_{1u}$	12.09	3 $^6T_{2u}$					
4 Γ_{8u}	2.556	320	31436		85.19	1 $^6T_{1u}$							
3 Γ_{7u}	2.556	321	31449		85.26	1 $^6T_{1u}$	10.79	2 ^6E_u					
$4f^7(^6I_{7/2,9/2,11/2,13/2,15/2,17/2})$ [c]													
3 Γ_{6u}	2.555	321	35200		75.84	1 $^6T_{2u}$	21.32	1 ^6E_u					
5 Γ_{8u}	2.555	321	35207		81.55	1 $^6T_{2u}$	15.16	1 ^6E_u					
4 Γ_{7u}	2.555	321	35219		93.60	1 $^6T_{2u}$							
6 Γ_{8u}	2.555	321	35227		80.56	1 $^6T_{2u}$	12.84	1 ^6E_u					
4 Γ_{6u}	2.555	321	35238		88.00	1 $^6T_{2u}$							

7 Γ_{8u}	2.555	321	35239	90.00	1 $^6T_{2u}$							
5 Γ_{7u}	2.555	322	35438	83.34	1 ^6E_u	13.74	2 $^6T_{1u}$					
8 Γ_{8u}	2.555	321	35456	49.53	1 ^6E_u	25.17	2 $^6T_{2u}$	20.16	1 $^6A_{2u}$			
9 Γ_{8u}	2.555	321	35500	61.53	1 ^6E_u	14.74	2 $^6T_{2u}$	12.28	1 $^6T_{2u}$			
5 Γ_{6u}	2.556	320	35515	52.30	2 $^6T_{2u}$	18.56	1 $^6A_{2u}$	10.53	2 $^6T_{1u}$	10.08	1 ^6E_u	
10 Γ_{8u}	2.557	320	35534	67.19	2 $^6T_{2u}$	26.86	2 $^6T_{1u}$					
6 Γ_{7u}	2.557	320	35535	65.71	2 $^6T_{2u}$	29.35	2 $^6T_{1u}$					
6 Γ_{6u}	2.556	321	35541	69.71	2 $^6T_{2u}$	12.94	2 $^6T_{1u}$					
11 Γ_{8u}	2.557	321	35560	43.46	2 $^6T_{1u}$	33.19	1 $^6A_{1u}$	14.65	2 $^6T_{2u}$			
12 Γ_{8u}	2.557	320	35592	47.53	2 $^6T_{1u}$	32.75	2 $^6T_{2u}$	11.11	1 ^6E_u			
7 Γ_{7u}	2.557	321	35594	55.79	1 $^6A_{1u}$	25.47	2 $^6T_{1u}$	13.17	2 $^6T_{2u}$			
7 Γ_{6u}	2.556	321	35603	35.44	1 ^6E_u	34.28	2 $^6T_{2u}$	17.18	2 $^6T_{1u}$			
13 Γ_{8u}	2.556	321	35643	26.51	2 $^6T_{2u}$	21.32	1 ^6E_u	19.98	1 $^6A_{1u}$	11.30	1 $^6T_{2u}$	
				10.47	2 $^6T_{1u}$	10.10	1 $^6A_{2u}$					
8 Γ_{6u}	2.556	321	35650	46.03	1 $^6A_{2u}$	25.28	1 ^6E_u	15.30	2 $^6T_{1u}$	12.96	1 $^6T_{2u}$	
8 Γ_{7u}	2.556	321	35664	72.30	2 $^6T_{1u}$							
14 Γ_{8u}	2.556	321	35685	30.24	1 $^6A_{2u}$	26.55	2 $^6T_{1u}$	17.77	2 $^6T_{2u}$	10.46	1 $^6A_{1u}$	
15 Γ_{8u}	2.557	321	35713	47.09	2 $^6T_{1u}$	26.04	2 $^6T_{2u}$	20.59	1 $^6A_{2u}$			
16 Γ_{8u}	2.556	321	35779	48.58	2 $^6T_{2u}$	37.39	2 $^6T_{1u}$					
9 Γ_{6u}	2.556	321	35815	41.55	2 $^6T_{1u}$	38.93	2 $^6T_{2u}$	16.64	1 $^6A_{2u}$			
17 Γ_{8u}	2.557	321	35842	48.33	2 $^6T_{1u}$	26.15	1 $^6A_{1u}$	18.56	2 $^6T_{2u}$			
9 Γ_{7u}	2.557	321	35846	56.08	2 $^6T_{1u}$	29.68	1 $^6A_{1u}$	12.22	2 $^6T_{2u}$			
$4f^7(^6D_{1/2,3/2,5/2,7/2})$ [c]												
18 Γ_{8u}	2.555	318	37970	75.16	3 $^6T_{2u}$	21.53	2 ^6E_u					
10 Γ_{6u}	2.556	321	38067	91.35	2 ^6E_u							
19 Γ_{8u}	2.555	319	38077	52.48	2 ^6E_u	44.18	3 $^6T_{2u}$					
11 Γ_{6u}	2.555	317	38310	95.44	3 $^6T_{2u}$							
20 Γ_{8u}	2.555	319	38547	53.00	3 $^6T_{2u}$	38.68	2 ^6E_u					
21 Γ_{8u}	2.555	320	38757	62.34	2 ^6E_u	23.24	3 $^6T_{2u}$	10.80	1 $^6T_{1u}$			
10 Γ_{7u}	2.556	321	38807	81.49	2 ^6E_u	11.78	1 $^6T_{1u}$					
12 Γ_{6u}	2.555	317	38925	80.69	3 $^6T_{2u}$	12.31	1 $^6T_{1u}$					
22 Γ_{8u}	2.556	317	38975	78.78	3 $^6T_{2u}$	11.38	1 $^6T_{1u}$					
11 Γ_{7u}	2.556	317	39028	84.34	3 $^6T_{2u}$	10.67	1 $^6T_{1u}$					
$4f^7(^6G_{3/2,5/2,7/2,9/2,11/2,13/2})$ [c]												
23 Γ_{8u}	2.554	323	48442	56.69	4 $^6T_{2u}$	20.47	2 $^6A_{2u}$	12.50	3 ^6E_u			
13 Γ_{6u}	2.555	323	48461	49.25	4 $^6T_{2u}$	18.14	2 $^6A_{2u}$	17.03	3 ^6E_u	10.61	5 $^6T_{2u}$	
24 Γ_{8u}	2.555	322	48511	34.25	4 $^6T_{2u}$	26.51	3 ^6E_u	20.63	3 $^6T_{1u}$			
14 Γ_{6u}	2.555	321	48649	33.97	3 ^6E_u	30.54	5 $^6T_{2u}$	20.49	4 $^6T_{2u}$			
12 Γ_{7u}	2.554	320	48703	55.93	3 $^6T_{1u}$	31.92	3 ^6E_u					
25 Γ_{8u}	2.555	320	48765	29.30	3 $^6T_{1u}$	22.02	3 ^6E_u	16.17	2 $^6A_{1u}$	10.84	4 $^6T_{1u}$	
				10.81	5 $^6T_{2u}$							
26 Γ_{8u}	2.555	322	48794	36.75	3 $^6T_{1u}$	28.14	5 $^6T_{2u}$	13.43	3 ^6E_u	12.12	4 $^6T_{2u}$	
15 Γ_{6u}	2.554	321	48794	67.38	3 $^6T_{1u}$	16.52	5 $^6T_{2u}$					
13 Γ_{7u}	2.555	321	48833	29.12	3 $^6T_{1u}$	28.55	5 $^6T_{2u}$	17.22	2 $^6A_{1u}$	14.76	4 $^6T_{2u}$	
27 Γ_{8u}	2.555	321	49003	40.36	4 $^6T_{2u}$	17.26	4 $^6T_{1u}$	15.24	3 ^6E_u	10.12	3 $^6T_{1u}$	
28 Γ_{8u}	2.557	321	49255	71.56	4 $^6T_{1u}$	13.82	3 $^6T_{1u}$					
14 Γ_{7u}	2.557	321	49434	39.67	4 $^6T_{1u}$	28.60	2 $^6A_{1u}$	19.93	5 $^6T_{2u}$			
29 Γ_{8u}	2.557	321	49832	23.82	4 $^6T_{1u}$	23.57	2 $^6A_{1u}$	18.43	5 $^6T_{2u}$	14.28	3 ^6E_u	
16 Γ_{6u}	2.554	323	50292	66.06	4 $^6T_{2u}$	15.36	3 ^6E_u					
30 Γ_{8u}	2.555	323	50352	55.24	4 $^6T_{2u}$	15.54	3 ^6E_u	14.71	3 $^6T_{1u}$			
15 Γ_{7u}	2.555	322	50401	47.32	4 $^6T_{2u}$	21.72	3 $^6T_{1u}$	11.43	3 ^6E_u			
16 Γ_{7u}	2.555	321	50510	36.87	3 $^6T_{1u}$	31.09	3 ^6E_u	12.37	4 $^6T_{1u}$			
31 Γ_{8u}	2.555	320	50544	42.05	3 $^6T_{1u}$	19.93	3 ^6E_u	18.11	4 $^6T_{1u}$	12.17	2 $^6A_{1u}$	
$4f^7(^6F_{1/2,3/2,5/2,7/2,9/2,11/2})$ [c]												
17 Γ_{6u}	2.555	321	51069	43.54	5 $^6T_{2u}$	23.35	4 $^6T_{1u}$	20.75	2 $^6A_{2u}$			
32 Γ_{8u}	2.555	321	51942	23.87	5 $^6T_{2u}$	18.71	2 $^6A_{2u}$	16.29	3 $^6T_{1u}$	15.12	4 $^6T_{2u}$	
				11.65	4 $^6T_{1u}$							
33 Γ_{8u}	2.554	321	52392	66.04	3 $^6T_{1u}$	13.45	4 $^6T_{1u}$					
17 Γ_{7u}	2.554	321	52395	41.66	5 $^6T_{2u}$	22.95	3 $^6T_{1u}$	16.40	4 $^6T_{2u}$			

34 Γ_{8u}	2.555	322	52531	21.28	4 $^6T_{2u}$	20.73	2 $^6A_{2u}$	20.22	5 $^6T_{2u}$	10.52	3 ^6E_u
18 Γ_{6u}	2.555	321	52666	42.23	2 $^6A_{2u}$	29.79	5 $^6T_{2u}$	15.76	4 $^6T_{2u}$		
18 Γ_{7u}	2.556	321	52792	42.71	4 $^6T_{1u}$	22.80	2 $^6A_{1u}$	13.94	3 $^6T_{1u}$		
35 Γ_{8u}	2.555	320	52836	57.11	5 $^6T_{2u}$	12.22	3 ^6E_u	10.99	2 $^6A_{2u}$		
36 Γ_{8u}	2.556	322	52916	36.37	5 $^6T_{2u}$	32.68	4 $^6T_{1u}$	13.76	4 $^6T_{2u}$		
19 Γ_{6u}	2.555	321	53001	50.89	5 $^6T_{2u}$	23.28	3 ^6E_u	16.26	4 $^6T_{2u}$		
37 Γ_{8u}	2.555	321	53005	34.24	4 $^6T_{1u}$	17.99	3 $^6T_{1u}$	17.80	2 $^6A_{1u}$		
20 Γ_{6u}	2.557	321	53066	63.69	4 $^6T_{1u}$	10.22	5 $^6T_{2u}$				
19 Γ_{7u}	2.557	321	53079	71.99	4 $^6T_{1u}$						
38 Γ_{8u}	2.556	321	53279	53.07	5 $^6T_{2u}$	25.73	4 $^6T_{1u}$				
$4f^7(^6H_{5/2,7/2,9/2,11/2,13/2,15/2})$ [c]											
20 Γ_{7u}	2.554	321	56062	54.56	5 $^6T_{1u}$	28.19	4 ^6E_u				
39 Γ_{8u}	2.555	320	56168	34.33	5 $^6T_{1u}$	21.18	4 ^6E_u	19.85	6 $^6T_{2u}$	19.24	6 $^6T_{1u}$
40 Γ_{8u}	2.554	320	56414	76.92	5 $^6T_{1u}$	10.90	4 ^6E_u				
41 Γ_{8u}	2.554	321	56455	44.29	5 $^6T_{1u}$	23.74	4 ^6E_u	22.56	6 $^6T_{1u}$		
21 Γ_{6u}	2.554	321	56473	48.86	5 $^6T_{1u}$	17.72	4 ^6E_u	16.43	6 $^6T_{2u}$		
21 Γ_{7u}	2.554	321	56478	40.34	5 $^6T_{1u}$	36.74	4 ^6E_u	20.92	6 $^6T_{1u}$		
42 Γ_{8u}	2.554	321	56485	57.56	4 ^6E_u	27.08	5 $^6T_{1u}$				
22 Γ_{7u}	2.555	321	56565	39.95	6 $^6T_{2u}$	36.11	6 $^6T_{1u}$	14.25	4 ^6E_u		
43 Γ_{8u}	2.554	320	56663	68.02	5 $^6T_{1u}$	11.72	6 $^6T_{1u}$				
22 Γ_{6u}	2.554	320	56674	35.37	4 ^6E_u	33.11	5 $^6T_{1u}$	18.52	6 $^6T_{1u}$		
23 Γ_{6u}	2.555	322	56707	65.93	6 $^6T_{1u}$	22.27	4 ^6E_u				
23 Γ_{7u}	2.554	321	56710	84.63	5 $^6T_{1u}$						
44 Γ_{8u}	2.555	320	56732	58.55	6 $^6T_{1u}$	16.50	6 $^6T_{2u}$	14.40	4 ^6E_u		
45 Γ_{8u}	2.555	321	56788	37.85	6 $^6T_{1u}$	30.05	4 ^6E_u	12.95	6 $^6T_{2u}$		
46 Γ_{8u}	2.556	321	56892	48.23	6 $^6T_{1u}$	27.45	6 $^6T_{2u}$				
24 Γ_{7u}	2.555	321	56900	75.19	6 $^6T_{1u}$	12.09	4 ^6E_u				
24 Γ_{6u}	2.555	321	56909	74.14	6 $^6T_{2u}$	14.35	4 ^6E_u				
47 Γ_{8u}	2.557	321	57058	76.36	6 $^6T_{2u}$						
48 Γ_{8u}	2.557	321	57113	51.81	6 $^6T_{2u}$	33.06	6 $^6T_{1u}$				
25 Γ_{6u}	2.557	321	57120	79.65	6 $^6T_{2u}$						
49 Γ_{8u}	2.557	321	57140	57.72	6 $^6T_{2u}$	27.98	6 $^6T_{1u}$				
25 Γ_{7u}	2.557	321	57164	45.93	6 $^6T_{1u}$	42.91	6 $^6T_{2u}$				

Eu^{3+}-doped BaF_2

$4f^6(^7F_{0-6})$											
1 A_{1g}	2.363	402	0	37.34	1 $^7T_{2g}$	32.60	1 $^7T_{1g}$	24.29	1 $^7A_{2g}$		
1 T_{1g}	2.363	402	363	37.36	1 $^7T_{2g}$	29.96	1 $^7T_{1g}$	27.80	1 $^7A_{2g}$		
1 T_{2g}	2.362	403	902	46.42	1 $^7A_{2g}$	37.51	1 $^7T_{2g}$	12.52	1 $^7T_{1g}$		
1 E_g	2.364	401	1297	62.81	1 $^7T_{1g}$	33.50	1 $^7T_{2g}$				
2 T_{1g}	2.363	402	1980	39.42	1 $^7T_{1g}$	30.83	1 $^7T_{2g}$	27.17	1 $^7A_{2g}$		
2 T_{2g}	2.363	402	2055	60.00	1 $^7T_{1g}$	25.21	1 $^7T_{2g}$	12.20	1 $^7A_{2g}$		
1 A_{2g}	2.364	401	2238	49.65	1 $^7T_{1g}$	47.81	1 $^7T_{2g}$				
2 A_{1g}	2.362	403	2640	56.46	1 $^7A_{2g}$	41.43	1 $^7T_{1g}$				
3 T_{1g}	2.363	403	3069	45.70	1 $^7T_{2g}$	33.81	1 $^7T_{1g}$	18.40	1 $^7A_{2g}$		
3 T_{2g}	2.364	400	3277	77.98	1 $^7T_{1g}$	17.42	1 $^7T_{2g}$				
2 E_g	2.364	402	3341	80.00	1 $^7T_{2g}$	17.96	1 $^7T_{1g}$				
4 T_{2g}	2.363	403	4124	36.64	1 $^7T_{1g}$	35.17	1 $^7T_{2g}$	25.84	1 $^7A_{2g}$		
4 T_{1g}	2.363	403	4320	72.00	1 $^7T_{2g}$	14.27	1 $^7T_{1g}$	11.38	1 $^7A_{2g}$		
3 E_g	2.364	401	4490	49.19	1 $^7T_{2g}$	48.48	1 $^7T_{1g}$				
5 T_{1g}	2.364	401	4490	52.42	1 $^7T_{2g}$	45.18	1 $^7T_{1g}$				
3 A_{1g}	2.363	403	5471	58.33	1 $^7T_{2g}$	22.06	1 $^7T_{1g}$	16.37	1 $^7A_{2g}$		
6 T_{1g}	2.363	403	5515	53.10	1 $^7T_{2g}$	31.32	1 $^7T_{1g}$	12.33	1 $^7A_{2g}$		
5 T_{2g}	2.363	402	5538	46.19	1 $^7T_{1g}$	40.41	1 $^7T_{2g}$	10.14	1 $^7A_{2g}$		
4 E_g	2.364	401	5709	64.60	1 $^7T_{1g}$	32.07	1 $^7T_{2g}$				
6 T_{2g}	2.364	401	5713	58.49	1 $^7T_{1g}$	38.16	1 $^7T_{2g}$				
2 A_{2g}	2.364	401	5720	49.23	1 $^7T_{2g}$	47.42	1 $^7T_{1g}$				
$4f^6(^5D_{0-3})$											
4 A_{1g}	2.362	400	20083	55.58	1 $^5T_{2g}$	38.63	1 ^5E_g				

7 T_{1g}	2.362	400	20893	55.64	1 $^5T_{2g}$	39.15	1 ^5E_g						
5 E_g	2.362	400	22513	54.65	1 ^5E_g	40.93	1 $^5T_{2g}$						
7 T_{2g}	2.362	400	22625	65.55	1 $^5T_{2g}$	29.93	1 ^5E_g						
3 A_{2g}	2.361	400	25196	95.64	1 ^5E_g								
8 T_{2g}	2.362	400	25264	50.80	1 $^5T_{2g}$	44.95	1 ^5E_g						
8 T_{1g}	2.362	400	25272	87.09	1 $^5T_{2g}$								
$4f^6(^5D_4,^5L_{6-10},^5G_{2-6})$													
6 E_g	2.360	399	28248	34.77	1 $^5T_{1g}$	19.72	2 ^5E_g	14.63	1 $^5A_{1g}$	12.71	2 $^5T_{1g}$		
9 T_{2g}	2.360	399	28250	35.83	1 $^5T_{1g}$	25.18	2 ^5E_g	10.14	2 $^5T_{1g}$				
4 A_{2g}	2.360	399	28271	40.22	1 $^5T_{1g}$	33.61	2 ^5E_g	12.15	3 ^5E_g				
9 T_{1g}	2.360	398	28485	33.47	2 ^5E_g	26.06	1 $^5T_{1g}$	21.43	2 $^5T_{2g}$				
10 T_{2g}	2.360	399	28493	49.35	2 $^5T_{2g}$	11.89	1 $^5T_{2g}$						
7 E_g	2.360	398	28606	38.89	2 $^5T_{2g}$	13.74	1 $^5T_{2g}$	11.31	1 ^5E_g	10.69	2 ^5E_g		
10 T_{1g}	2.361	399	28617	36.20	1 $^5T_{1g}$	22.34	2 $^5T_{2g}$						
5 A_{1g}	2.360	398	28619	57.38	2 ^5E_g	15.58	2 $^5T_{2g}$						
5 A_{2g}	2.362	400	28739	33.52	3 ^5E_g	31.37	2 $^5T_{1g}$	14.98	2 ^5E_g				
11 T_{2g}	2.361	398	28745	19.77	2 ^5E_g	15.97	2 $^5T_{2g}$	14.21	2 $^5T_{1g}$	12.44	1 $^5T_{1g}$		
				10.21	3 ^5E_g								
12 T_{2g}	2.361	401	28795	33.33	1 $^5T_{1g}$	15.04	3 ^5E_g	13.65	1 $^5A_{1g}$	13.14	2 $^5T_{1g}$		
8 E_g	2.362	400	28937	32.88	2 $^5T_{1g}$	16.09	3 ^5E_g	13.90	1 $^5T_{1g}$	10.80	2 $^5A_{1g}$		
13 T_{2g}	2.363	400	28984	25.27	3 $^5T_{2g}$	18.17	1 $^5T_{2g}$	14.06	3 $^5T_{1g}$	11.46	4 $^5T_{2g}$		
11 T_{1g}	2.362	397	29013	30.07	2 $^5T_{1g}$	23.97	3 ^5E_g	12.12	1 $^5T_{1g}$	11.36	3 $^5T_{2g}$		
12 T_{1g}	2.362	398	29085	20.73	4 $^5T_{2g}$	15.04	3 $^5T_{2g}$	11.84	3 $^5T_{1g}$	11.15	1 $^5T_{2g}$		
				10.69	1 ^5E_g	10.24	4 ^5E_g						
14 T_{2g}	2.362	400	29091	26.86	2 $^5T_{1g}$	16.85	1 $^5T_{2g}$	13.09	2 $^5T_{2g}$				
13 T_{1g}	2.361	404	29115	24.37	1 $^5T_{1g}$	15.67	2 ^5E_g	10.29	2 $^5T_{2g}$				
6 A_{1g}	2.363	397	29123	44.82	1 ^5E_g	29.55	1 $^5T_{2g}$	10.42	4 $^5T_{2g}$	10.41	4 ^5E_g		
7 A_{1g}	2.363	405	29196	40.16	4 $^5T_{2g}$	23.86	4 ^5E_g	10.75	1 ^5E_g				
9 E_g	2.362	398	29242	29.69	1 $^5T_{2g}$	21.41	1 ^5E_g	18.51	2 ^5E_g	15.74	1 $^5A_{1g}$		
14 T_{1g}	2.362	399	29266	27.38	2 $^5T_{2g}$	19.14	1 $^5T_{2g}$	18.14	1 ^5E_g				
10 E_g	2.361	401	29267	32.15	2 $^5T_{2g}$	11.76	2 ^5E_g	11.42	1 $^5A_{1g}$				
15 T_{2g}	2.363	400	29298	17.69	1 $^5T_{2g}$	14.74	3 $^5T_{1g}$	13.86	2 $^5T_{1g}$	10.81	2 $^5A_{1g}$		
				10.68	2 $^5T_{2g}$								
15 T_{1g}	2.361	401	29318	29.07	1 $^5T_{1g}$	16.35	2 $^5T_{2g}$	12.78	2 $^5T_{1g}$	10.26	3 ^5E_g		
16 T_{2g}	2.362	400	29350	21.66	2 $^5T_{2g}$	13.36	1 $^5A_{1g}$	10.96	2 $^5A_{1g}$	10.47	1 $^5T_{1g}$		
6 A_{2g}	2.362	401	29420	54.86	3 $^5T_{1g}$	27.52	4 ^5E_g	11.48	2 $^5T_{1g}$				
17 T_{2g}	2.364	403	29491	43.76	3 $^5T_{2g}$	27.68	4 $^5T_{2g}$						
16 T_{1g}	2.363	400	29627	28.76	2 $^5T_{1g}$	19.92	4 $^5T_{2g}$	16.66	3 $^5T_{2g}$	15.72	4 ^5E_g		
11 E_g	2.364	401	29637	31.12	4 ^5E_g	23.39	4 $^5T_{2g}$	13.24	3 $^5T_{2g}$	11.70	3 $^5T_{1g}$		
17 T_{1g}	2.362	402	29753	37.67	2 $^5T_{1g}$	25.50	3 $^5T_{1g}$						
8 A_{1g}	2.361	400	29831	68.36	3 ^5E_g	10.20	3 $^5T_{2g}$						
12 E_g	2.362	401	29901	34.30	3 ^5E_g	28.43	2 $^5A_{1g}$						
18 T_{2g}	2.362	399	30084	20.95	3 $^5T_{1g}$	14.36	2 $^5T_{1g}$	13.16	4 $^5T_{2g}$	11.78	1 $^5T_{1g}$		
13 E_g	2.362	400	30093	29.26	3 $^5T_{2g}$	18.75	1 $^5T_{1g}$	10.53	1 $^5A_{1g}$	10.03	2 $^5A_{1g}$		
18 T_{1g}	2.363	400	30175	25.49	4 $^5T_{2g}$	20.77	3 $^5T_{2g}$	11.34	2 $^5T_{2g}$				
19 T_{2g}	2.361	400	30187	22.79	4 ^5E_g	17.17	3 $^5T_{1g}$	16.65	1 $^5A_{1g}$	10.66	1 $^5T_{1g}$		
7 A_{2g}	2.361	399	30209	35.50	1 $^5T_{1g}$	34.16	2 ^5E_g						
9 A_{1g}	2.361	399	30277	50.11	2 $^5T_{2g}$	14.53	5 ^5E_g	13.60	3 ^5E_g				
20 T_{2g}	2.361	399	30312	29.77	2 $^5T_{2g}$	21.86	1 $^5T_{1g}$	11.72	2 ^5E_g				
19 T_{1g}	2.362	402	30327	33.14	2 $^5T_{2g}$	13.17	2 ^5E_g	11.83	4 $^5T_{2g}$				
14 E_g	2.362	401	30387	23.47	3 $^5T_{2g}$	12.74	4 ^5E_g	10.69	1 $^5T_{1g}$				
21 T_{2g}	2.363	402	30432	26.73	4 $^5T_{2g}$	21.10	3 $^5T_{1g}$	14.66	4 ^5E_g	10.90	1 $^5T_{1g}$		
20 T_{1g}	2.362	401	30648	42.62	3 ^5E_g	36.46	2 $^5T_{1g}$						
22 T_{2g}	2.362	401	30703	26.59	2 $^5A_{1g}$	25.03	2 $^5T_{1g}$	16.19	3 ^5E_g				
21 T_{1g}	2.363	401	31007	34.93	3 $^5T_{2g}$	25.86	3 $^5T_{1g}$	15.35	4 ^5E_g				
15 E_g	2.363	402	31051	39.10	3 $^5T_{1g}$	22.68	4 $^5T_{2g}$						
10 A_{1g}	2.363	401	31080	59.08	3 $^5T_{2g}$	21.94	4 ^5E_g						
22 T_{1g}	2.363	402	31190	51.24	4 $^5T_{2g}$	25.02	3 $^5T_{2g}$	17.45	3 $^5T_{1g}$				
23 T_{2g}	2.363	402	31245	40.44	4 $^5T_{2g}$	27.18	3 $^5T_{1g}$	19.85	4 ^5E_g				
8 A_{2g}	2.363	401	31268	65.55	4 ^5E_g	29.29	3 $^5T_{1g}$						
9 A_{2g}	2.361	401	31703	44.96	3 ^5E_g	37.65	2 $^5T_{1g}$						

24 T_{2g}	2.362	401	31727	35.20	2 $^5T_{1g}$	29.29	3 ^5E_g	13.87	2 $^5A_{1g}$				
16 E_g	2.361	401	31741	35.15	2 $^5T_{1g}$	21.20	3 ^5E_g	20.54	2 $^5A_{1g}$				
25 T_{2g}	2.363	403	32097	49.91	3 $^5T_{2g}$	25.18	3 $^5T_{1g}$						
23 T_{1g}	2.362	402	32114	49.04	3 $^5T_{1g}$	32.20	3 $^5T_{2g}$						
11 A_{1g}	2.363	404	32305	39.00	4 $^5T_{2g}$	37.50	4 ^5E_g	17.62	3 $^5T_{2g}$				
24 T_{1g}	2.363	402	32334	35.21	4 ^5E_g	34.04	4 $^5T_{2g}$	19.27	3 $^5T_{1g}$				
17 E_g	2.363	401	32351	33.10	4 $^5T_{2g}$	32.75	4 ^5E_g	24.44	3 $^5T_{1g}$				
26 T_{2g}	2.363	402	32374	55.09	4 $^5T_{2g}$	19.70	4 ^5E_g	13.89	3 $^5T_{2g}$	10.05	3 $^5T_{1g}$		

[a] Absorption oscillator strengths for 1 $\Gamma_{6u,8u,7u} \rightarrow i$ transitions are calculated at $d_{\mathrm{Eu-F}}$= 2.550 Å; the reference value is f_{ref} = 1.688×10^{-2}. Emission oscillator strengths for 1 $\Gamma_{8g} \rightarrow$1 Γ_{6u},1 Γ_{8u},1 Γ_{7u} and radiative emission lifetime are calculated at $d_{\mathrm{Eu-F}}$= 2.550 Å; the reference value is f_{ref} = 2.227×10^{-3}.

[b] The analyses of the wave functions have been done at $d_{\mathrm{Eu-F}}$= 2.550 Å ($4f^7$), 2.550 Å ($4f^6(5d^1 + ITE^1_{a_{1g}})$), 2.350 Å ($4f^6$).

[c] C.f. Table S7.

[d] C.f. Table S8.

[e] Low-spin ($S = 5/2$) wave functions of the $4f^6(^7F_J)(5dt^1_{2g} + ITE^1_{a_{1g}})$ configurations have not been included in the spin-orbit calculations.

TABLE S12: Spectroscopic constants and analyses of the spin-orbit wave functions of the ground and lowest lying excited states of Eu^{2+} and Eu^{3+} -doped CaS octahedral defects. Eu–S bond distances ($d_{\mathrm{Eu-S},e}$ in Å), EuS_6 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), minimum-to-minimum energy differences (T_e in cm^{-1}), and relative absorption and emission oscillator strengths (f_i^{abs}/f_{ref} and f_i^{emi}/f_{ref}) are given. Calculated radiative emission lifetime for the $4f^6(^7F_J)5de_g^1$ – 1 Γ_{8g} excited state is 0.437 μs. Local distortion around the Eu^{2+}impurity, relative to experimental crystal structure d_{Ca-F}= 2.855 Å, is $d_{\mathrm{Eu-S},e}(1\Gamma_{6u}) - d_{\mathrm{Ca-S}} = +0.021$; ionic radii mismatch is +0.13 Å[31]. See Fig. 3, S3 and text for details.

State	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e	f_i^{abs}/f_{ref} [a]	f_i^{emi}/f_{ref} [a]	weights of terms larger than 10% [b]					
Eu^{2+}-doped CaS											
$4f^7(^8S_{7/2})$ [c]											
1 Γ_{6u}	2.876	286	0		1.00	97.68	1 $^8A_{1g}$				
1 Γ_{8u}	2.876	286	0		0.34	97.69	1 $^8A_{1g}$				
1 Γ_{7u}	2.876	286	0		0.06	97.68	1 $^8A_{1g}$				
$4f^6(5d+6s)^1$ excited states											
$4f^6(^7F_J)5dt_{2g}^1$ High-Spin coupling [d]											
1 Γ_{8g}	2.849	283	17309	1.00		34.99	1 $^8T_{1g}$	30.29	1 ^8E_g	16.99	1 $^8T_{2g}$
2 Γ_{8g}	2.849	284	17710	1.11		29.71	1 $^8T_{2g}$	27.02	1 ^8E_g	26.24	1 $^8T_{1g}$
1 Γ_{7g}	2.849	283	18010	1.74		46.09	1 $^8T_{2g}$	26.16	2 $^8T_{1g}$	13.32	1 ^8E_g
3 Γ_{8g}	2.849	284	18252	1.30		40.05	1 $^8T_{2g}$	30.26	1 ^8E_g	12.91	1 $^8T_{1g}$
1 Γ_{6g}	2.849	284	18269	0.72		41.49	1 ^8E_g	36.98	1 $^8T_{1g}$		
2 Γ_{7g}	2.849	283	18582	1.99		39.05	1 $^8T_{2g}$	26.84	2 $^8T_{1g}$	18.65	1 ^8E_g
4 Γ_{8g}	2.849	283	19003	2.18		34.97	1 $^8T_{2g}$	20.15	1 $^8T_{1g}$	18.45	1 ^8E_g
2 Γ_{6g}	2.849	283	19090	0.28		46.65	1 $^8T_{1g}$	15.62	2 $^8T_{1g}$	15.24	1 ^8E_g
5 Γ_{8g}	2.848	282	19404	6.10		35.53	2 $^8T_{1g}$	29.36	1 $^8T_{1g}$	24.36	1 $^8T_{2g}$
6 Γ_{8g}	2.849	283	19799	2.47		33.03	1 $^8T_{1g}$	19.87	1 ^8E_g	14.89	2 $^8T_{1g}$
3 Γ_{7g}	2.848	283	19805	1.79		31.79	2 $^8T_{1g}$	16.56	2 $^8T_{2g}$	13.38	2 ^8E_g
7 Γ_{8g}	2.848	283	19883	1.73		33.48	1 $^8T_{2g}$	16.40	2 ^8E_g	10.60	2 $^8T_{1g}$
3 Γ_{6g}	2.847	284	19938	0.16		34.28	2 ^8E_g	21.03	3 $^8T_{1g}$	14.77	2 $^8T_{2g}$
8 Γ_{8g}	2.848	282	20109	2.68		19.25	1 $^8T_{1g}$	14.53	1 $^8T_{2g}$	12.83	2 $^8T_{1g}$
						10.26	3 $^8T_{1g}$				
4 Γ_{7g}	2.848	284	20143	2.14		28.04	1 ^8E_g	17.33	2 ^8E_g	14.54	2 $^8T_{1g}$
4 Γ_{6g}	2.848	282	20269	1.66		37.87	2 $^8T_{1g}$	31.36	1 $^8T_{2g}$	17.16	1 $^8T_{1g}$
9 Γ_{8g}	2.848	282	20487	1.63		21.21	2 ^8E_g	19.16	1 ^8E_g	14.94	1 $^8T_{2g}$
						13.61	1 $^8T_{1g}$				
5 Γ_{7g}	2.848	282	20685	1.28		45.46	1 $^8T_{1g}$	27.90	1 $^8T_{2g}$		
5 Γ_{6g}	2.848	283	20713	1.01		26.70	1 $^8T_{2g}$	19.98	2 $^8T_{2g}$	15.38	2 $^8T_{1g}$
10 Γ_{8g}	2.848	283	20768	0.07		37.44	2 ^8E_g	21.83	2 $^8T_{2g}$	10.04	3 $^8T_{1g}$
11 Γ_{8g}	2.848	282	20993	2.47		21.58	2 ^8E_g	19.02	2 $^8T_{1g}$	18.78	1 $^8T_{1g}$
						10.98	3 $^8T_{1g}$				
6 Γ_{7g}	2.848	283	21014	2.56		40.97	1 $^8T_{1g}$	21.79	2 $^8T_{1g}$	16.30	1 $^8T_{2g}$
12 Γ_{8g}	2.848	285	21024	3.34		21.65	1 $^8T_{2g}$	20.86	1 ^8E_g	19.74	2 $^8T_{1g}$
7 Γ_{7g}	2.848	283	21231	0.53		24.51	1 $^8T_{2g}$	18.99	3 $^8T_{1g}$	10.46	2 $^8T_{1g}$
6 Γ_{6g}	2.848	282	21238	1.34		30.34	1 $^8T_{1g}$	17.93	1 $^8T_{2g}$	13.64	2 $^8T_{1g}$
7 Γ_{6g}	2.848	282	21610	5.12		32.89	1 $^8T_{1g}$	25.07	2 $^8T_{1g}$	17.06	1 $^8T_{2g}$
13 Γ_{8g}	2.848	282	21646	5.04		23.39	1 $^8T_{1g}$	15.34	2 $^8T_{1g}$	12.41	2 ^8E_g
						11.97	1 ^8E_g				
14 Γ_{8g}	2.848	282	21696	1.65		23.77	1 $^8T_{2g}$	21.52	2 ^8E_g	17.47	1 ^8E_g
15 Γ_{8g}	2.848	283	21781	1.54		28.30	1 $^8T_{2g}$	17.17	1 $^8T_{1g}$	11.63	2 ^8E_g
8 Γ_{7g}	2.847	284	21799	0.29		27.01	2 ^8E_g	10.73	3 $^8T_{1g}$		
16 Γ_{8g}	2.848	283	21823	2.08		19.60	1 $^8T_{2g}$	12.42	1 $^8T_{1g}$	11.19	2 ^8E_g
						10.65	2 $^8T_{1g}$				
9 Γ_{7g}	2.849	283	22246	2.25		36.41	2 $^8T_{1g}$	15.66	3 $^8T_{1g}$	11.64	1 $^8T_{2g}$
17 Γ_{8g}	2.848	283	22256	3.99		29.88	2 $^8T_{1g}$	15.21	2 $^8T_{2g}$	14.16	3 $^8T_{1g}$
8 Γ_{6g}	2.848	283	22358	0.45		34.30	2 $^8T_{2g}$	10.51	3 $^8T_{1g}$		
9 Γ_{6g}	2.848	283	22399	0.02		40.80	1 $^8T_{2g}$	27.20	2 ^8E_g		

18 Γ_{8g}	2.848	282	22449	6.99	34.93	2 $^8T_{1g}$	21.38	2 $^8T_{2g}$	18.50	1 $^8T_{1g}$	10.13	3 $^8T_{1g}$
19 Γ_{8g}	2.848	282	22564	0.09	23.06	1 $^8T_{1g}$	23.04	1 $^8T_{2g}$	16.27	2 ^8E_g	11.16	1 ^8E_g
10 Γ_{7g}	2.848	283	22700	0.02	33.12	1 $^8T_{1g}$	18.49	1 $^8T_{2g}$	14.29	2 $^8T_{1g}$	10.95	1 ^8E_g
20 Γ_{8g}	2.848	283	22860	9.55	39.66	2 $^8T_{1g}$	20.47	1 $^8T_{1g}$	11.33	1 ^8E_g		
10 Γ_{6g}	2.848	283	22881	4.21	49.68	2 $^8T_{1g}$	16.60	1 $^8T_{2g}$				
21 Γ_{8g}	2.848	283	23096	8.96	41.57	2 $^8T_{1g}$	22.74	2 $^8T_{2g}$	16.90	1 $^8T_{2g}$		
11 Γ_{6g}	2.848	283	23256	0.83	38.11	2 $^8T_{2g}$	13.86	2 ^8E_g	12.64	2 $^8T_{1g}$	10.59	1 $^8T_{2g}$
22 Γ_{8g}	2.848	283	23354	2.35	42.88	2 $^8T_{2g}$	16.82	3 $^8T_{1g}$				
23 Γ_{8g}	2.848	282	23438	0.74	53.39	2 $^8T_{2g}$	15.30	3 $^8T_{1g}$	11.97	1 $^8T_{1g}$		
11 Γ_{7g}	2.848	282	23444	0.10	58.05	2 $^8T_{2g}$	10.04	1 $^8T_{1g}$				
12 Γ_{6g}	2.848	283	23516	1.91	37.50	3 $^8T_{1g}$	25.41	2 $^8T_{2g}$				
24 Γ_{8g}	2.848	283	23763	0.75	59.75	3 $^8T_{1g}$	19.70	2 $^8T_{2g}$				
12 Γ_{7g}	2.848	283	23766	0.49	62.66	3 $^8T_{1g}$						
25 Γ_{8g}	2.848	282	24028	0.21	37.07	2 $^8T_{2g}$	16.76	2 ^8E_g				
13 Γ_{7g}	2.847	283	24153	0.01	54.92	2 $^8T_{2g}$	10.45	2 ^8E_g				
26 Γ_{8g}	2.849	284	24185	0.01	68.88	1 $^6T_{1g}$	21.51	2 $^8T_{2g}$				
13 Γ_{6g}	2.847	283	24624	0.34	48.23	3 $^8T_{1g}$	34.85	2 $^8T_{2g}$				
28 Γ_{8g}	2.847	283	24685	1.05	61.49	3 $^8T_{1g}$	15.90	2 $^8T_{2g}$	14.54	2 ^8E_g		
14 Γ_{7g}	2.847	283	24946	0.31	49.03	3 $^8T_{1g}$	13.04	2 $^8T_{2g}$				
29 Γ_{8g}	2.847	283	24982	0.68	52.97	3 $^8T_{1g}$						
14 Γ_{6g}	2.847	283	24994	0.38	53.88	3 $^8T_{1g}$						
$4f^6(^7F_J)5dt^1_{2g}$ Low-Spin coupling [d]												
15 Γ_{7g}	2.849	283	25411	0.01	78.49	1 $^6T_{1g}$	11.03	1 $^6T_{2g}$				
30 Γ_{8g}	2.849	283	25414	0.01	80.32	1 $^6T_{1g}$						
16 Γ_{7g}	2.846	283	26839	0.01	38.70	2 $^6T_{1g}$	35.96	1 ^6E_g	18.90	1 $^6T_{1g}$		
15 Γ_{6g}	2.847	282	27064	0.06	49.69	1 $^6T_{1g}$	32.01	1 $^6T_{2g}$	12.40	2 $^6T_{1g}$		
31 Γ_{8g}	2.847	282	27089	0.10	47.68	1 $^6T_{1g}$	33.08	1 $^6T_{2g}$				
32 Γ_{8g}	2.845	284	27251	0.01	48.90	2 $^6T_{1g}$	28.04	1 ^6E_g				
17 Γ_{7g}	2.846	283	27344	0.03	30.50	1 $^6T_{2g}$	28.89	1 $^6T_{1g}$	26.30	2 $^6T_{1g}$		
16 Γ_{6g}	2.845	283	27462		24.02	2 $^6T_{1g}$	19.35	1 $^6T_{2g}$	16.37	1 ^6E_g	15.62	2 $^6T_{2g}$
					10.98	1 $^6T_{1g}$						
33 Γ_{8g}	2.845	283	27767	0.02	22.36	2 $^6T_{1g}$	21.92	2 $^6T_{2g}$	19.63	1 ^6E_g	16.07	1 $^6A_{2g}$
18 Γ_{7g}	2.847	284	27991	0.01	45.12	1 $^6T_{1g}$	24.45	2 $^6T_{1g}$	13.37	1 $^6T_{2g}$		
17 Γ_{6g}	2.845	283	28081	0.02	39.33	1 $^6T_{2g}$	37.80	2 $^6T_{1g}$				
34 Γ_{8g}	2.845	283	28267	0.01	20.04	1 $^6A_{2g}$	18.50	2 $^6T_{2g}$	12.78	1 $^6T_{1g}$	11.90	2 $^6T_{1g}$
					11.32	1 ^6E_g	10.12	1 $^6T_{2g}$				
18 Γ_{6g}	2.844	283	28448	0.01	38.67	1 $^6A_{2g}$	25.41	2 $^6T_{2g}$				
35 Γ_{8g}	2.845	283	28490	0.07	35.18	2 $^6T_{1g}$	34.47	1 $^6T_{2g}$	15.18	1 ^6E_g		
36 Γ_{8g}	2.845	283	28670	0.05	26.77	1 ^6E_g	20.03	1 $^6T_{2g}$	18.18	2 $^6T_{1g}$	10.59	3 $^6T_{1g}$
19 Γ_{6g}	2.846	283	29080	0.04	35.27	1 ^6E_g	28.73	1 $^6T_{2g}$	23.06	2 $^6T_{2g}$		
37 Γ_{8g}	2.844	283	29154	0.06	21.75	3 $^6T_{1g}$	21.44	2 $^6T_{2g}$	17.18	1 ^6E_g	15.37	2 ^6E_g
					12.51	2 $^6T_{1g}$						
38 Γ_{8g}	2.844	284	29250	0.03	22.89	1 $^6T_{2g}$	17.95	2 $^6T_{2g}$	16.67	2 $^6T_{1g}$	11.70	2 ^6E_g
					11.43	3 $^6T_{1g}$						
19 Γ_{7g}	2.845	282	29513	0.02	35.54	2 $^6T_{1g}$	35.46	1 $^6T_{2g}$				
20 Γ_{6g}	2.844	283	29626	0.01	35.82	2 ^6E_g	22.97	1 ^6E_g	22.86	2 $^6T_{2g}$		
20 Γ_{7g}	2.844	285	29661	0.02	34.02	3 $^6T_{1g}$	28.56	2 $^6T_{1g}$	13.85	2 ^6E_g		
2 Γ_{7u}	2.870	212	29871		89.54	1 $^6T_{1u}$						
2 Γ_{8u}	2.870	212	29883		89.81	1 $^6T_{1u}$						
39 Γ_{8g}	2.844	283	29916	0.02	22.86	2 ^6E_g	19.84	2 $^6T_{2g}$	15.05	1 $^6A_{2g}$	14.14	3 $^6T_{1g}$
21 Γ_{6g}	2.846	283	30059	0.04	47.57	1 $^6T_{2g}$	15.82	3 $^6T_{1g}$	10.45	1 $^6T_{1g}$		
40 Γ_{8g}	2.845	283	30163	0.02	28.65	2 $^6T_{1g}$	26.68	1 $^6T_{2g}$	18.02	2 $^6T_{2g}$		
3 Γ_{8u}	2.870	210	30250		94.06	1 $^6T_{1u}$						
41 Γ_{8g}	2.844	284	30325	0.05	29.81	2 $^6T_{2g}$	22.25	3 $^6T_{1g}$	15.41	1 $^6T_{2g}$	11.90	2 $^6T_{1g}$
21 Γ_{7g}	2.844	281	30363	0.03	33.22	2 $^6T_{1g}$	26.10	3 $^6T_{1g}$	15.74	1 ^6E_g	15.70	2 $^6T_{2g}$
2 Γ_{6u}	2.870	215	30527		85.44	1 $^6T_{1u}$	11.88	3 $^6T_{2u}$				
4 Γ_{8u}	2.870	216	30532		85.58	1 $^6T_{1u}$						
3 Γ_{7u}	2.870	217	30541		85.79	1 $^6T_{1u}$	10.37	2 ^6E_u				
42 Γ_{8g}	2.845	284	30591	0.07	29.45	1 $^6T_{2g}$	29.24	2 $^6T_{1g}$	15.31	1 ^6E_g	10.21	3 $^6T_{1g}$
22 Γ_{7g}	2.844	283	30612	0.02	29.10	2 ^6E_g	22.11	1 ^6E_g	17.14	3 $^6T_{1g}$		
43 Γ_{8g}	2.845	283	30903	0.12	51.00	1 $^6T_{2g}$	16.37	1 ^6E_g	13.43	2 $^6T_{1g}$		

23 Γ_{7g}	2.844	283	31141	0.01	54.68	2 $^6T_{2g}$	22.58	1 $^6A_{1g}$				
44 Γ_{8g}	2.844	283	31270	0.02	21.75	2 $^6T_{2g}$	20.26	1 $^6A_{1g}$	13.20	2 ^6E_g	12.00	3 $^6T_{1g}$
					10.52	1 $^6A_{2g}$						
22 Γ_{6g}	2.843	283	31297	0.01	27.92	3 $^6T_{1g}$	25.03	1 $^6A_{2g}$	21.62	2 $^6T_{2g}$	17.80	1 $^6T_{2g}$
45 Γ_{8g}	2.843	283	31473	0.03	27.03	2 $^6T_{2g}$	25.47	2 ^6E_g	23.73	3 $^6T_{1g}$	12.01	1 $^6T_{2g}$
46 Γ_{8g}	2.844	283	31511	0.01	61.79	3 $^6T_{1g}$	14.93	2 $^6T_{1g}$				
23 Γ_{6g}	2.844	283	32559	0.01	38.53	3 $^6T_{1g}$	38.09	2 $^6T_{2g}$	13.63	1 $^6A_{2g}$		
47 Γ_{8g}	2.843	283	32595		43.07	2 $^6T_{2g}$	26.22	2 ^6E_g	15.95	1 $^6A_{2g}$		
24 Γ_{7g}	2.843	283	32728	0.01	53.20	3 $^6T_{1g}$	34.08	2 ^6E_g				
48 Γ_{8g}	2.843	283	32742	0.01	35.13	3 $^6T_{1g}$	33.48	2 ^6E_g	24.27	2 $^6T_{2g}$		
24 Γ_{6g}	2.843	283	32782		44.48	2 ^6E_g	41.12	2 $^6T_{2g}$				
25 Γ_{7g}	2.843	283	33073		47.77	1 $^6A_{1g}$	41.36	3 $^6T_{1g}$				
49 Γ_{8g}	2.843	283	33090		45.65	1 $^6A_{1g}$	42.60	3 $^6T_{1g}$				
$4f^6(^7F_J)(5de_g^1+6sa_{1g}^1)$ High-, Low- and Mixed-Spin coupling [d]												
50 Γ_{8g}	2.882	275	40030	7.55	62.01	3 $^8T_{2g}$	28.58	4 $^8T_{1g}$				
26 Γ_{7g}	2.883	275	40125	3.43	68.95	3 $^8T_{2g}$	26.64	4 $^8T_{1g}$				
51 Γ_{8g}	2.883	275	40271	1.08	79.75	3 $^8T_{2g}$						
27 Γ_{7g}	2.881	275	40746	6.95	50.82	4 $^8T_{1g}$	34.94	3 $^8T_{2g}$				
52 Γ_{8g}	2.883	261	41065	0.10	30.81	3 $^8T_{2g}$	22.49	4 $^8T_{1g}$	19.35	3 $^6T_{2g}$		
25 Γ_{6g}	2.882	275	41125	2.72	51.91	3 $^8T_{2g}$	25.49	4 $^8T_{1g}$	11.49	5 $^8T_{1g}$		
53 Γ_{8g}	2.861	326	41289	9.26	38.29	3 $^6T_{2g}$	17.31	3 $^8T_{2g}$	12.06	4 $^8T_{1g}$		
54 Γ_{8g}	2.872	395	41685	13.75	54.45	4 $^8T_{1g}$	30.78	3 $^8T_{2g}$				
26 Γ_{6g}	2.875	383	41732	3.67	29.48	3 $^8T_{2g}$	26.06	4 $^8T_{1g}$	20.77	3 ^8E_g	12.59	4 $^8T_{2g}$
					10.06	5 $^8T_{1g}$						
28 Γ_{7g}	2.882	261	41980	0.20	34.64	4 $^8T_{1g}$	26.72	3 $^8T_{2g}$				
55 Γ_{8g}	2.881	303	42104	0.05	32.29	4 $^8T_{2g}$	28.56	3 $^8T_{2g}$	20.58	3 ^8E_g	10.83	4 $^8T_{1g}$
29 Γ_{7g}	2.855	360	42271	5.26	20.50	5 $^6T_{1g}$	19.00	3 ^6E_g	17.45	4 $^6T_{1g}$	13.69	3 $^8T_{2g}$
56 Γ_{8g}	2.881	282	42379	2.99	24.54	5 $^8T_{1g}$	21.00	4 $^8T_{2g}$	19.50	4 $^8T_{1g}$	17.68	3 $^8T_{2g}$
27 Γ_{6g}	2.880	553	42402	0.05	27.84	4 $^8T_{2g}$	18.01	4 $^8T_{1g}$	16.80	5 $^6T_{1g}$	12.14	3 $^6T_{2g}$
57 Γ_{8g}	2.879	368	42486	0.39	16.51	3 $^6T_{2g}$	16.49	3 ^6E_g	15.34	5 $^8T_{1g}$	14.57	3 ^8E_g
					13.48	4 $^6T_{1g}$						
58 Γ_{8g}	2.861	317	42642	4.62	28.98	5 $^8T_{1g}$	24.55	3 ^8E_g				
28 Γ_{6g}	2.857	343	42663	3.21	22.91	5 $^6T_{1g}$	16.04	4 $^8T_{2g}$	14.87	4 $^8T_{1g}$	14.75	3 $^6T_{2g}$
59 Γ_{8g}	2.876	315	43058	1.54	27.22	4 $^8T_{1g}$	16.36	4 $^6T_{2g}$	14.27	3 $^6T_{2g}$	10.17	4 $^6T_{1g}$
60 Γ_{8g}	2.870	311	43061	12.56	27.64	4 $^8T_{1g}$	22.61	3 $^8T_{2g}$	13.92	5 $^8T_{1g}$		
30 Γ_{7g}	2.879	565	43079	0.13	28.33	4 $^8T_{1g}$	13.40	4 $^6T_{2g}$	12.26	4 $^6T_{1g}$	11.95	5 $^6T_{1g}$
31 Γ_{7g}	2.879	459	43148	9.03	37.10	4 $^8T_{1g}$	23.02	3 $^8T_{2g}$	13.10	5 $^8T_{1g}$		
29 Γ_{6g}	2.877	326	43163	1.21	34.54	4 $^8T_{2g}$	28.79	5 $^8T_{1g}$	19.05	3 $^8T_{2g}$	12.01	4 $^8T_{1g}$
61 Γ_{8g}	2.861	334	43326	2.83	29.19	4 $^8T_{2g}$	16.93	3 ^8E_g	16.82	4 $^8T_{1g}$	15.49	5 $^8T_{1g}$
					10.56	3 $^8T_{2g}$						
30 Γ_{6g}	2.881	321	43389	2.37	60.48	3 $^8T_{2g}$	18.67	5 $^8T_{1g}$	13.81	4 $^8T_{1g}$		
32 Γ_{7g}	2.858	356	43412	0.40	24.49	4 $^8T_{2g}$	19.86	3 ^8E_g	11.00	5 $^8T_{1g}$		
31 Γ_{6g}	2.880	300	43685	1.27	41.37	4 $^8T_{2g}$	29.12	3 ^8E_g	12.32	4 $^8T_{1g}$	11.30	5 $^8T_{1g}$
62 Γ_{8g}	2.877	312	43693	0.93	35.79	3 ^8E_g	30.20	4 $^8T_{2g}$	18.40	5 $^8T_{1g}$		
63 Γ_{8g}	2.879	539	43738	9.01	43.21	4 $^8T_{1g}$	18.05	3 $^8T_{2g}$	17.14	3 ^8E_g	11.07	4 $^8T_{2g}$
64 Γ_{8g}	2.881	290	44218	0.71	31.95	3 $^8T_{2g}$	28.03	3 ^8E_g	16.87	4 $^8T_{2g}$	13.78	5 $^8T_{1g}$
33 Γ_{7g}	2.881	291	44343		48.56	5 $^8T_{1g}$	21.29	4 $^8T_{2g}$				
65 Γ_{8g}	2.880	463	44491	0.06	19.87	5 $^6T_{1g}$	17.61	4 $^6T_{1g}$	13.00	5 $^8T_{1g}$	12.98	4 $^8T_{1g}$
32 Γ_{6g}	2.865	208	44557	0.11	39.90	4 $^6T_{2g}$	37.21	3 ^6E_g	12.18	5 $^6T_{1g}$		
34 Γ_{7g}	2.860	328	44616	0.01	26.59	4 $^6T_{1g}$	18.69	5 $^6T_{1g}$	15.03	2 $^6A_{1g}$	13.39	4 $^6T_{2g}$
66 Γ_{8g}	2.869	239	44639	0.12	17.73	4 $^6T_{1g}$	13.17	5 $^8T_{1g}$	12.50	5 $^6T_{1g}$	10.08	3 ^6E_g
67 Γ_{8g}	2.857	300	44765	0.60	27.49	3 $^6T_{2g}$	15.36	5 $^6T_{1g}$	14.73	4 $^6T_{2g}$	13.77	4 $^6T_{1g}$
34 Γ_{6g}	2.860	350	44824	8.24	67.99	4 $^8T_{1g}$	20.60	3 $^8T_{2g}$				
33 Γ_{6g}	2.855	255	44836	0.05	39.96	4 $^6T_{2g}$	28.52	3 $^6T_{2g}$	19.52	4 $^6T_{1g}$		
68 Γ_{8g}	2.859	323	44870	7.38	18.47	4 $^6T_{1g}$	17.48	3 ^6E_g	14.85	5 $^6T_{1g}$	12.77	4 $^8T_{1g}$
					10.92	4 $^6T_{2g}$	10.87	3 $^6T_{2g}$				
69 Γ_{8g}	2.861	343	44916	15.94	41.70	4 $^8T_{1g}$	19.32	5 $^8T_{1g}$	10.71	4 $^8T_{2g}$		
35 Γ_{7g}	2.876	549	45013	0.01	59.37	4 $^8T_{2g}$	28.86	3 ^8E_g				
70 Γ_{8g}	2.868	317	45216	3.08	52.50	4 $^8T_{2g}$	27.29	5 $^8T_{1g}$	11.42	3 ^8E_g		
35 Γ_{6g}	2.876	396	45278	1.96	48.37	4 $^8T_{2g}$	41.22	5 $^8T_{1g}$				
71 Γ_{8g}	2.880	366	45727	4.89	51.00	5 $^8T_{1g}$	31.81	3 ^8E_g	12.26	4 $^8T_{1g}$		

36 Γ_{6g}	2.881	291	45775	0.40
72 Γ_{8g}	2.882	263	46059	0.31
36 Γ_{7g}	2.875	417	46169	0.03
73 Γ_{8g}	2.865	304	46294	1.10
74 Γ_{8g}	2.880	500	46610	0.02
75 Γ_{8g}	2.881	271	46793	
37 Γ_{7g}	2.881	267	46816	
38 Γ_{7g}	2.855	357	47084	0.01
76 Γ_{8g}	2.855	326	47110	0.28
37 Γ_{6g}	2.851	292	47136	0.01
38 Γ_{6g}	2.851	286	47338	0.02
77 Γ_{8g}	2.851	290	47374	0.02
78 Γ_{8g}	2.850	298	47470	0.12
39 Γ_{7g}	2.853	275	47488	0.02
40 Γ_{7g}	2.876	575	47845	0.01
79 Γ_{8g}	2.876	573	47993	0.01
80 Γ_{8g}	2.855	292	48316	0.01
39 Γ_{6g}	2.867	214	49006	
81 Γ_{8g}	2.857	245	49133	
40 Γ_{6g}	2.876	634	49137	
82 Γ_{8g}	2.860	260	49147	
41 Γ_{7g}	2.857	246	49167	
42 Γ_{7g}	2.853	304	49208	
83 Γ_{8g}	2.853	272	49253	
41 Γ_{6g}	2.855	269	49260	
84 Γ_{8g}	2.854	266	49303	
43 Γ_{7g}	2.851	277	49415	
44 Γ_{7g}	2.851	294	49445	
85 Γ_{8g}	2.855	249	49450	
86 Γ_{8g}	2.855	264	49473	
87 Γ_{8g}	2.854	255	49549	
42 Γ_{6g}	2.876	582	49562	
45 Γ_{7g}	2.851	281	49596	
88 Γ_{8g}	2.857	247	49623	
46 Γ_{7g}	2.857	294	49669	
89 Γ_{8g}	2.855	255	49740	
43 Γ_{6g}	2.855	252	49786	
90 Γ_{8g}	2.876	630	49844	
47 Γ_{7g}	2.857	280	49861	
91 Γ_{8g}	2.855	260	49906	
44 Γ_{6g}	2.856	253	49948	
92 Γ_{8g}	2.857	248	49973	
93 Γ_{8g}	2.853	271	50010	
48 Γ_{7g}	2.852	286	50013	
45 Γ_{6g}	2.857	252	50029	
94 Γ_{8g}	2.855	292	50049	
49 Γ_{7g}	2.857	306	50075	
46 Γ_{6g}	2.855	290	50081	
95 Γ_{8g}	2.856	291	50099	
50 Γ_{7g}	2.858	319	50158	
96 Γ_{8g}	2.858	276	50225	
47 Γ_{6g}	2.858	242	50295	
97 Γ_{8g}	2.857	262	50336	
98 Γ_{8g}	2.858	259	50371	
48 Γ_{6g}	2.850	279	50375	
99 Γ_{8g}	2.857	276	50389	
100 Γ_{8g}	2.858	277	50428	
101 Γ_{8g}	2.857	297	50433	
51 Γ_{7g}	2.855	295	50442	
102 Γ_{8g}	2.857	291	50479	
49 Γ_{6g}	2.853	268	50480	

61.41	5 $^8T_{1g}$	27.54	3 ^8E_g					
63.63	5 $^8T_{1g}$	19.37	3 ^8E_g					
76.81	5 $^8T_{1g}$	11.23	3 ^8E_g					
27.37	4 $^6T_{1g}$	19.94	6 $^6T_{1g}$	15.18	5 $^6T_{1g}$	12.62	4 $^6T_{2g}$	
11.28	3 ^6E_g							
78.24	4 $^8T_{2g}$							
68.49	4 $^8T_{2g}$	28.55	5 $^8T_{1g}$					
71.98	4 $^8T_{2g}$	26.00	5 $^8T_{1g}$					
52.75	5 $^6T_{1g}$	33.66	4 $^6T_{1g}$					
39.01	4 $^6T_{1g}$	24.19	5 $^6T_{1g}$	17.33	3 $^6T_{2g}$	14.36	4 $^6T_{2g}$	
44.80	4 $^6T_{1g}$	32.63	3 $^6T_{2g}$	12.36	4 $^6T_{2g}$			
33.37	3 $^6T_{2g}$	27.24	4 $^6T_{2g}$	22.65	3 ^6E_g			
26.73	3 $^6T_{2g}$	21.81	3 ^6E_g	20.34	5 $^6T_{1g}$	16.97	4 $^6T_{2g}$	
45.97	4 $^6T_{2g}$	17.44	5 $^6T_{1g}$	17.16	2 $^6A_{1g}$			
28.63	4 $^6T_{2g}$	23.74	5 $^6T_{1g}$	18.41	2 $^6A_{1g}$	14.24	3 $^6T_{2g}$	
54.52	6 $^6T_{1g}$	14.19	4 $^6T_{1g}$	12.44	2 $^6A_{1g}$			
55.42	6 $^6T_{1g}$	19.22	4 $^6T_{1g}$	10.96	2 $^6A_{1g}$			
65.60	6 $^6T_{1g}$	11.85	3 ^6E_g					
24.77	5 $^6T_{2g}$	23.04	6 $^6T_{1g}$	10.37	4 ^6E_g			
33.77	9 $^6T_{1g}$	28.01	7 $^6T_{2g}$					
32.86	5 $^6T_{2g}$	15.10	4 ^6E_g	12.73	6 $^6T_{1g}$			
31.78	6 $^6T_{1g}$							
39.20	7 $^6T_{2g}$	23.33	9 $^6T_{1g}$					
32.89	6 $^6T_{1g}$	17.44	4 $^6T_{1g}$	10.21	7 $^6T_{1g}$			
36.05	5 $^6T_{2g}$	17.79	4 ^6E_g					
24.48	2 $^6A_{2g}$	17.71	6 $^6T_{2g}$	17.08	5 $^6T_{2g}$	10.53	8 $^6T_{1g}$	
24.56	5 $^6T_{2g}$	23.10	2 $^6A_{2g}$	13.40	7 $^6T_{1g}$	12.58	6 $^6T_{2g}$	
35.75	10 $^6T_{1g}$	28.90	5 ^6E_g					
23.84	7 $^6T_{1g}$	16.84	3 $^6A_{1g}$	12.92	8 $^6T_{1g}$			
20.36	6 $^6T_{2g}$	14.35	7 $^6T_{1g}$	14.02	5 $^6T_{2g}$	12.52	8 $^6T_{1g}$	
20.33	7 $^6T_{1g}$	16.35	3 $^6A_{1g}$	12.65	2 $^6A_{2g}$			
29.88	10 $^6T_{1g}$	20.74	5 ^6E_g	11.95	4 $^6A_{1g}$			
34.97	6 $^6T_{2g}$	13.67	7 $^6T_{1g}$	12.77	7 $^6T_{2g}$			
28.20	6 $^6T_{2g}$	26.70	5 $^6T_{2g}$	12.68	4 ^6E_g			
19.07	6 $^6T_{2g}$	18.58	7 $^6T_{1g}$	11.67	5 $^6T_{2g}$			
51.53	6 $^8T_{1g}$	38.22	5 $^8T_{2g}$					
42.38	9 $^6T_{1g}$	13.09	7 $^6T_{2g}$					
43.37	7 $^6T_{2g}$							
16.36	4 ^6E_g	14.94	5 $^6T_{2g}$					
24.72	7 $^6T_{1g}$	19.55	5 $^6T_{2g}$					
21.79	10 $^6T_{2g}$	13.45	9 $^6T_{2g}$	10.23	6 ^6E_g	10.23	11 $^6T_{1g}$	
18.11	7 $^6T_{1g}$	17.36	11 $^6T_{1g}$	16.04	9 $^6T_{2g}$			
54.82	6 $^8T_{1g}$	36.29	5 $^8T_{2g}$					
12.87	7 $^6T_{1g}$							
18.19	11 $^6T_{1g}$	14.77	4 $^6A_{1g}$	12.64	10 $^6T_{1g}$			
15.17	7 $^6T_{1g}$	11.35	11 $^6T_{1g}$	10.77	9 $^6T_{2g}$	10.71	6 $^6T_{2g}$	
11.95	8 $^6T_{1g}$	10.76	7 $^6T_{1g}$					
19.41	3 $^6A_{1g}$	19.20	6 $^6T_{2g}$	17.88	4 ^6E_g			
23.74	6 $^6T_{2g}$	11.90	5 $^6T_{2g}$					
23.93	8 $^6T_{1g}$							
29.24	8 $^6T_{1g}$	19.30	7 $^6T_{1g}$	13.36	7 ^6E_g			
13.59	10 $^6T_{2g}$	13.30	5 ^6E_g	12.36	10 $^6T_{1g}$			
23.70	10 $^6T_{2g}$	23.20	6 ^6E_g	11.38	12 $^6T_{2g}$	10.09	9 $^6T_{2g}$	
23.19	9 $^6T_{1g}$							
20.09	8 $^6T_{1g}$	13.98	4 ^6E_g					
39.22	7 $^6T_{2g}$	11.88	10 $^6T_{1g}$	10.67	9 $^6T_{1g}$			
63.12	6 $^8T_{1g}$	30.74	5 $^8T_{2g}$					
26.64	3 $^6T_{2g}$							
37.61	3 $^6T_{2g}$	15.56	5 $^6T_{1g}$					
13.38	5 $^6T_{1g}$							
18.60	3 $^6T_{2g}$	11.35	4 ^6E_g	11.07	8 $^6T_{2g}$			

50 Γ_{6g}	2.853	280	50515		20.30	5 $^6T_{2g}$	12.03	8 $^6T_{1g}$				
52 Γ_{7g}	2.853	297	50556		23.75	8 $^6T_{1g}$	18.75	7 $^6T_{1g}$	10.00	3 $^6T_{2g}$		
103 Γ_{8g}	2.857	280	50575		14.85	4 $^6T_{2g}$	10.97	5 $^6T_{1g}$	10.23	6 $^6T_{2g}$		
53 Γ_{7g}	2.853	312	50632		26.88	11 $^6T_{1g}$	22.12	6 ^6E_g	12.45	9 $^6T_{2g}$		
104 Γ_{8g}	2.858	273	50642		10.82	5 $^6T_{2g}$						
54 Γ_{7g}	2.850	346	50659		49.92	5 $^8T_{2g}$	24.93	6 $^8T_{1g}$				
105 Γ_{8g}	2.857	280	50674									
51 Γ_{6g}	2.856	242	50713	0.01	24.79	10 $^6T_{1g}$	12.37	5 ^6E_g	10.65	9 $^6T_{2g}$		
106 Γ_{8g}	2.857	274	50757		12.14	7 $^6T_{1g}$	10.68	11 $^6T_{2g}$				
107 Γ_{8g}	2.855	274	50790		24.43	10 $^6T_{2g}$	10.52	12 $^6T_{1g}$	10.02	9 $^6T_{2g}$		
55 Γ_{7g}	2.853	326	50825		26.50	12 $^6T_{1g}$	11.78	6 ^6E_g				
108 Γ_{8g}	2.855	269	50843		23.96	12 $^6T_{1g}$	11.37	12 $^6T_{2g}$				
52 Γ_{6g}	2.848	235	50872		11.44	8 $^6T_{2g}$						
109 Γ_{8g}	2.855	286	50879	0.03	31.64	11 $^6T_{2g}$	25.21	8 $^6T_{2g}$				
110 Γ_{8g}	2.854	293	50887		11.00	12 $^6T_{2g}$						
56 Γ_{7g}	2.851	323	50913		29.18	4 ^6E_g	22.43	8 $^6T_{1g}$				
53 Γ_{6g}	2.852	231	50965		13.10	8 $^6T_{2g}$	10.46	12 $^6T_{2g}$				
111 Γ_{8g}	2.855	277	50966		13.60	8 $^6T_{1g}$	13.30	4 $^6T_{2g}$	11.31	7 ^6E_g		
57 Γ_{7g}	2.853	325	51014									
112 Γ_{8g}	2.857	261	51039		13.87	8 $^6T_{1g}$						
58 Γ_{7g}	2.850	338	51079		37.14	9 $^6T_{1g}$	13.31	10 $^6T_{1g}$				
54 Γ_{6g}	2.847	247	51092		32.67	8 $^6T_{2g}$	18.07	11 $^6T_{2g}$				
113 Γ_{8g}	2.854	263	51095									
114 Γ_{8g}	2.855	276	51098		21.84	8 $^6T_{2g}$	13.40	11 $^6T_{2g}$				
115 Γ_{8g}	2.855	265	51168		11.33	11 $^6T_{2g}$						
55 Γ_{6g}	2.848	261	51170		11.16	2 $^6A_{2g}$	10.89	11 $^6T_{2g}$				
56 Γ_{6g}	2.849	274	51208		12.00	13 $^6T_{1g}$	10.63	13 $^6T_{2g}$	10.61	6 ^6E_g	10.51	8 ^6E_g
116 Γ_{8g}	2.856	273	51222		11.01	13 $^6T_{2g}$	10.79	10 $^6T_{1g}$				
117 Γ_{8g}	2.856	278	51243		48.63	6 $^8T_{1g}$	30.00	5 $^8T_{2g}$				
59 Γ_{7g}	2.850	314	51273		42.22	5 $^8T_{2g}$	32.14	6 $^8T_{1g}$				
60 Γ_{7g}	2.849	322	51280		20.80	14 $^6T_{2g}$	14.82	14 $^6T_{1g}$				
57 Γ_{6g}	2.849	265	51283		47.28	5 $^8T_{2g}$	35.88	6 $^8T_{1g}$				
58 Γ_{6g}	2.852	279	51308		15.20	11 $^6T_{2g}$	14.23	7 ^6E_g				
61 Γ_{7g}	2.850	324	51316		14.04	11 $^6T_{1g}$	13.67	6 $^6T_{1g}$	12.35	12 $^6T_{2g}$		
118 Γ_{8g}	2.857	270	51323		13.80	6 $^6T_{1g}$	13.62	2 $^6A_{1g}$	12.11	4 $^6T_{1g}$		
119 Γ_{8g}	2.857	276	51340	0.04	11.76	9 $^6T_{2g}$						
59 Γ_{6g}	2.854	277	51416		20.11	9 $^6T_{2g}$	14.75	5 ^6E_g	13.19	10 $^6T_{1g}$		
120 Γ_{8g}	2.857	260	51417									
62 Γ_{7g}	2.849	321	51418		14.27	13 $^6T_{1g}$	12.53	12 $^6T_{1g}$				
63 Γ_{7g}	2.849	318	51467		15.15	6 $^6T_{1g}$	10.09	12 $^6T_{2g}$				
121 Γ_{8g}	2.855	270	51474									
60 Γ_{6g}	2.856	301	51482		24.64	10 $^6T_{2g}$						
122 Γ_{8g}	2.853	268	51518		13.59	5 $^6T_{2g}$						
123 Γ_{8g}	2.853	276	51540									
64 Γ_{7g}	2.850	313	51550	0.01	10.87	6 $^6T_{1g}$	10.06	14 $^6T_{2g}$				
124 Γ_{8g}	2.853	267	51608		13.71	13 $^6T_{2g}$	13.63	13 $^6T_{1g}$				
65 Γ_{7g}	2.850	345	51612		21.95	12 $^6T_{1g}$	12.07	8 ^6E_g	11.54	10 $^6T_{2g}$		
125 Γ_{8g}	2.857	275	51640		23.13	14 $^6T_{2g}$						
61 Γ_{6g}	2.857	280	51646									
126 Γ_{8g}	2.857	261	51738		12.99	7 $^6T_{2g}$	11.20	10 $^6T_{1g}$				
127 Γ_{8g}	2.857	272	51774									
62 Γ_{6g}	2.855	265	51808		20.49	16 $^6T_{2g}$	12.83	15 $^6T_{2g}$	11.58	9 ^6E_g	10.43	15 $^6T_{1g}$
66 Γ_{7g}	2.850	295	51821		16.59	16 $^6T_{1g}$	13.07	10 ^6E_g				
128 Γ_{8g}	2.859	264	51827		12.22	7 ^6E_g	10.91	8 $^6T_{2g}$	10.05	11 $^6T_{2g}$		
67 Γ_{7g}	2.849	315	51868		13.08	16 $^6T_{1g}$	11.02	16 $^6T_{2g}$				
63 Γ_{6g}	2.853	302	51868		16.63	13 $^6T_{1g}$	10.59	13 $^6T_{2g}$				
68 Γ_{7g}	2.849	329	51875		24.02	15 $^6T_{1g}$						
129 Γ_{8g}	2.857	254	51935									
130 Γ_{8g}	2.857	254	51971		12.75	12 $^6T_{2g}$						
64 Γ_{6g}	2.854	278	52000									
131 Γ_{8g}	2.857	251	52006									
69 Γ_{7g}	2.849	303	52019		18.07	9 $^6T_{1g}$	15.81	10 $^6T_{1g}$				

132 Γ_{8g}	2.853	266	52048		13.28	7 ^6E_g	11.68	16 $^6T_{2g}$				
70 Γ_{7g}	2.848	313	52049		18.78	13 $^6T_{1g}$	14.03	9 $^6T_{1g}$	11.57	11 $^6T_{1g}$		
133 Γ_{8g}	2.853	266	52066		10.24	7 $^6T_{2g}$						
65 Γ_{6g}	2.853	265	52070		11.69	14 $^6T_{2g}$						
134 Γ_{8g}	2.853	275	52083		56.41	6 $^8T_{1g}$	27.04	5 $^8T_{2g}$				
66 Γ_{6g}	2.851	282	52089		17.40	16 $^6T_{2g}$	13.79	15 $^6T_{2g}$	10.59	4 $^6A_{2g}$	10.06	9 ^6E_g
135 Γ_{8g}	2.853	282	52099									
71 Γ_{7g}	2.847	304	52122		10.69	9 $^6T_{1g}$						
67 Γ_{6g}	2.853	292	52122		17.43	12 $^6T_{2g}$	12.26	11 $^6T_{2g}$				
136 Γ_{8g}	2.853	274	52152		23.03	11 $^6T_{2g}$	11.10	15 $^6T_{1g}$				
137 Γ_{8g}	2.853	280	52163									
138 Γ_{8g}	2.853	284	52182		10.30	8 $^6T_{2g}$						
72 Γ_{7g}	2.849	313	52184	0.01	38.02	11 $^6T_{2g}$						
139 Γ_{8g}	2.853	271	52249	0.03	11.17	10 $^6T_{1g}$						
68 Γ_{6g}	2.855	271	52250	0.01	21.42	11 $^6T_{2g}$						
140 Γ_{8g}	2.852	270	52268	0.01	10.67	12 $^6T_{1g}$						
69 Γ_{6g}	2.855	268	52274		37.47	6 $^8T_{1g}$	16.21	5 $^8T_{2g}$				
141 Γ_{8g}	2.853	277	52285	0.01	59.39	5 $^8T_{2g}$	18.76	6 $^8T_{1g}$				
142 Γ_{8g}	2.852	287	52293		18.92	7 ^6E_g	12.86	11 $^6T_{2g}$				
73 Γ_{7g}	2.848	282	52320		23.53	13 $^6T_{1g}$	10.14	13 $^6T_{2g}$				
143 Γ_{8g}	2.854	286	52341		16.46	7 ^6E_g						
74 Γ_{7g}	2.851	297	52342		10.45	10 $^6T_{2g}$						
70 Γ_{6g}	2.851	291	52355		24.39	7 ^6E_g	14.65	11 $^6T_{2g}$				
144 Γ_{8g}	2.853	284	52385		14.87	12 $^6T_{1g}$						
71 Γ_{6g}	2.854	289	52435		14.05	14 $^6T_{2g}$						
145 Γ_{8g}	2.855	288	52441		18.69	14 $^6T_{1g}$						
146 Γ_{8g}	2.855	296	52459		21.42	14 $^6T_{1g}$						
147 Γ_{8g}	2.857	302	52490		12.09	11 $^6T_{2g}$						
72 Γ_{6g}	2.857	294	52530		20.29	15 $^6T_{2g}$	10.07	16 $^6T_{2g}$				
148 Γ_{8g}	2.857	280	52587		13.83	15 $^6T_{2g}$						
75 Γ_{7g}	2.876	730	52600		24.02	16 $^6T_{2g}$	17.16	9 ^6E_g	10.74	15 $^6T_{1g}$		
149 Γ_{8g}	2.857	268	52684									
73 Γ_{6g}	2.858	257	52740		14.55	13 $^6T_{2g}$	10.34	14 $^6T_{2g}$	10.19	9 $^6T_{2g}$		
150 Γ_{8g}	2.857	269	52741		11.90	11 $^6T_{1g}$	10.47	5 ^6E_g				
151 Γ_{8g}	2.858	267	52785		12.30	13 $^6T_{1g}$	10.48	15 $^6T_{1g}$				
76 Γ_{7g}	2.855	239	52813		23.78	13 $^6T_{1g}$	11.00	9 $^6T_{1g}$	10.53	12 $^6T_{1g}$		
152 Γ_{8g}	2.854	290	52819									
74 Γ_{6g}	2.853	270	52826		22.90	14 $^6T_{2g}$	14.97	13 $^6T_{2g}$	11.89	12 $^6T_{2g}$		
77 Γ_{7g}	2.849	280	52830		28.57	14 $^6T_{1g}$						
75 Γ_{6g}	2.854	298	52844		14.46	13 $^6T_{2g}$	11.94	12 $^6T_{2g}$				
153 Γ_{8g}	2.855	293	52859		10.60	13 $^6T_{2g}$						
154 Γ_{8g}	2.855	278	52925		11.63	10 $^6T_{1g}$						
76 Γ_{6g}	2.856	286	52970		39.62	9 $^6T_{1g}$	26.35	7 $^6T_{2g}$				
155 Γ_{8g}	2.856	269	53010		12.77	9 $^6T_{1g}$	11.27	10 $^6T_{1g}$				
78 Γ_{7g}	2.855	248	53011		17.54	10 $^6T_{1g}$	12.37	5 ^6E_g				
156 Γ_{8g}	2.854	278	53024	0.04	28.46	7 $^6T_{2g}$	19.07	9 $^6T_{1g}$				
77 Γ_{6g}	2.857	281	53097		12.93	12 $^6T_{1g}$	12.21	13 $^6T_{2g}$				
157 Γ_{8g}	2.854	273	53098		13.32	11 $^6T_{1g}$	10.16	6 ^6E_g				
79 Γ_{7g}	2.851	265	53101		17.48	10 $^6T_{2g}$	12.60	12 $^6T_{1g}$				
158 Γ_{8g}	2.855	274	53157									
159 Γ_{8g}	2.854	276	53177		12.59	9 $^6T_{2g}$	12.00	11 $^6T_{1g}$	11.60	14 $^6T_{2g}$		
80 Γ_{7g}	2.851	270	53190		24.30	15 $^6T_{1g}$	13.29	16 $^6T_{2g}$				
78 Γ_{6g}	2.857	270	53214	0.01	16.94	16 $^6T_{2g}$	10.06	4 $^6A_{2g}$				
160 Γ_{8g}	2.855	270	53226	0.01	13.21	15 $^6T_{1g}$	12.44	17 $^6T_{2g}$	10.82	9 ^6E_g		
79 Γ_{6g}	2.857	293	53231		29.10	6 $^8T_{1g}$	22.19	5 $^8T_{2g}$	14.84	12 $^6T_{1g}$		
80 Γ_{6g}	2.857	314	53240		22.44	6 $^8T_{1g}$	16.23	5 $^8T_{2g}$	14.24	16 $^6T_{1g}$	12.30	12 $^6T_{1g}$
161 Γ_{8g}	2.855	276	53270		52.99	6 $^8T_{1g}$	41.65	5 $^8T_{2g}$				
162 Γ_{8g}	2.857	288	53296		18.49	16 $^6T_{2g}$	17.76	15 $^6T_{2g}$				
81 Γ_{7g}	2.853	258	53312		17.88	5 $^6A_{1g}$						
82 Γ_{7g}	2.851	287	53322		59.84	6 $^8T_{1g}$						
83 Γ_{7g}	2.855	311	53383		29.42	14 $^6T_{1g}$						
163 Γ_{8g}	2.858	267	53407		20.34	17 $^6T_{2g}$						

164 Γ_{8g}	2.857	274	53449	
165 Γ_{8g}	2.853	297	53525	
81 Γ_{6g}	2.851	292	53566	
84 Γ_{7g}	2.857	279	53569	
166 Γ_{8g}	2.854	287	53581	
167 Γ_{8g}	2.853	286	53615	
82 Γ_{6g}	2.855	313	53647	
85 Γ_{7g}	2.860	303	53652	
168 Γ_{8g}	2.853	280	53715	
169 Γ_{8g}	2.853	294	53733	
170 Γ_{8g}	2.855	287	53800	
86 Γ_{7g}	2.860	276	53848	
83 Γ_{6g}	2.857	266	53888	
171 Γ_{8g}	2.859	295	53889	
87 Γ_{7g}	2.876	734	53906	
84 Γ_{6g}	2.861	305	53909	0.02
86 Γ_{6g}	2.857	364	53928	
85 Γ_{6g}	2.856	338	53933	
172 Γ_{8g}	2.858	281	53959	
88 Γ_{7g}	2.876	622	54064	0.02
87 Γ_{6g}	2.857	347	54090	
173 Γ_{8g}	2.861	268	54117	0.04
174 Γ_{8g}	2.876	696	54257	
175 Γ_{8g}	2.876	679	54312	
89 Γ_{7g}	2.876	898	54327	
88 Γ_{6g}	2.856	317	54384	
176 Γ_{8g}	2.876	706	54397	
90 Γ_{7g}	2.876	744	54412	
177 Γ_{8g}	2.876	784	54465	0.01
89 Γ_{6g}	2.853	318	54531	
178 Γ_{8g}	2.858	240	54581	
91 Γ_{7g}	2.876	770	54629	
179 Γ_{8g}	2.876	598	54648	
92 Γ_{7g}	2.867	378	54664	0.01
90 Γ_{6g}	2.852	310	54674	
91 Γ_{6g}	2.857	349	54677	
180 Γ_{8g}	2.861	255	54679	
181 Γ_{8g}	2.860	257	54700	
92 Γ_{6g}	2.856	432	54704	
182 Γ_{8g}	2.864	295	54756	
93 Γ_{7g}	2.857	414	54814	0.01
183 Γ_{8g}	2.864	298	54822	
184 Γ_{8g}	2.862	273	54994	
94 Γ_{7g}	2.851	426	55071	
185 Γ_{8g}	2.876	623	55096	
93 Γ_{6g}	2.850	407	55110	
186 Γ_{8g}	2.858	310	55248	
187 Γ_{8g}	2.876	608	55540	0.04
94 Γ_{6g}	2.854	324	55608	0.01
188 Γ_{8g}	2.850	276	55646	
189 Γ_{8g}	2.851	293	55652	
190 Γ_{8g}	2.853	292	55720	0.01
95 Γ_{7g}	2.851	278	55735	
96 Γ_{7g}	2.849	275	55798	0.01
191 Γ_{8g}	2.851	271	55844	
192 Γ_{8g}	2.850	279	55905	
97 Γ_{7g}	2.849	270	55905	
193 Γ_{8g}	2.850	282	55963	

69.05	5 $^8T_{2g}$	15.13	6 $^8T_{1g}$					
12.60	9 $^6T_{2g}$	11.81	11 $^6T_{1g}$					
15.07	9 $^6T_{2g}$	14.88	3 $^6A_{2g}$	13.40	13 $^6T_{2g}$	11.21	10 $^6T_{2g}$	
10.31	12 $^6T_{2g}$							
27.98	16 $^6T_{1g}$	10.81	13 $^6T_{2g}$					
19.82	12 $^6T_{2g}$	14.96	10 $^6T_{2g}$	10.92	13 $^6T_{2g}$	10.39	6 ^6E_g	
15.15	16 $^6T_{1g}$	10.36	13 $^6T_{1g}$					
17.70	12 $^6T_{2g}$	17.56	10 $^6T_{2g}$	16.92	13 $^6T_{2g}$	11.15	6 ^6E_g	
26.75	13 $^6T_{1g}$	19.13	13 $^6T_{2g}$					
22.45	13 $^6T_{1g}$	18.30	12 $^6T_{2g}$	15.84	13 $^6T_{2g}$			
36.62	13 $^6T_{1g}$	10.03	14 $^6T_{2g}$					
31.33	13 $^6T_{1g}$							
20.62	13 $^6T_{2g}$	14.86	15 $^6T_{2g}$	12.21	13 $^6T_{1g}$	12.13	16 $^6T_{1g}$	
23.58	16 $^6T_{2g}$	13.87	4 $^6A_{2g}$	10.58	10 ^6E_g			
13.33	15 $^6T_{2g}$	12.14	13 $^6T_{2g}$					
34.36	12 $^6T_{1g}$	15.47	15 $^6T_{1g}$	10.87	8 ^6E_g			
18.09	16 $^6T_{1g}$	12.49	16 $^6T_{2g}$					
13.16	13 $^6T_{2g}$	11.97	16 $^6T_{1g}$					
20.11	13 $^6T_{2g}$	11.44	8 ^6E_g					
13.09	12 $^6T_{1g}$	10.47	16 $^6T_{2g}$					
16.58	15 $^6T_{2g}$	16.17	9 ^6E_g	12.01	12 $^6T_{1g}$	11.52	15 $^6T_{1g}$	
10.82	10 ^6E_g							
25.14	16 $^6T_{2g}$	17.45	10 ^6E_g	11.87	15 $^6T_{2g}$			
23.30	15 $^6T_{2g}$	15.77	16 $^6T_{2g}$					
16.64	18 $^6T_{2g}$	13.36	11 ^6E_g	10.12	19 $^6T_{2g}$			
15.05	11 ^6E_g	10.66	19 $^6T_{2g}$					
24.43	15 $^6T_{1g}$	18.36	5 $^6A_{1g}$	11.89	14 $^6T_{2g}$	11.04	15 $^6T_{2g}$	
10.97	14 $^6T_{1g}$							
32.19	14 $^6T_{1g}$	27.90	14 $^6T_{2g}$					
19.25	15 $^6T_{1g}$	15.31	5 $^6A_{1g}$	13.07	14 $^6T_{2g}$			
50.34	6 $^8T_{1g}$	48.04	5 $^8T_{2g}$					
21.78	14 $^6T_{2g}$	16.55	18 $^6T_{2g}$					
20.33	18 $^6T_{1g}$	20.31	19 $^6T_{2g}$	15.47	17 $^6T_{2g}$	10.78	5 $^6A_{2g}$	
56.16	6 $^8T_{1g}$	41.05	5 $^8T_{2g}$					
31.78	5 $^8T_{2g}$	17.04	6 $^8T_{1g}$	10.44	10 ^6E_g			
34.96	17 $^6T_{2g}$	12.30	18 $^6T_{2g}$					
24.33	10 ^6E_g	22.61	16 $^6T_{1g}$	13.75	5 $^8T_{2g}$			
27.67	17 $^6T_{2g}$	12.62	15 $^6T_{2g}$					
31.48	15 $^6T_{2g}$	15.68	4 $^6A_{2g}$	14.84	9 ^6E_g			
28.63	15 $^6T_{2g}$	21.67	9 ^6E_g	19.12	4 $^6A_{2g}$	14.00	16 $^6T_{2g}$	
20.66	16 $^6T_{1g}$	15.09	9 ^6E_g	11.39	15 $^6T_{2g}$			
18.44	9 ^6E_g	16.16	15 $^6T_{2g}$	13.05	15 $^6T_{1g}$	11.77	17 $^6T_{2g}$	
11.72	16 $^6T_{2g}$							
49.08	5 $^8T_{2g}$	18.68	6 $^8T_{1g}$					
50.61	5 $^8T_{2g}$	14.25	6 $^8T_{1g}$					
25.93	16 $^6T_{1g}$	22.39	10 ^6E_g	14.37	16 $^6T_{2g}$			
34.08	16 $^6T_{2g}$	14.34	10 ^6E_g					
21.60	11 ^6E_g	15.39	17 $^6T_{1g}$	13.49	19 $^6T_{1g}$	12.42	18 $^6T_{1g}$	
21.69	18 $^6T_{2g}$	17.53	19 $^6T_{2g}$	15.68	18 $^6T_{1g}$	11.30	5 $^6A_{2g}$	
28.19	18 $^6T_{2g}$	17.18	11 ^6E_g					
17.58	18 $^6T_{2g}$	16.99	17 $^6T_{1g}$	14.73	18 $^6T_{1g}$	10.85	11 ^6E_g	
22.01	17 $^6T_{1g}$	11.12	19 $^6T_{2g}$					
25.79	11 ^6E_g	21.31	18 $^6T_{2g}$					
28.71	11 ^6E_g	20.51	17 $^6T_{1g}$					
26.77	17 $^6T_{1g}$	25.77	11 ^6E_g	12.76	6 $^6A_{1g}$			
19.41	11 ^6E_g	15.31	17 $^6T_{2g}$					
42.31	17 $^6T_{1g}$	17.00	17 $^6T_{2g}$					
31.53	18 $^6T_{1g}$	18.37	19 $^6T_{2g}$	13.29	17 $^6T_{1g}$			
13.92	18 $^6T_{2g}$	13.60	18 $^6T_{1g}$	11.29	19 $^6T_{1g}$			
28.37	17 $^6T_{2g}$	11.72	18 $^6T_{2g}$					
32.05	17 $^6T_{1g}$	25.04	17 $^6T_{2g}$					
44.08	17 $^6T_{1g}$							

95 Γ_{6g}	2.855	268	55981	52.05	17 $^6T_{2g}$	14.89	13 ^6E_g				
194 Γ_{8g}	2.849	279	56019	15.30	11 ^6E_g	14.25	12 ^6E_g	14.17	17 $^6T_{1g}$	10.64	17 $^6T_{2g}$
98 Γ_{7g}	2.849	275	56050	22.81	19 $^6T_{1g}$	13.97	21 $^6T_{2g}$	11.05	6 $^6A_{1g}$		
195 Γ_{8g}	2.848	280	56063	16.57	20 $^6T_{2g}$	10.15	19 $^6T_{2g}$	10.10	17 $^6T_{1g}$		
99 Γ_{7g}	2.850	274	56162	50.17	6 $^6A_{1g}$	11.11	19 $^6T_{1g}$				
96 Γ_{6g}	2.847	284	56273	20.47	5 $^6A_{2g}$	15.52	18 $^6T_{2g}$	12.08	18 $^6T_{1g}$	10.61	20 $^6T_{2g}$
196 Γ_{8g}	2.849	272	56301	38.85	17 $^6T_{1g}$						
197 Γ_{8g}	2.850	280	56354	42.46	6 $^6A_{1g}$	16.73	11 ^6E_g				
100 Γ_{7g}	2.849	274	56362	19.59	18 $^6T_{1g}$	17.01	19 $^6T_{1g}$	15.29	17 $^6T_{1g}$	10.06	6 $^6A_{1g}$
198 Γ_{8g}	2.850	272	56420	14.42	20 $^6T_{2g}$	12.14	19 $^6T_{2g}$	11.08	20 $^6T_{1g}$		
97 Γ_{6g}	2.851	258	56428	35.82	17 $^6T_{1g}$	16.21	20 $^6T_{2g}$	10.83	18 $^6T_{2g}$		
98 Γ_{6g}	2.849	295	56469	48.65	18 $^6T_{2g}$	16.25	12 ^6E_g				
199 Γ_{8g}	2.849	275	56486	18.88	18 $^6T_{1g}$	11.63	20 $^6T_{2g}$	10.46	12 ^6E_g		
101 Γ_{7g}	2.853	262	56546	24.69	13 ^6E_g	21.80	18 $^6T_{1g}$	14.09	20 $^6T_{1g}$		
99 Γ_{6g}	2.848	277	56616	33.27	19 $^6T_{2g}$	17.09	21 $^6T_{2g}$				
200 Γ_{8g}	2.853	263	56651	26.90	18 $^6T_{2g}$	10.40	12 ^6E_g	10.16	19 $^6T_{2g}$		
102 Γ_{7g}	2.849	259	56683	18.28	21 $^6T_{2g}$	17.92	20 $^6T_{2g}$	12.76	12 ^6E_g		
201 Γ_{8g}	2.848	278	56717	25.05	18 $^6T_{2g}$	17.49	19 $^6T_{1g}$	11.28	19 $^6T_{2g}$	10.10	12 ^6E_g
100 Γ_{6g}	2.849	282	56757	23.00	19 $^6T_{2g}$	12.13	20 $^6T_{2g}$	11.82	5 $^6A_{2g}$		
103 Γ_{7g}	2.849	259	56809	29.41	18 $^6T_{2g}$	12.65	21 $^6T_{2g}$	10.79	19 $^6T_{1g}$		
202 Γ_{8g}	2.849	279	56838	20.26	19 $^6T_{2g}$	16.36	13 ^6E_g	11.70	19 $^6T_{1g}$		
101 Γ_{6g}	2.848	276	56946	25.92	12 ^6E_g	21.55	21 $^6T_{2g}$	21.47	18 $^6T_{2g}$		
203 Γ_{8g}	2.850	275	56957	26.63	13 ^6E_g	18.92	20 $^6T_{2g}$				
204 Γ_{8g}	2.848	274	57025	21.38	21 $^6T_{2g}$	18.29	19 $^6T_{2g}$	13.86	12 ^6E_g	12.45	19 $^6T_{1g}$
205 Γ_{8g}	2.849	290	57062	49.04	20 $^6T_{2g}$						
102 Γ_{6g}	2.848	280	57165	32.81	19 $^6T_{1g}$	14.66	18 $^6T_{1g}$	10.62	20 $^6T_{1g}$	10.15	20 $^6T_{2g}$
104 Γ_{7g}	2.848	276	57248	32.87	19 $^6T_{1g}$	16.00	18 $^6T_{1g}$				
206 Γ_{8g}	2.848	281	57283	30.58	13 ^6E_g	13.34	18 $^6T_{1g}$				
103 Γ_{6g}	2.848	288	57368	27.36	21 $^6T_{2g}$	24.61	19 $^6T_{1g}$	12.41	20 $^6T_{1g}$		
207 Γ_{8g}	2.849	277	57425	33.18	19 $^6T_{1g}$	19.72	18 $^6T_{1g}$	17.22	21 $^6T_{2g}$		
104 Γ_{6g}	2.849	277	57430	36.39	20 $^6T_{1g}$	14.59	21 $^6T_{2g}$	10.68	13 ^6E_g		
208 Γ_{8g}	2.850	281	57452	24.90	21 $^6T_{2g}$	22.46	20 $^6T_{1g}$				
105 Γ_{7g}	2.848	280	57485	31.85	19 $^6T_{2g}$	27.86	18 $^6T_{1g}$				
209 Γ_{8g}	2.848	283	57518	35.48	20 $^6T_{1g}$	13.91	18 $^6T_{1g}$	10.38	19 $^6T_{2g}$	10.25	20 $^6T_{2g}$
210 Γ_{8g}	2.848	286	57541	16.05	19 $^6T_{2g}$	14.01	20 $^6T_{1g}$	13.27	5 $^6A_{2g}$	10.85	20 $^6T_{2g}$
105 Γ_{6g}	2.850	286	57541	17.43	19 $^6T_{2g}$	14.65	21 $^6T_{2g}$	12.32	5 $^6A_{2g}$	10.25	13 ^6E_g
211 Γ_{8g}	2.849	280	57619	22.04	19 $^6T_{1g}$	18.92	18 $^6T_{1g}$	14.91	20 $^6T_{1g}$	13.81	12 ^6E_g
				10.93	19 $^6T_{2g}$						
106 Γ_{6g}	2.849	281	57624	34.44	19 $^6T_{1g}$	24.06	12 ^6E_g	10.50	18 $^6T_{1g}$		
106 Γ_{7g}	2.847	299	57649	28.15	20 $^6T_{2g}$	26.44	21 $^6T_{2g}$	10.13	18 $^6T_{1g}$		
107 Γ_{6g}	2.846	290	57695	28.32	21 $^6T_{2g}$	21.58	20 $^6T_{1g}$	15.85	18 $^6T_{1g}$	15.73	19 $^6T_{2g}$
212 Γ_{8g}	2.847	281	57754	28.25	21 $^6T_{2g}$	15.27	19 $^6T_{1g}$	10.31	20 $^6T_{1g}$		
213 Γ_{8g}	2.847	284	57778	60.07	20 $^6T_{1g}$						
214 Γ_{8g}	2.848	283	57963	39.97	20 $^6T_{1g}$	15.77	21 $^6T_{2g}$	11.97	20 $^6T_{2g}$		
107 Γ_{7g}	2.848	271	58071	54.95	20 $^6T_{1g}$	14.15	20 $^6T_{2g}$				
215 Γ_{8g}	2.846	286	58130	23.53	21 $^6T_{2g}$	18.66	20 $^6T_{1g}$	13.67	20 $^6T_{2g}$	13.32	13 ^6E_g
108 Γ_{6g}	2.846	291	58151	34.97	20 $^6T_{2g}$	21.06	21 $^6T_{2g}$	17.68	13 ^6E_g		
216 Γ_{8g}	2.847	284	58208	25.93	21 $^6T_{2g}$	25.39	20 $^6T_{1g}$	16.14	20 $^6T_{2g}$		
217 Γ_{8g}	2.846	288	58250	35.16	20 $^6T_{1g}$	25.57	21 $^6T_{2g}$	13.62	20 $^6T_{2g}$		
108 Γ_{7g}	2.846	280	58259	41.82	20 $^6T_{1g}$	28.94	13 ^6E_g				
109 Γ_{6g}	2.848	280	58285	53.00	20 $^6T_{1g}$	22.19	20 $^6T_{2g}$				

$4f^7$ excited states

$4f^7(^6P_{3/2,5/2,7/2})$ [c]											
2 Γ_{7u}	2.870	212	29871	89.54	1 $^6T_{1u}$						
2 Γ_{8u}	2.870	212	29883	89.81	1 $^6T_{1u}$						
3 Γ_{8u}	2.870	210	30250	94.06	1 $^6T_{1u}$						
2 Γ_{6u}	2.870	215	30527	85.44	1 $^6T_{1u}$	11.88	3 $^6T_{2u}$				
4 Γ_{8u}	2.870	216	30532	85.58	1 $^6T_{1u}$						
3 Γ_{7u}	2.870	217	30541	85.79	1 $^6T_{1u}$	10.37	2 ^6E_u				

$4f^7(^6I_{7/2,9/2,11/2,13/2,15/2,17/2})$ [c]											
3 Γ_{6u}	2.869	280	34401	73.40	1 $^6T_{2u}$	21.14	1 ^6E_u				
5 Γ_{8u}	2.869	279	34406	72.80	1 $^6T_{2u}$	14.95	1 ^6E_u				
4 Γ_{7u}	2.869	280	34444	47.81	2 $^6T_{1u}$	26.30	2 $^6T_{2u}$	23.12	1 $^6A_{1u}$		
6 Γ_{8u}	2.869	279	34445	75.02	1 $^6T_{2u}$	12.65	1 ^6E_u				
4 Γ_{6u}	2.869	279	34453	82.61	1 $^6T_{2u}$						
7 Γ_{8u}	2.869	278	34477	42.41	1 $^6T_{2u}$	28.55	2 $^6T_{1u}$	13.88	1 $^6A_{1u}$	13.43	2 $^6T_{2u}$
8 Γ_{8u}	2.869	282	34481	60.25	1 $^6T_{2u}$	15.36	2 $^6T_{1u}$	11.71	1 $^6A_{1u}$	11.20	2 $^6T_{2u}$
5 Γ_{7u}	2.869	280	34483	90.68	1 $^6T_{2u}$						
9 Γ_{8u}	2.869	281	34530	45.43	2 $^6T_{1u}$	35.10	2 $^6T_{2u}$	14.67	1 $^6A_{1u}$		
5 Γ_{6u}	2.869	281	34546	48.10	2 $^6T_{2u}$	43.09	2 $^6T_{1u}$				
6 Γ_{7u}	2.869	280	34584	33.51	1 $^6A_{1u}$	31.30	2 $^6T_{1u}$	28.46	2 $^6T_{2u}$		
10 Γ_{8u}	2.869	280	34596	71.22	2 $^6T_{1u}$	19.31	2 $^6T_{2u}$				
6 Γ_{6u}	2.869	281	34625	85.97	2 $^6T_{2u}$						
7 Γ_{7u}	2.869	280	34644	36.08	2 $^6T_{1u}$	31.69	1 ^6E_u	18.85	1 $^6A_{1u}$	13.29	2 $^6T_{2u}$
11 Γ_{8u}	2.869	281	34676	43.04	2 $^6T_{2u}$	18.29	1 $^6A_{1u}$	17.23	2 $^6T_{1u}$	14.38	1 ^6E_u
12 Γ_{8u}	2.869	280	34688	33.31	2 $^6T_{1u}$	27.18	2 $^6T_{2u}$	19.05	1 ^6E_u	12.72	1 $^6A_{1u}$
13 Γ_{8u}	2.869	279	34704	60.24	1 ^6E_u	20.95	2 $^6T_{2u}$				
8 Γ_{7u}	2.869	279	34708	62.08	1 ^6E_u	32.42	2 $^6T_{1u}$				
14 Γ_{8u}	2.869	280	34730	53.21	1 ^6E_u	14.31	2 $^6T_{1u}$	13.78	2 $^6T_{2u}$		
7 Γ_{6u}	2.869	280	34746	57.70	1 ^6E_u	14.35	1 $^6T_{2u}$	11.45	1 $^6A_{2u}$		
9 Γ_{7u}	2.869	280	34787	52.13	2 $^6T_{1u}$	24.14	2 $^6T_{2u}$	22.36	1 $^6A_{1u}$		
8 Γ_{6u}	2.869	281	34788	31.73	2 $^6T_{2u}$	24.64	2 $^6T_{1u}$	19.32	1 ^6E_u	15.24	1 $^6A_{2u}$
15 Γ_{8u}	2.869	281	34793	33.77	2 $^6T_{1u}$	30.15	2 $^6T_{2u}$	14.69	1 ^6E_u	11.67	1 $^6A_{1u}$
16 Γ_{8u}	2.869	282	34814	72.30	2 $^6T_{2u}$	18.02	2 $^6T_{1u}$				
17 Γ_{8u}	2.870	280	34834	73.28	1 $^6A_{2u}$						
9 Γ_{6u}	2.870	280	34838	64.17	1 $^6A_{2u}$	18.80	2 $^6T_{2u}$				
$4f^7(^6D_{1/2,3/2,5/2,7/2})$ [c]											
10 Γ_{6u}	2.869	279	37105	95.23	3 $^6T_{2u}$						
18 Γ_{8u}	2.869	279	37295	72.05	3 $^6T_{2u}$	27.60	2 ^6E_u				
19 Γ_{8u}	2.869	279	37322	78.35	3 $^6T_{2u}$	21.58	2 ^6E_u				
11 Γ_{6u}	2.869	279	37361	89.25	2 ^6E_u	10.72	3 $^6T_{2u}$				
20 Γ_{8u}	2.869	279	37622	47.26	2 ^6E_u	46.96	3 $^6T_{2u}$				
10 Γ_{7u}	2.869	279	37958	87.19	3 $^6T_{2u}$	10.60	1 $^6T_{1u}$				
21 Γ_{8u}	2.869	279	38070	52.12	3 $^6T_{2u}$	37.46	2 ^6E_u	10.38	1 $^6T_{1u}$		
12 Γ_{6u}	2.869	279	38156	82.13	3 $^6T_{2u}$	12.21	1 $^6T_{1u}$				
22 Γ_{8u}	2.869	279	38222	54.33	2 ^6E_u	33.82	3 $^6T_{2u}$	11.67	1 $^6T_{1u}$		
11 Γ_{7u}	2.869	279	38279	86.10	2 ^6E_u	11.74	1 $^6T_{1u}$				

Eu^{3+}-doped CaS

$4f^6(^7F_{0-6})$											
1 A_{1g}	2.729	308	0	48.45	1 $7T_{1g}$	36.36	1 $7T_{2g}$				
1 T_{1g}	2.729	308	372	50.79	1 $7T_{1g}$	35.76	1 $7T_{2g}$				
1 E_g	2.728	308	945	68.06	1 $7T_{1g}$	28.25	1 $7T_{2g}$				
1 T_{2g}	2.729	308	1142	46.15	1 $7T_{1g}$	38.40	1 $7T_{2g}$	11.82	1 $7A_{2g}$		
1 A_{2g}	2.728	308	1944	55.53	1 $7T_{1g}$	41.97	1 $7T_{2g}$				
2 T_{2g}	2.729	308	2026	45.50	1 $7T_{1g}$	32.90	1 $7T_{2g}$	19.00	1 $7A_{2g}$		
2 T_{1g}	2.729	308	2074	46.78	1 $7T_{2g}$	37.51	1 $7T_{1g}$	13.15	1 $7A_{2g}$		
3 T_{2g}	2.728	308	2933	69.23	1 $7T_{1g}$	24.82	1 $7T_{2g}$				
2 E_g	2.729	308	3171	73.32	1 $7T_{2g}$	24.62	1 $7T_{1g}$				
3 T_{1g}	2.729	308	3211	44.25	1 $7T_{2g}$	29.17	1 $7T_{1g}$	24.51	1 $7A_{2g}$		
2 A_{1g}	2.729	308	3252	48.85	1 $7A_{2g}$	37.23	1 $7T_{1g}$	11.83	1 $7T_{2g}$		
4 T_{1g}	2.728	308	4172	51.04	1 $7T_{1g}$	44.38	1 $7T_{2g}$				
3 E_g	2.728	308	4204	51.45	1 $7T_{2g}$	46.18	1 $7T_{1g}$				
4 T_{2g}	2.729	308	4251	64.79	1 $7T_{1g}$	24.40	1 $7A_{2g}$				
5 T_{1g}	2.729	308	4416	73.81	1 $7T_{2g}$	12.74	1 $7T_{1g}$	11.07	1 $7A_{2g}$		
4 E_g	2.728	308	5369	54.99	1 $7T_{1g}$	41.70	1 $7T_{2g}$				
5 T_{2g}	2.728	308	5391	50.60	1 $7T_{1g}$	45.30	1 $7T_{2g}$				
2 A_{2g}	2.728	308	5446	55.11	1 $7T_{2g}$	41.55	1 $7T_{1g}$				
6 T_{2g}	2.729	308	5653	44.03	1 $7T_{2g}$	37.12	1 $7A_{2g}$	15.53	1 $7T_{1g}$		

6 T_{1g}	2.729	308	5687	46.35	1 $7T_{2g}$	37.60	1 $7A_{2g}$	12.73	1 $7T_{1g}$				
3 A_{1g}	2.729	308	5715	47.40	1 $7T_{2g}$	38.81	1 $7A_{2g}$	10.44	1 $7T_{1g}$				
$4f^6(^5D_{0-3})$													
4 A_{1g}	2.727	307	19893	57.55	1 $5T_{2g}$	36.69	1 $5E_g$						
7 T_{1g}	2.727	307	20699	58.17	1 $5T_{2g}$	36.63	1 $5E_g$						
7 T_{2g}	2.727	307	22337	70.60	1 $5T_{2g}$	24.94	1 $5E_g$						
5 E_g	2.727	307	22440	53.99	1 $5E_g$	41.49	1 $5T_{2g}$						
8 T_{1g}	2.727	307	25019	85.55	1 $5T_{2g}$	10.13	1 $5E_g$						
8 T_{2g}	2.727	307	25063	50.23	1 $5E_g$	45.42	1 $5T_{2g}$						
3 A_{2g}	2.727	307	25100	95.34	1 $5E_g$								
$4f^6(^5D_4,^5L_{6-10},^5G_{2-6})$													
9 T_{2g}	2.726	307	28200	23.26	1 $5T_{1g}$	22.66	2 $5E_g$	16.25	4 $5T_{2g}$	14.50	2 $5T_{1g}$		
5 A_{1g}	2.725	307	28212	54.31	3 $5T_{2g}$	33.41	3 $5E_g$						
4 A_{2g}	2.726	307	28225	37.63	1 $5T_{1g}$	36.55	2 $5E_g$	13.47	2 $5T_{1g}$				
9 T_{1g}	2.725	307	28234	32.05	3 $5T_{2g}$	13.37	1 $5T_{1g}$	13.35	2 $5T_{1g}$	13.30	3 $5E_g$		
				11.10	2 $5E_g$								
10 T_{2g}	2.726	307	28378	43.45	1 $5T_{1g}$	14.42	2 $5E_g$	10.37	3 $5T_{2g}$	10.01	4 $5T_{1g}$		
11 T_{2g}	2.726	307	28379	41.40	1 $5T_{1g}$	35.38	1 $5A_{1g}$						
6 E_g	2.726	307	28413	44.78	1 $5T_{1g}$	22.10	2 $5E_g$	18.46	1 $5A_{1g}$				
12 T_{2g}	2.726	307	28463	26.80	4 $5T_{2g}$	16.11	1 $5T_{1g}$	14.57	2 $5E_g$	10.03	3 $5T_{2g}$		
10 T_{1g}	2.726	307	28513	44.39	1 $5T_{1g}$	20.58	2 $5T_{2g}$						
7 E_g	2.726	307	28514	32.42	1 $5A_{1g}$	16.62	2 $5E_g$	11.16	2 $5T_{2g}$	10.23	1 $5T_{2g}$		
13 T_{2g}	2.727	307	28529	22.05	4 $5T_{2g}$	21.42	3 $5T_{2g}$	17.97	3 $5T_{1g}$	13.05	4 $5E_g$		
				12.66	2 $5T_{1g}$								
6 A_{1g}	2.727	307	28605	64.54	2 $5E_g$	13.87	2 $5T_{2g}$	13.80	5 $5T_{2g}$				
8 E_g	2.727	308	28625	31.75	3 $5T_{1g}$	20.52	4 $5T_{2g}$	17.19	4 $5E_g$	10.56	2 $5A_{1g}$		
5 A_{2g}	2.727	307	28635	40.31	2 $5T_{1g}$	18.85	4 $5E_g$	12.64	3 $5E_g$				
14 T_{2g}	2.727	308	28745	71.97	2 $5T_{2g}$								
11 T_{1g}	2.726	307	28821	24.19	2 $5T_{1g}$	20.91	3 $5T_{2g}$	10.84	4 $5T_{2g}$				
7 A_{1g}	2.726	307	28845	56.55	1 $5E_g$	36.10	1 $5T_{2g}$						
9 E_g	2.727	307	28901	33.09	3 $5E_g$	13.60	4 $5T_{2g}$	11.82	2 $5T_{1g}$	11.74	2 $5T_{2g}$		
12 T_{1g}	2.727	307	28915	30.47	1 $5E_g$	30.35	1 $5T_{2g}$	10.42	2 $5T_{2g}$				
15 T_{2g}	2.727	307	28924	25.04	3 $5T_{2g}$	12.73	2 $5T_{1g}$	11.66	4 $5E_g$	10.55	4 $5T_{2g}$		
10 E_g	2.727	307	28968	41.04	1 $5T_{2g}$	30.69	1 $5E_g$	11.76	2 $5E_g$				
16 T_{2g}	2.727	307	29021	25.86	2 $5E_g$	17.03	1 $5T_{1g}$	10.86	2 $5T_{2g}$				
17 T_{2g}	2.727	307	29022	18.59	2 $5E_g$	16.29	1 $5T_{1g}$	11.54	1 $5A_{1g}$	11.23	2 $5T_{2g}$		
18 T_{2g}	2.727	308	29028	34.63	1 $5T_{2g}$	15.48	2 $5T_{2g}$	13.15	1 $5T_{1g}$				
13 T_{1g}	2.727	307	29088	23.07	4 $5T_{2g}$	20.41	4 $5E_g$	19.17	3 $5T_{1g}$	13.58	2 $5T_{2g}$		
6 A_{2g}	2.727	308	29114	40.96	3 $5T_{1g}$	24.46	4 $5E_g$	21.32	3 $5E_g$				
11 E_g	2.727	308	29137	55.16	2 $5T_{2g}$								
14 T_{1g}	2.727	307	29154	34.92	2 $5T_{2g}$								
19 T_{2g}	2.727	308	29165	28.97	3 $5T_{1g}$	18.79	2 $5A_{1g}$	18.04	2 $5T_{1g}$	12.45	3 $5E_g$		
				11.04	4 $5T_{2g}$								
12 E_g	2.726	307	29573	51.15	3 $5T_{2g}$	19.91	2 $5T_{1g}$	14.36	4 $5T_{2g}$				
20 T_{2g}	2.726	307	29601	32.48	2 $5T_{1g}$	27.26	3 $5E_g$	14.31	4 $5T_{2g}$	10.27	3 $5T_{2g}$		
15 T_{1g}	2.726	308	29686	25.67	3 $5T_{2g}$	16.70	4 $5T_{2g}$	13.79	4 $5E_g$	12.98	3 $5E_g$		
				11.62	2 $5T_{1g}$	10.73	3 $5T_{1g}$						
21 T_{2g}	2.727	308	29787	35.80	3 $5T_{1g}$	13.95	4 $5E_g$	12.17	4 $5T_{2g}$				
16 T_{1g}	2.727	308	29823	48.22	3 $5T_{1g}$	20.88	2 $5T_{1g}$	18.84	4 $5T_{2g}$				
8 A_{1g}	2.727	307	29867	54.65	4 $5E_g$	24.86	4 $5T_{2g}$	14.68	3 $5T_{2g}$				
13 E_g	2.726	307	29901	31.66	1 $5T_{1g}$	17.23	2 $5E_g$	15.46	1 $5A_{1g}$				
22 T_{2g}	2.726	307	29938	35.49	1 $5T_{1g}$	23.00	2 $5E_g$	12.90	1 $5A_{1g}$				
14 E_g	2.727	308	29949	22.14	2 $5A_{1g}$	18.69	2 $5T_{1g}$	16.04	4 $5T_{2g}$	13.77	4 $5E_g$		
7 A_{2g}	2.727	307	29982	38.00	1 $5T_{1g}$	35.33	2 $5E_g$	12.44	4 $5T_{1g}$				
9 A_{1g}	2.727	307	30116	58.63	2 $5T_{2g}$	15.11	5 $5E_g$	14.43	2 $5E_g$				
17 T_{1g}	2.727	307	30120	51.65	2 $5T_{2g}$								
23 T_{2g}	2.727	307	30143	48.89	2 $5T_{2g}$	12.53	5 $5T_{1g}$	11.75	1 $5T_{1g}$				
8 A_{2g}	2.726	307	30532	58.93	3 $5E_g$	25.10	2 $5T_{1g}$						
24 T_{2g}	2.726	307	30536	30.14	2 $5T_{1g}$	28.59	3 $5T_{2g}$	19.51	4 $5T_{2g}$				
18 T_{1g}	2.726	307	30538	41.47	3 $5T_{2g}$	21.47	2 $5T_{1g}$	21.02	4 $5T_{2g}$				
10 A_{1g}	2.726	308	30632	33.15	3 $5E_g$	29.79	4 $5E_g$	25.36	3 $5T_{2g}$				

19 T_{1g}	2.727	308	30652	41.25	3 $5T_{1g}$	22.04	4 $5T_{2g}$	13.91	3 $5E_g$		
15 E_g	2.727	307	30725	30.90	4 $5E_g$	22.99	4 $5T_{2g}$	19.41	2 $5A_{1g}$		
25 T_{2g}	2.727	308	30815	26.82	2 $5A_{1g}$	22.32	2 $5T_{1g}$	20.50	4 $5T_{2g}$	12.53	4 $5E_g$
				12.52	3 $5T_{1g}$						
20 T_{1g}	2.727	308	30843	42.32	3 $5T_{1g}$	36.79	4 $5E_g$				
21 T_{1g}	2.725	307	31577	57.80	3 $5T_{2g}$	20.90	3 $5E_g$	13.20	2 $5T_{1g}$		
16 E_g	2.726	307	31632	31.49	3 $5T_{2g}$	31.00	2 $5T_{1g}$	28.83	3 $5E_g$		
22 T_{1g}	2.726	307	31652	40.58	2 $5T_{1g}$	25.89	3 $5E_g$	18.08	3 $5T_{2g}$		
11 A_{1g}	2.726	308	31704	60.74	4 $5T_{2g}$	24.63	3 $5E_g$	11.78	4 $5E_g$		
23 T_{1g}	2.727	307	31755	39.44	4 $5T_{2g}$	24.09	2 $5T_{1g}$	16.00	4 $5E_g$	12.58	3 $5T_{1g}$
26 T_{2g}	2.727	308	31799	36.28	4 $5T_{2g}$	28.85	3 $5T_{1g}$	11.58	4 $5E_g$		
9 A_{2g}	2.727	308	31982	50.80	4 $5E_g$	40.85	3 $5T_{1g}$				
27 T_{2g}	2.727	308	32020	43.26	3 $5T_{1g}$	26.92	4 $5E_g$	24.22	2 $5A_{1g}$		
17 E_g	2.727	308	32034	42.99	3 $5T_{1g}$	30.67	2 $5A_{1g}$	21.76	4 $5E_g$		

[a] Absorption oscillator strengths for 1 $\Gamma_{6u,8u,7u} \rightarrow i$ transitions are calculated at $d_{\mathrm{Eu-F}}$= 2.850 Å; the reference value is f_{ref} = 5.062×10^{-3}. Emission oscillator strengths for 1 $\Gamma_{8g} \rightarrow$1 Γ_{6u},1 Γ_{8u},1 Γ_{7u} and radiative emission lifetime are calculated at $d_{\mathrm{Eu-F}}$= 2.800 Å; the reference value is f_{ref} = 8.993×10^{-4}.
[b] The analyses of the wave functions have been done at $d_{\mathrm{Eu-F}}$= 2.850 Å ($4f^7$), 2.850 Å ($4f^6(5d^1 + 6sa^1_{1g})$), 2.700 Å ($4f^6$).
[c] C.f. Table S7.
[d] C.f. Table S8.

TABLE S13: Spectroscopic constants and analyses of the spin-orbit wave functions of the ground and lowest lying excited states of Eu^{2+} and Eu^{3+} -doped SrS octahedral defects. Eu–S bond distances ($d_{\mathrm{Eu-S},e}$ in Å), EuS_6 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), minimum-to-minimum energy differences (T_e in cm^{-1}), and relative absorption and emission oscillator strengths (f_i^{abs}/f_{ref} and f_i^{emi}/f_{ref}) are given. Calculated radiative emission lifetime for the $4f^6(^7F_J)5dt_{2g}^1$ – 1 Γ_{8g} excited state is 0.306 μs. Local distortion around the Eu^{2+}impurity, relative to experimental crystal structure d_{Sr-F}= 3.010 Å, is $d_{\mathrm{Eu-S},e}(1\Gamma_{6u}) - d_{\mathrm{Sr-S}} = -0.035$; ionic radii mismatch is –0.01 Å[31]. See Fig. 3, S3 and text for details.

State	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e	f_i^{abs}/f_{ref} [a]	f_i^{emi}/f_{ref} [a]	weights of terms larger than 10% [b]							
						Eu^{2+}-doped SrS							
$4f^7(^8S_{7/2})$ [c]													
1 Γ_{8u}	2.975	273	0		0.39	97.71	1 $^8A_{1g}$						
1 Γ_{6u}	2.975	273	0		1.00	97.70	1 $^8A_{1g}$						
1 Γ_{7u}	2.975	273	0		0.06	97.70	1 $^8A_{1g}$						
						$4f^6(5d+6s)^1$ excited states							
$4f^6(^7F_J)5dt_{2g}^1$ High-Spin coupling [d]													
1 Γ_{8g}	2.945	263	18978	1.00		35.23	1 $^8T_{1g}$	24.67	1 ^8E_g	20.92	1 $^8T_{2g}$	11.57	2 $^8T_{1g}$
2 Γ_{8g}	2.945	263	19368	0.88		31.83	1 $^8T_{2g}$	28.46	1 $^8T_{1g}$	22.31	1 ^8E_g	11.17	2 $^8T_{1g}$
1 Γ_{7g}	2.944	264	19626	1.44		51.15	1 $^8T_{2g}$	28.10	2 $^8T_{1g}$				
3 Γ_{8g}	2.944	263	19949	1.43		40.37	1 $^8T_{2g}$	24.78	1 ^8E_g	16.40	1 $^8T_{1g}$	10.40	2 $^8T_{1g}$
1 Γ_{6g}	2.944	263	19993	0.51		42.98	1 $^8T_{1g}$	30.45	1 ^8E_g				
2 Γ_{7g}	2.944	264	20246	2.22		34.97	1 $^8T_{2g}$	32.16	2 $^8T_{1g}$	16.73	1 ^8E_g	10.13	1 $^8T_{1g}$
4 Γ_{8g}	2.944	263	20670	1.70		34.79	1 $^8T_{2g}$	24.41	1 $^8T_{1g}$	17.07	1 ^8E_g	15.64	2 $^8T_{1g}$
2 Γ_{6g}	2.944	263	20743	0.41		47.02	1 $^8T_{1g}$	20.98	1 ^8E_g	12.56	2 $^8T_{1g}$	10.58	1 $^8T_{2g}$
5 Γ_{8g}	2.944	263	21010	5.73		38.76	2 $^8T_{1g}$	27.90	1 $^8T_{1g}$	24.40	1 $^8T_{2g}$		
6 Γ_{8g}	2.944	263	21491	1.78		41.74	1 $^8T_{1g}$	18.74	1 ^8E_g	13.90	2 $^8T_{1g}$	11.69	1 $^8T_{2g}$
3 Γ_{7g}	2.943	262	21536	2.68		36.34	2 $^8T_{1g}$	13.29	2 $^8T_{2g}$	12.90	1 ^8E_g	10.03	1 $^8T_{2g}$
7 Γ_{8g}	2.943	264	21596	3.23		45.56	1 $^8T_{2g}$	14.19	1 $^8T_{1g}$	14.19	2 $^8T_{1g}$		
3 Γ_{6g}	2.943	263	21786	0.61		26.15	2 ^8E_g	24.06	1 $^8T_{2g}$	18.39	3 $^8T_{1g}$	14.63	2 $^8T_{2g}$
8 Γ_{8g}	2.943	264	21902	0.95		18.32	2 $^8T_{2g}$	17.27	2 ^8E_g	16.89	3 $^8T_{1g}$	10.70	2 $^8T_{1g}$
4 Γ_{6g}	2.943	263	21903	1.11		39.62	2 $^8T_{1g}$	19.12	1 $^8T_{2g}$	17.25	1 $^8T_{1g}$		
4 Γ_{7g}	2.943	262	22004	1.11		19.35	2 ^8E_g	18.87	1 ^8E_g	16.83	2 $^8T_{2g}$	12.97	3 $^8T_{1g}$
						10.69	1 $^8T_{1g}$						
9 Γ_{8g}	2.944	263	22242	1.61		21.57	1 ^8E_g	21.27	1 $^8T_{2g}$	16.46	2 $^8T_{1g}$	15.96	1 $^8T_{1g}$
						10.54	2 ^8E_g						
5 Γ_{7g}	2.943	263	22331	1.18		49.84	1 $^8T_{1g}$	28.33	1 $^8T_{2g}$				
5 Γ_{6g}	2.943	263	22459	1.19		37.32	1 $^8T_{2g}$	17.50	2 $^8T_{1g}$	16.33	2 $^8T_{2g}$		
10 Γ_{8g}	2.943	263	22662	0.55		30.33	2 ^8E_g	28.39	2 $^8T_{2g}$	11.58	3 $^8T_{1g}$		
6 Γ_{7g}	2.943	262	22697	2.84		35.94	1 $^8T_{1g}$	23.14	2 $^8T_{1g}$	19.72	1 ^8E_g	14.51	1 $^8T_{2g}$
11 Γ_{8g}	2.943	262	22770	3.72		38.20	2 $^8T_{1g}$	33.14	1 ^8E_g	11.81	1 $^8T_{2g}$		
12 Γ_{8g}	2.943	264	22852	0.68		35.35	2 ^8E_g	21.15	3 $^8T_{1g}$				
7 Γ_{7g}	2.943	263	22966	0.65		25.44	1 $^8T_{2g}$	18.65	3 $^8T_{1g}$	17.00	2 $^8T_{1g}$	12.59	2 $^8T_{2g}$
6 Γ_{6g}	2.943	263	22966	0.82		26.60	1 $^8T_{1g}$	22.40	2 $^8T_{2g}$	10.77	2 $^8T_{1g}$		
7 Γ_{6g}	2.943	263	23284	4.50		27.20	2 $^8T_{1g}$	25.01	1 $^8T_{1g}$	23.36	1 $^8T_{2g}$	14.11	1 ^8E_g
13 Γ_{8g}	2.943	262	23354	6.19		25.96	2 $^8T_{1g}$	23.85	1 $^8T_{2g}$	21.86	1 $^8T_{1g}$	12.67	1 ^8E_g
14 Γ_{8g}	2.943	263	23453	0.78		39.39	1 $^8T_{2g}$	20.03	1 ^8E_g	14.08	2 $^8T_{2g}$	10.00	2 ^8E_g
15 Γ_{8g}	2.943	264	23528	2.35		20.34	1 $^8T_{1g}$	18.53	1 ^8E_g	17.31	2 ^8E_g	16.03	2 $^8T_{1g}$
16 Γ_{8g}	2.943	263	23736	1.16		23.66	2 ^8E_g	15.60	2 $^8T_{2g}$	12.07	1 $^8T_{1g}$		
8 Γ_{7g}	2.943	263	23760	1.21		20.43	3 $^8T_{1g}$	12.34	2 ^8E_g	11.93	2 $^8T_{1g}$		
9 Γ_{7g}	2.943	263	23974	1.17		20.98	2 $^8T_{1g}$	19.54	3 $^8T_{1g}$	14.14	2 ^8E_g	10.76	1 $^8T_{1g}$
17 Γ_{8g}	2.943	264	24016	2.65		23.51	2 $^8T_{1g}$	18.79	3 $^8T_{1g}$	14.26	2 $^8T_{2g}$		
18 Γ_{8g}	2.943	264	24118	5.16		32.06	2 $^8T_{1g}$	19.95	2 $^8T_{2g}$	17.00	1 $^8T_{1g}$	13.37	3 $^8T_{1g}$
8 Γ_{6g}	2.943	263	24121	0.75		31.05	2 $^8T_{2g}$	16.39	1 ^8E_g	11.85	1 $^8T_{2g}$		
9 Γ_{6g}	2.943	264	24254	0.30		27.47	1 $^8T_{2g}$	17.68	2 ^8E_g				
19 Γ_{8g}	2.943	264	24304	0.37		24.42	1 $^8T_{2g}$	24.27	1 $^8T_{1g}$	15.60	2 ^8E_g	14.67	1 ^8E_g
10 Γ_{7g}	2.943	263	24412	0.03		34.81	1 $^8T_{1g}$	18.07	1 $^8T_{2g}$	14.73	1 ^8E_g	11.97	2 ^8E_g

					11.33	$2\ ^8T_{1g}$						
10 Γ_{6g}	2.943	264	24567	5.08	53.95	$2\ ^8T_{1g}$	17.78	$1\ ^8T_{2g}$				
20 Γ_{8g}	2.943	263	24581	9.50	38.50	$2\ ^8T_{1g}$	20.12	$1\ ^8T_{1g}$	11.88	$1\ ^8E_g$		
21 Γ_{8g}	2.943	264	24702	8.09	39.14	$2\ ^8T_{1g}$	21.27	$2\ ^8T_{2g}$	13.53	$1\ ^8T_{2g}$	10.28	$3\ ^8T_{1g}$
11 Γ_{6g}	2.943	263	25055	0.06	29.50	$2\ ^8T_{2g}$	27.15	$2\ ^8E_g$	10.81	$1\ ^8T_{1g}$		
22 Γ_{8g}	2.943	264	25122	0.56	52.90	$2\ ^8T_{2g}$	16.19	$3\ ^8T_{1g}$	11.49	$2\ ^8E_g$		
23 Γ_{8g}	2.943	263	25134	0.89	41.89	$2\ ^8T_{2g}$	13.13	$2\ ^8E_g$	12.44	$3\ ^8T_{1g}$		
11 Γ_{7g}	2.943	264	25194	0.01	63.17	$2\ ^8T_{2g}$						
12 Γ_{6g}	2.942	264	25306	1.30	44.91	$3\ ^8T_{1g}$	15.07	$2\ ^8T_{2g}$				
24 Γ_{8g}	2.943	264	25408	0.86	56.33	$3\ ^8T_{1g}$	17.91	$2\ ^8T_{2g}$				
12 Γ_{7g}	2.943	263	25437	0.47	58.48	$3\ ^8T_{1g}$	10.67	$2\ ^8E_g$				
25 Γ_{8g}	2.945	264	25676	0.01	85.38	$1\ ^6T_{1g}$						
26 Γ_{8g}	2.942	263	25901	0.20	49.51	$2\ ^8T_{2g}$	14.51	$2\ ^8E_g$				
13 Γ_{7g}	2.942	263	26000	0.01	48.72	$2\ ^8T_{2g}$	11.87	$2\ ^8E_g$				
27 Γ_{8g}	2.942	264	26303	0.83	51.39	$3\ ^8T_{1g}$	26.44	$2\ ^8T_{2g}$	11.18	$2\ ^8E_g$		
13 Γ_{6g}	2.942	264	26332	0.27	40.46	$3\ ^8T_{1g}$	36.63	$2\ ^8T_{2g}$				
28 Γ_{8g}	2.942	264	26418	0.89	57.44	$3\ ^8T_{1g}$	18.11	$2\ ^8E_g$	14.92	$2\ ^8T_{2g}$		
14 Γ_{7g}	2.942	263	26757	0.36	44.20	$3\ ^8T_{1g}$						
29 Γ_{8g}	2.942	263	26815	0.76	47.40	$3\ ^8T_{1g}$						
14 Γ_{6g}	2.942	263	26836	0.40	47.76	$3\ ^8T_{1g}$						
$4f^6(^7F_J)5dt^1_{2g}$ Low-Spin coupling [d]												
30 Γ_{8g}	2.944	264	26963		79.64	$1\ ^6T_{1g}$						
15 Γ_{7g}	2.944	264	26976		78.16	$1\ ^6T_{1g}$	10.26	$1\ ^6T_{2g}$				
16 Γ_{7g}	2.941	263	28524	0.01	36.27	$2\ ^6T_{1g}$	34.88	$1\ ^6E_g$	22.23	$1\ ^6T_{1g}$		
15 Γ_{6g}	2.942	264	28704	0.05	53.53	$1\ ^6T_{1g}$	29.25	$1\ ^6T_{2g}$				
31 Γ_{8g}	2.942	264	28727	0.09	52.96	$1\ ^6T_{1g}$	28.41	$1\ ^6T_{2g}$				
32 Γ_{8g}	2.940	264	28961	0.01	51.52	$2\ ^6T_{1g}$	25.80	$1\ ^6E_g$				
17 Γ_{7g}	2.941	264	29020	0.03	29.11	$1\ ^6T_{2g}$	28.60	$1\ ^6T_{1g}$	27.74	$2\ ^6T_{1g}$		
16 Γ_{6g}	2.940	264	29178	0.01	28.13	$2\ ^6T_{1g}$	20.56	$1\ ^6T_{2g}$	16.55	$1\ ^6E_g$	13.93	$2\ ^6T_{2g}$
33 Γ_{8g}	2.940	264	29496	0.03	24.36	$2\ ^6T_{1g}$	22.18	$1\ ^6E_g$	19.51	$2\ ^6T_{2g}$	13.81	$1\ ^6A_{2g}$
18 Γ_{7g}	2.942	264	29636	0.02	40.70	$1\ ^6T_{1g}$	25.53	$2\ ^6T_{1g}$	16.22	$1\ ^6T_{2g}$		
17 Γ_{6g}	2.940	263	29807	0.02	39.50	$1\ ^6T_{2g}$	38.31	$2\ ^6T_{1g}$				
34 Γ_{8g}	2.940	263	30012	0.01	21.98	$1\ ^6A_{2g}$	20.77	$2\ ^6T_{2g}$	12.55	$1\ ^6T_{1g}$	11.57	$1\ ^6T_{2g}$
					11.15	$2\ ^6T_{1g}$						
35 Γ_{8g}	2.941	264	30196	0.08	31.41	$2\ ^6T_{1g}$	27.92	$1\ ^6T_{2g}$	15.85	$1\ ^6E_g$		
18 Γ_{6g}	2.939	263	30217	0.01	28.22	$1\ ^6A_{2g}$	18.90	$2\ ^6T_{2g}$	16.15	$2\ ^6T_{1g}$	12.28	$1\ ^6T_{2g}$
36 Γ_{8g}	2.940	264	30399	0.07	28.29	$1\ ^6E_g$	22.84	$1\ ^6T_{2g}$	18.28	$2\ ^6T_{1g}$		
19 Γ_{6g}	2.941	264	30768	0.06	38.32	$1\ ^6E_g$	29.13	$1\ ^6T_{2g}$	20.59	$2\ ^6T_{2g}$		
37 Γ_{8g}	2.939	262	30949	0.08	21.44	$1\ ^6E_g$	20.69	$3\ ^6T_{1g}$	19.72	$2\ ^6T_{1g}$	12.31	$2\ ^6T_{2g}$
38 Γ_{8g}	2.939	264	31031	0.04	28.94	$2\ ^6T_{2g}$	19.43	$1\ ^6T_{2g}$	19.27	$2\ ^6E_g$	13.54	$3\ ^6T_{1g}$
19 Γ_{7g}	2.941	263	31235		47.34	$2\ ^6T_{1g}$	33.05	$1\ ^6T_{2g}$				
20 Γ_{6g}	2.939	263	31433	0.01	36.41	$2\ ^6E_g$	25.06	$2\ ^6T_{2g}$	19.00	$1\ ^6E_g$		
20 Γ_{7g}	2.938	263	31480	0.06	37.00	$3\ ^6T_{1g}$	17.75	$2\ ^6T_{1g}$	16.08	$2\ ^6E_g$	12.37	$1\ ^6A_{1g}$
39 Γ_{8g}	2.938	264	31727	0.03	23.40	$2\ ^6E_g$	20.67	$2\ ^6T_{2g}$	15.51	$1\ ^6A_{2g}$	15.13	$3\ ^6T_{1g}$
21 Γ_{6g}	2.941	263	31754	0.06	47.69	$1\ ^6T_{2g}$	14.66	$3\ ^6T_{1g}$	10.39	$2\ ^6T_{1g}$	10.05	$1\ ^6E_g$
40 Γ_{8g}	2.941	263	31880	0.04	34.51	$2\ ^6T_{1g}$	25.89	$1\ ^6T_{2g}$	14.99	$2\ ^6T_{2g}$		
21 Γ_{7g}	2.940	263	32108	0.02	35.16	$2\ ^6T_{1g}$	23.00	$1\ ^6E_g$	18.87	$3\ ^6T_{1g}$	15.96	$2\ ^6T_{2g}$
41 Γ_{8g}	2.938	264	32128	0.07	32.73	$2\ ^6T_{2g}$	22.27	$3\ ^6T_{1g}$	15.72	$1\ ^6T_{2g}$	11.85	$1\ ^6A_{1g}$
42 Γ_{8g}	2.941	264	32298	0.10	32.53	$2\ ^6T_{1g}$	30.51	$1\ ^6T_{2g}$	15.63	$1\ ^6E_g$		
22 Γ_{7g}	2.938	264	32406	0.03	34.70	$2\ ^6E_g$	25.74	$3\ ^6T_{1g}$	16.59	$1\ ^6E_g$		
43 Γ_{8g}	2.941	263	32613	0.19	52.54	$1\ ^6T_{2g}$	17.31	$1\ ^6E_g$	14.62	$2\ ^6T_{1g}$		
23 Γ_{7g}	2.938	263	32967	0.02	55.75	$2\ ^6T_{2g}$	23.03	$1\ ^6A_{1g}$				
44 Γ_{8g}	2.938	263	33093	0.04	23.61	$2\ ^6T_{2g}$	20.46	$1\ ^6A_{1g}$	13.95	$2\ ^6E_g$	12.31	$3\ ^6T_{1g}$
					11.19	$1\ ^6A_{2g}$						
22 Γ_{6g}	2.938	263	33127	0.01	28.55	$3\ ^6T_{1g}$	25.18	$1\ ^6A_{2g}$	22.33	$2\ ^6T_{2g}$	16.63	$1\ ^6T_{2g}$
45 Γ_{8g}	2.939	262	33293	0.01	33.04	$3\ ^6T_{1g}$	23.86	$2\ ^6T_{2g}$	20.38	$2\ ^6E_g$		
46 Γ_{8g}	2.938	264	33316	0.03	49.36	$3\ ^6T_{1g}$	17.08	$2\ ^6E_g$	11.03	$2\ ^6T_{2g}$	10.01	$2\ ^6T_{1g}$
23 Γ_{6g}	2.938	263	34376	0.02	39.61	$3\ ^6T_{1g}$	37.39	$2\ ^6T_{2g}$	13.38	$1\ ^6A_{2g}$		
47 Γ_{8g}	2.938	263	34426	0.01	42.28	$2\ ^6T_{2g}$	26.28	$2\ ^6E_g$	15.49	$1\ ^6A_{2g}$	10.09	$3\ ^6T_{1g}$
24 Γ_{7g}	2.938	263	34557	0.02	52.89	$3\ ^6T_{1g}$	34.56	$2\ ^6E_g$				
48 Γ_{8g}	2.938	263	34575	0.03	34.40	$2\ ^6E_g$	34.02	$3\ ^6T_{1g}$	24.51	$2\ ^6T_{2g}$		

24 Γ_{6g}	2.938	263	34624	0.01	45.15	2 ^6E_g	41.07	2 $^6T_{2g}$				
$4f^6(^7F_J)(5de_g^1+6sa_{1g}^1)$ High-, Low- and Mixed-Spin coupling [d]												
50 Γ_{8g}	2.983	262	39417	6.41	61.54	3 $^8T_{2g}$	28.77	4 $^8T_{1g}$				
26 Γ_{7g}	2.983	263	39514	2.87	68.46	3 $^8T_{2g}$	26.90	4 $^8T_{1g}$				
51 Γ_{8g}	2.983	262	39646	0.85	79.34	3 $^8T_{2g}$	10.10	3 ^8E_g				
27 Γ_{7g}	2.982	262	40133	6.08	50.61	4 $^8T_{1g}$	35.09	3 $^8T_{2g}$				
52 Γ_{8g}	2.982	262	40430	7.78	47.28	3 $^8T_{2g}$	33.84	4 $^8T_{1g}$	13.05	3 ^8E_g		
25 Γ_{6g}	2.983	262	40503	2.33	50.70	3 $^8T_{2g}$	25.42	4 $^8T_{1g}$	11.56	5 $^8T_{1g}$		
53 Γ_{8g}	2.982	262	40987	12.68	55.03	4 $^8T_{1g}$	30.22	3 $^8T_{2g}$				
26 Γ_{6g}	2.982	262	41085	3.09	29.87	3 $^8T_{2g}$	24.87	4 $^8T_{1g}$	21.34	3 ^8E_g	12.37	4 $^8T_{2g}$
					10.44	5 $^8T_{1g}$						
28 Γ_{7g}	2.982	262	41340	4.95	42.58	4 $^8T_{1g}$	38.40	3 $^8T_{2g}$	13.96	3 ^8E_g		
54 Γ_{8g}	2.982	261	41477	3.29	29.91	3 $^8T_{2g}$	29.27	4 $^8T_{2g}$	22.42	3 ^8E_g	11.96	4 $^8T_{1g}$
55 Γ_{8g}	2.982	261	41746	2.18	30.19	5 $^8T_{1g}$	27.82	3 ^8E_g	13.16	4 $^8T_{2g}$		
27 Γ_{6g}	2.982	262	41809	2.79	42.71	4 $^8T_{2g}$	34.32	4 $^8T_{1g}$	13.92	5 $^8T_{1g}$		
56 Γ_{8g}	2.982	261	41837	2.78	30.33	5 $^8T_{1g}$	22.43	4 $^8T_{1g}$	15.13	4 $^8T_{2g}$	13.88	3 $^8T_{2g}$
					12.57	3 ^8E_g						
57 Γ_{8g}	2.984	256	42319	10.74	46.34	3 $^6T_{2g}$	15.37	5 $^6T_{1g}$	10.73	3 ^6E_g		
29 Γ_{7g}	2.982	262	42471	8.20	68.41	4 $^8T_{1g}$	17.74	3 $^8T_{2g}$				
58 Γ_{8g}	2.982	258	42507	2.67	52.23	4 $^8T_{1g}$	23.40	3 $^8T_{2g}$	17.93	5 $^8T_{1g}$		
28 Γ_{6g}	2.982	262	42512	1.06	33.66	4 $^8T_{2g}$	28.58	5 $^8T_{1g}$	18.88	3 $^8T_{2g}$	12.72	4 $^8T_{1g}$
30 Γ_{7g}	2.982	261	42533	0.27	29.75	4 $^8T_{2g}$	22.71	3 $^8T_{2g}$	21.99	3 ^8E_g	20.50	5 $^8T_{1g}$
29 Γ_{6g}	2.983	262	42774	2.33	58.57	3 $^8T_{2g}$	19.74	5 $^8T_{1g}$	12.03	4 $^8T_{1g}$		
59 Γ_{8g}	2.962	290	42798	0.04	30.76	4 $^8T_{2g}$	19.65	3 ^8E_g	18.39	4 $^8T_{1g}$	16.32	5 $^8T_{1g}$
					13.06	3 $^8T_{2g}$						
30 Γ_{6g}	2.982	261	43064	1.14	40.70	4 $^8T_{2g}$	25.66	3 ^8E_g	13.36	4 $^8T_{1g}$		
60 Γ_{8g}	2.974	501	43071	1.74	35.13	3 ^8E_g	30.06	4 $^8T_{2g}$	17.18	5 $^8T_{1g}$		
61 Γ_{8g}	2.971	449	43226	7.28	41.52	4 $^8T_{1g}$	18.22	3 $^8T_{2g}$	17.87	3 ^8E_g	11.60	4 $^8T_{2g}$
62 Γ_{8g}	2.982	298	43549	0.45	25.79	3 ^6E_g	25.67	3 $^6T_{2g}$	18.69	5 $^6T_{1g}$		
31 Γ_{7g}	2.978	568	43698	0.01	35.21	5 $^6T_{1g}$	24.39	3 ^6E_g	13.90	4 $^6T_{2g}$	10.23	4 $^6T_{1g}$
63 Γ_{8g}	2.982	291	43826	6.85	31.92	3 $^8T_{2g}$	28.93	3 ^8E_g	17.75	4 $^8T_{2g}$	14.67	5 $^8T_{1g}$
32 Γ_{7g}	2.959	343	43883	2.29	53.70	5 $^8T_{1g}$	23.09	4 $^8T_{2g}$				
31 Γ_{6g}	2.986	254	44025	0.01	42.60	5 $^6T_{1g}$	26.85	3 $^6T_{2g}$	11.85	4 $^6T_{2g}$		
64 Γ_{8g}	2.979	198	44065	0.14	25.29	4 $^6T_{2g}$	21.85	4 $^6T_{1g}$	21.56	3 $^6T_{2g}$		
33 Γ_{7g}	2.967	313	44108	0.01	23.42	4 $^6T_{2g}$	23.04	4 $^6T_{1g}$	19.64	5 $^6T_{1g}$	13.70	3 ^6E_g
65 Γ_{8g}	2.961	280	44255	14.59	29.17	5 $^8T_{1g}$	26.85	4 $^8T_{1g}$	19.20	4 $^8T_{2g}$	13.42	3 ^8E_g
34 Γ_{7g}	2.954	374	44515	0.01	60.70	4 $^8T_{2g}$	27.42	3 ^8E_g				
66 Γ_{8g}	2.975	481	44567	0.02	57.55	4 $^8T_{1g}$	17.81	5 $^8T_{1g}$	11.22	4 $^8T_{2g}$		
67 Γ_{8g}	2.961	331	44647	2.55	53.38	4 $^8T_{2g}$	26.41	5 $^8T_{1g}$	11.53	3 ^8E_g		
32 Γ_{6g}	2.984	252	44651	5.16	69.16	4 $^8T_{1g}$	20.80	3 $^8T_{2g}$				
35 Γ_{7g}	2.959	462	44723	0.05	36.40	5 $^6T_{1g}$	16.79	2 $^6A_{1g}$	14.40	4 $^6T_{1g}$	14.19	4 $^6T_{2g}$
33 Γ_{6g}	2.992	365	44775	1.59	49.04	4 $^8T_{2g}$	40.52	5 $^8T_{1g}$				
68 Γ_{8g}	2.981	306	45035	4.75	46.47	5 $^8T_{1g}$	27.59	3 ^8E_g	11.81	4 $^8T_{1g}$		
34 Γ_{6g}	3.000	406	45185	0.38	61.87	5 $^8T_{1g}$	25.82	3 ^8E_g				
69 Γ_{8g}	2.981	255	45387	0.08	58.24	4 $^6T_{1g}$	10.31	3 $^6T_{2g}$				
70 Γ_{8g}	2.974	365	45459	0.90	26.05	4 $^6T_{1g}$	18.32	3 $^6T_{2g}$	17.58	5 $^6T_{1g}$	12.50	2 $^6A_{1g}$
36 Γ_{7g}	2.956	355	45707		77.16	5 $^8T_{1g}$	10.48	3 ^8E_g				
71 Γ_{8g}	2.979	487	46016	0.01	64.38	5 $^8T_{1g}$	18.24	3 ^8E_g				
37 Γ_{7g}	2.960	381	46102		72.45	4 $^8T_{2g}$	25.46	5 $^8T_{1g}$				
35 Γ_{6g}	2.946	214	46150	0.01	41.57	4 $^6T_{2g}$	36.14	3 ^6E_g				
72 Γ_{8g}	2.975	447	46152	0.22	29.66	3 ^6E_g	21.21	5 $^6T_{1g}$	16.56	4 $^6T_{1g}$	14.68	3 $^6T_{2g}$
					10.58	4 $^6T_{2g}$						
73 Γ_{8g}	2.965	307	46181	0.02	76.53	4 $^8T_{2g}$						
36 Γ_{6g}	2.881	738	46274	0.03	39.72	4 $^6T_{2g}$	26.48	3 $^6T_{2g}$	25.16	4 $^6T_{1g}$		
74 Γ_{8g}	2.964	325	46340	0.12	68.56	4 $^8T_{2g}$	27.44	5 $^8T_{1g}$				
38 Γ_{7g}	2.956	526	46385		40.48	6 $^6T_{1g}$	36.88	4 $^6T_{1g}$				
75 Γ_{8g}	2.952	288	46814		22.12	6 $^6T_{1g}$	19.60	4 $^6T_{2g}$	19.17	4 $^6T_{1g}$	12.70	3 $^6T_{2g}$
					10.04	5 $^6T_{1g}$						
39 Γ_{7g}	2.958	375	47480		73.81	4 $^6T_{1g}$	14.20	5 $^6T_{1g}$				
76 Γ_{8g}	2.962	297	47733	0.01	40.81	4 $^6T_{1g}$	23.27	6 $^6T_{1g}$	14.10	3 $^6T_{2g}$		
37 Γ_{6g}	3.006	282	47762		30.89	4 $^6T_{1g}$	26.09	3 $^6T_{2g}$	14.47	4 $^6T_{2g}$	11.39	5 $^6T_{1g}$

77 Γ_{8g}	2.970	243	47910	0.01	41.09	4 $^6T_{1g}$	14.80	6 $^6T_{1g}$	11.35	4 $^6T_{2g}$	10.51	5 $^6T_{1g}$	
40 Γ_{7g}	2.956	416	47933		27.23	4 $^6T_{2g}$	24.15	2 $^6A_{1g}$	16.99	5 $^6T_{1g}$	10.60	3 $^6T_{2g}$	
78 Γ_{8g}	2.990	330	48151	0.01	31.15	4 $^6T_{2g}$	26.95	2 $^6A_{1g}$	19.92	3 ^6E_g			
38 Γ_{6g}	2.983	314	48311		33.96	3 $^6T_{2g}$	21.31	4 $^6T_{2g}$	17.73	3 ^6E_g	14.62	5 $^6T_{1g}$	
79 Γ_{8g}	2.994	283	48517	0.01	31.38	4 $^6T_{2g}$	28.53	5 $^6T_{1g}$	18.87	3 $^6T_{2g}$			
41 Γ_{7g}	2.962	387	48834		29.58	6 $^6T_{1g}$	24.80	7 $^6T_{1g}$	12.69	5 $^6T_{1g}$			
80 Γ_{8g}	2.960	341	48854		33.05	6 $^6T_{1g}$	19.29	6 $^8T_{1g}$	13.42	5 $^8T_{2g}$			
39 Γ_{6g}	2.994	302	48921		50.20	6 $^8T_{1g}$	38.67	5 $^8T_{2g}$					
81 Γ_{8g}	2.964	303	48969	0.01	34.04	6 $^8T_{1g}$	23.82	5 $^8T_{2g}$	18.75	6 $^6T_{1g}$			
42 Γ_{7g}	2.970	688	49049		50.66	5 $^8T_{2g}$	22.24	6 $^8T_{1g}$					
82 Γ_{8g}	2.975	505	49206		35.57	6 $^6T_{1g}$	12.23	7 $^6T_{1g}$	11.17	3 $^6T_{2g}$			
40 Γ_{6g}	2.997	327	49329		21.47	6 $^6T_{1g}$	17.23	5 $^6T_{2g}$	12.62	5 $^6T_{1g}$	11.86	7 $^6T_{1g}$	
					11.81	4 $^6T_{2g}$							
41 Γ_{6g}	2.989	347	49526		46.75	5 $^6T_{2g}$	19.94	4 ^6E_g					
83 Γ_{8g}	2.981	292	49539		63.95	6 $^8T_{1g}$	31.97	5 $^8T_{2g}$					
43 Γ_{7g}	2.973	534	49595		24.34	5 $^6T_{2g}$	20.32	7 $^6T_{1g}$					
84 Γ_{8g}	2.961	301	49763	0.01	43.18	5 $^6T_{2g}$	17.93	4 ^6E_g					
44 Γ_{7g}	2.956	389	49803		45.69	7 $^6T_{2g}$	25.91	9 $^6T_{1g}$					
85 Γ_{8g}	2.967	298	49901		16.19	9 $^6T_{1g}$	15.87	7 $^6T_{1g}$	14.80	7 $^6T_{2g}$			
86 Γ_{8g}	2.967	269	50107		21.99	9 $^6T_{1g}$	18.59	7 $^6T_{1g}$	17.16	7 $^6T_{2g}$			
45 Γ_{7g}	2.960	328	50127		32.83	7 $^6T_{1g}$	17.00	5 $^6T_{2g}$					
42 Γ_{6g}	2.974	373	50224		23.68	6 $^6T_{2g}$	17.74	7 $^6T_{1g}$	17.40	2 $^6A_{2g}$	15.48	5 $^6T_{2g}$	
87 Γ_{8g}	2.982	329	50231		26.14	5 $^6T_{2g}$	15.10	7 $^6T_{1g}$	13.04	6 $^6T_{2g}$	12.74	2 $^6A_{2g}$	
43 Γ_{6g}	2.990	345	50253		35.40	7 $^6T_{1g}$	13.42	2 $^6A_{2g}$	10.03	4 $^6T_{1g}$			
88 Γ_{8g}	2.982	346	50299		17.51	6 $^6T_{2g}$	16.45	8 $^6T_{1g}$	14.89	7 $^6T_{1g}$	10.81	3 $^6A_{1g}$	
46 Γ_{7g}	2.950	361	50365		27.25	6 $^6T_{2g}$	18.26	8 $^6T_{1g}$	16.70	7 $^6T_{1g}$	10.44	5 $^6T_{2g}$	
44 Γ_{6g}	2.986	333	50450		48.74	5 $^8T_{2g}$	37.23	6 $^8T_{1g}$					
89 Γ_{8g}	2.963	239	50616	0.01	48.98	6 $^8T_{1g}$	29.02	5 $^8T_{2g}$					
47 Γ_{7g}	2.950	304	50627		45.72	5 $^8T_{2g}$	37.63	6 $^8T_{1g}$					
90 Γ_{8g}	2.962	258	50642		19.15	8 $^6T_{1g}$	17.52	7 $^6T_{1g}$	12.59	2 $^6A_{2g}$	11.41	6 $^6T_{2g}$	
48 Γ_{7g}	2.947	280	50793		37.66	10 $^6T_{1g}$	28.32	5 ^6E_g					
91 Γ_{8g}	2.955	256	50819		25.53	6 $^6T_{2g}$	11.69	8 $^6T_{1g}$	10.99	5 $^6T_{2g}$			
92 Γ_{8g}	2.953	265	50854		31.72	10 $^6T_{1g}$	23.07	5 ^6E_g	10.24	4 $^6A_{1g}$			
49 Γ_{7g}	2.954	314	50909		32.27	8 $^6T_{1g}$	24.72	4 ^6E_g					
93 Γ_{8g}	2.955	282	50924		20.21	9 $^6T_{1g}$	12.41	5 $^6T_{2g}$	11.04	6 $^6T_{2g}$			
45 Γ_{6g}	2.951	235	50965		25.16	6 $^6T_{2g}$	17.12	8 $^6T_{1g}$					
94 Γ_{8g}	2.954	272	51008		25.65	9 $^6T_{1g}$	12.89	5 $^6T_{2g}$	12.67	7 $^6T_{2g}$			
95 Γ_{8g}	2.957	292	51039		27.20	8 $^6T_{1g}$	12.06	5 $^6T_{2g}$					
46 Γ_{6g}	2.975	666	51111		56.05	7 $^6T_{2g}$	10.20	10 $^6T_{1g}$					
50 Γ_{7g}	2.957	292	51125		20.43	11 $^6T_{1g}$	15.64	4 $^6A_{1g}$	13.78	10 $^6T_{1g}$			
96 Γ_{8g}	2.960	268	51164		18.64	8 $^6T_{1g}$	13.16	7 $^6T_{1g}$	12.82	4 ^6E_g			
97 Γ_{8g}	2.956	274	51203		23.54	11 $^6T_{2g}$	11.11	10 $^6T_{2g}$					
47 Γ_{6g}	2.975	584	51263		21.69	8 $^6T_{2g}$	19.11	6 $^6T_{2g}$					
51 Γ_{7g}	2.952	287	51297		15.88	7 $^6T_{1g}$	15.05	6 $^6T_{2g}$					
98 Γ_{8g}	2.958	256	51302		19.59	10 $^6T_{1g}$	15.63	5 ^6E_g	10.19	12 $^6T_{1g}$			
99 Γ_{8g}	2.975	575	51419		22.26	8 $^6T_{2g}$	16.43	4 ^6E_g					
48 Γ_{6g}	2.975	699	51448		30.28	11 $^6T_{1g}$	12.74	10 $^6T_{2g}$					
100 Γ_{8g}	2.961	256	51463		42.08	6 $^8T_{1g}$	17.93	5 $^8T_{2g}$					
52 Γ_{7g}	2.946	281	51472		16.49	7 $^6T_{1g}$	14.06	3 $^6A_{1g}$	10.84	8 $^6T_{1g}$			
49 Γ_{6g}	2.975	677	51481		15.93	5 $^6T_{2g}$							
101 Γ_{8g}	2.956	268	51512		16.58	6 $^8T_{1g}$	12.07	11 $^6T_{2g}$					
53 Γ_{7g}	2.954	321	51532		27.95	3 $^6T_{2g}$	22.60	8 $^6T_{2g}$	12.95	5 $^6T_{1g}$			
102 Γ_{8g}	2.956	257	51608		23.70	4 $^6T_{2g}$	10.48	6 $^6T_{2g}$					
50 Γ_{6g}	2.975	653	51627		26.78	7 $^6T_{2g}$	10.89	10 $^6T_{1g}$	10.82	6 $^6T_{2g}$			
103 Γ_{8g}	2.955	257	51661		24.46	9 $^6T_{1g}$	18.59	7 $^6T_{2g}$					
51 Γ_{6g}	2.975	612	51698		27.27	11 $^6T_{2g}$	17.08	7 ^6E_g	10.26	12 $^6T_{2g}$			
104 Γ_{8g}	2.956	240	51732		18.84	5 $^6T_{1g}$	17.54	3 $^6T_{2g}$					
105 Γ_{8g}	2.954	242	51758		10.44	7 $^6T_{1g}$							
52 Γ_{6g}	2.957	213	51820	0.01	24.53	6 $^8T_{1g}$	10.31	5 $^8T_{2g}$					
106 Γ_{8g}	2.954	235	51832		66.50	5 $^8T_{2g}$	20.74	6 $^8T_{1g}$					
54 Γ_{7g}	2.953	306	51848		31.00	11 $^6T_{1g}$	16.70	7 ^6E_g	11.30	11 $^6T_{2g}$			
107 Γ_{8g}	2.951	250	51849	0.01	12.31	12 $^6T_{1g}$							

53 Γ_{6g}	2.957	207	51851		15.18	7 $^6T_{2g}$	10.65	4 ^6E_g	10.26	3 $^6T_{2g}$		
55 Γ_{7g}	2.950	344	51867		23.75	8 $^6T_{1g}$	15.22	4 ^6E_g	11.00	7 $^6T_{1g}$		
56 Γ_{7g}	2.949	366	51878		33.49	12 $^6T_{1g}$	14.01	11 $^6T_{2g}$				
108 Γ_{8g}	2.950	267	51884		12.03	6 $^6T_{2g}$	10.00	7 $^6T_{1g}$				
109 Γ_{8g}	2.952	265	51943		18.28	9 $^6T_{2g}$						
110 Γ_{8g}	2.954	263	51994		13.83	9 $^6T_{2g}$	12.04	11 $^6T_{1g}$				
111 Γ_{8g}	2.954	267	52082		11.28	8 $^6T_{2g}$						
54 Γ_{6g}	2.975	813	52107		13.70	6 ^6E_g	11.51	7 $^6T_{2g}$	10.17	6 $^6T_{2g}$		
112 Γ_{8g}	2.955	263	52137		23.54	12 $^6T_{1g}$						
57 Γ_{7g}	2.950	298	52183		25.70	12 $^6T_{1g}$	11.07	10 $^6T_{2g}$				
58 Γ_{7g}	2.952	306	52236		31.66	9 $^6T_{1g}$	18.53	10 $^6T_{1g}$				
55 Γ_{6g}	2.975	787	52255		25.08	10 $^6T_{1g}$	18.00	5 ^6E_g	11.62	7 $^6T_{2g}$	10.24	10 $^6T_{2g}$
113 Γ_{8g}	2.950	250	52259		11.07	11 $^6T_{2g}$	10.36	12 $^6T_{2g}$				
114 Γ_{8g}	2.953	257	52293		10.06	8 $^6T_{1g}$						
59 Γ_{7g}	2.956	310	52297		19.13	14 $^6T_{1g}$	16.06	14 $^6T_{2g}$				
56 Γ_{6g}	2.977	819	52301		14.96	12 $^6T_{2g}$	12.56	10 $^6T_{2g}$				
115 Γ_{8g}	2.952	243	52358		11.43	7 $^6T_{2g}$	11.32	12 $^6T_{2g}$				
116 Γ_{8g}	2.954	260	52367		17.54	8 $^6T_{2g}$						
117 Γ_{8g}	2.952	265	52383		16.29	9 $^6T_{2g}$						
60 Γ_{7g}	2.958	309	52415		19.55	11 $^6T_{1g}$						
118 Γ_{8g}	2.954	254	52455		10.61	7 $^6T_{2g}$						
119 Γ_{8g}	2.956	269	52502		11.83	13 $^6T_{2g}$						
61 Γ_{7g}	2.955	315	52514		14.33	14 $^6T_{1g}$	12.66	9 ^6E_g				
120 Γ_{8g}	2.958	267	52554		19.31	5 $^6T_{1g}$	12.56	7 $^6T_{1g}$				
57 Γ_{6g}	2.975	611	52579		28.07	9 $^6T_{2g}$						
121 Γ_{8g}	2.958	256	52615									
58 Γ_{6g}	2.975	576	52617		28.08	8 $^6T_{2g}$	10.43	2 $^6A_{2g}$				
59 Γ_{6g}	2.975	717	52669		13.98	13 $^6T_{1g}$	12.30	10 $^6T_{1g}$	10.62	10 $^6T_{2g}$	10.14	8 ^6E_g
62 Γ_{7g}	2.956	271	52689		16.89	9 $^6T_{1g}$	16.22	13 $^6T_{1g}$	10.04	12 $^6T_{2g}$		
122 Γ_{8g}	2.958	239	52720									
123 Γ_{8g}	2.960	245	52761		29.25	6 $^8T_{1g}$	22.44	5 $^8T_{2g}$				
63 Γ_{7g}	2.950	261	52814		20.09	6 $^8T_{1g}$	15.60	5 $^8T_{2g}$				
124 Γ_{8g}	2.975	562	52827		11.67	12 $^6T_{2g}$						
60 Γ_{6g}	2.975	777	52845		12.68	9 $^6T_{2g}$	12.37	3 $^6T_{2g}$	11.63	4 ^6E_g		
125 Γ_{8g}	2.959	244	52873									
64 Γ_{7g}	2.949	242	52893		26.86	6 $^8T_{1g}$	20.79	5 $^8T_{2g}$				
126 Γ_{8g}	2.957	236	52930		10.38	12 $^6T_{1g}$						
61 Γ_{6g}	2.975	740	52935		18.48	6 $^8T_{1g}$	13.14	5 $^8T_{2g}$				
127 Γ_{8g}	2.954	251	52960		12.94	5 $^8T_{2g}$	10.66	6 $^6T_{1g}$				
128 Γ_{8g}	2.952	256	52990		47.74	5 $^8T_{2g}$						
129 Γ_{8g}	2.953	263	53011									
62 Γ_{6g}	2.975	810	53020		35.15	6 $^8T_{1g}$	25.88	5 $^8T_{2g}$				
130 Γ_{8g}	2.951	263	53070		11.06	13 $^6T_{1g}$	10.42	14 $^6T_{1g}$				
65 Γ_{7g}	2.941	196	53088		58.87	6 $^8T_{1g}$						
131 Γ_{8g}	2.952	273	53088		10.09	7 $^6T_{2g}$						
63 Γ_{6g}	2.975	731	53121		20.71	11 $^6T_{2g}$	15.95	5 ^6E_g				
66 Γ_{7g}	2.943	203	53124		18.18	6 $^6T_{1g}$	13.36	3 ^6E_g				
132 Γ_{8g}	2.953	268	53144		11.93	16 $^6T_{1g}$						
133 Γ_{8g}	2.952	262	53191	0.01	14.48	14 $^6T_{1g}$	10.20	6 ^6E_g				
134 Γ_{8g}	2.953	277	53206	0.01	25.12	14 $^6T_{1g}$						
67 Γ_{7g}	2.944	188	53216	0.01	17.27	12 $^6T_{1g}$	10.03	6 $^6T_{1g}$				
135 Γ_{8g}	2.954	275	53256									
64 Γ_{6g}	2.975	684	53276		10.62	11 $^6T_{2g}$	10.38	8 $^6T_{2g}$				
68 Γ_{7g}	2.942	171	53305		14.98	12 $^6T_{1g}$						
136 Γ_{8g}	2.952	272	53308									
69 Γ_{7g}	2.952	220	53322		19.79	9 $^6T_{1g}$						
137 Γ_{8g}	2.954	281	53323									
65 Γ_{6g}	2.975	654	53335		15.97	14 $^6T_{2g}$	12.83	13 $^6T_{2g}$	11.24	9 $^6T_{2g}$		
138 Γ_{8g}	2.953	288	53347		12.91	7 $^6T_{2g}$	10.04	9 $^6T_{1g}$				
70 Γ_{7g}	2.949	217	53366		25.02	16 $^6T_{1g}$	14.84	15 $^6T_{2g}$	14.34	5 $^6A_{1g}$		
139 Γ_{8g}	2.952	291	53367									
71 Γ_{7g}	2.950	251	53374		17.70	11 $^6T_{1g}$	17.16	10 $^6T_{1g}$	12.01	13 $^6T_{1g}$		

66 Γ_{6g}	2.956	207	53382	13.74	15 $^6T_{2g}$	10.89	10 ^6E_g				
67 Γ_{6g}	2.954	214	53430	15.16	13 $^6T_{1g}$	11.94	5 ^6E_g	10.39	11 $^6T_{2g}$		
68 Γ_{6g}	2.952	227	53447	12.01	6 $^6T_{1g}$						
140 Γ_{8g}	2.953	277	53466	14.54	9 $^6T_{2g}$						
72 Γ_{7g}	2.947	240	53497	18.28	9 $^6T_{1g}$						
69 Γ_{6g}	2.948	252	53503								
141 Γ_{8g}	2.951	279	53518								
142 Γ_{8g}	2.950	282	53555	10.95	11 $^6T_{2g}$	10.62	16 $^6T_{1g}$				
143 Γ_{8g}	2.950	286	53569	12.76	9 ^6E_g						
73 Γ_{7g}	2.948	232	53590	10.07	6 ^6E_g						
70 Γ_{6g}	2.948	231	53615								
144 Γ_{8g}	2.952	274	53628	13.25	10 $^6T_{2g}$						
74 Γ_{7g}	2.947	243	53633	14.11	6 ^6E_g						
145 Γ_{8g}	2.950	287	53634	10.65	13 $^6T_{1g}$						
71 Γ_{6g}	2.952	229	53677								
75 Γ_{7g}	2.944	245	53680	31.15	9 $^6T_{2g}$	13.98	10 $^6T_{2g}$				
146 Γ_{8g}	2.951	286	53680								
147 Γ_{8g}	2.951	283	53738	11.27	6 ^6E_g	10.27	12 $^6T_{1g}$				
148 Γ_{8g}	2.950	284	53764	10.50	10 $^6T_{2g}$						
149 Γ_{8g}	2.952	281	53801	10.54	16 $^6T_{2g}$						
72 Γ_{6g}	2.975	637	53807	18.77	10 $^6T_{2g}$	14.59	9 ^6E_g				
150 Γ_{8g}	2.950	287	53814	15.06	15 $^6T_{1g}$	11.19	12 $^6T_{1g}$				
76 Γ_{7g}	2.947	224	53833	15.58	13 $^6T_{1g}$	13.11	14 $^6T_{1g}$				
151 Γ_{8g}	2.954	301	53848	16.03	17 $^6T_{2g}$						
152 Γ_{8g}	2.955	313	53871	11.53	12 $^6T_{2g}$	10.14	10 $^6T_{1g}$				
73 Γ_{6g}	2.955	227	53871								
153 Γ_{8g}	2.954	306	53918	13.45	15 $^6T_{1g}$						
154 Γ_{8g}	2.954	303	53955	57.87	6 $^8T_{1g}$	41.16	5 $^8T_{2g}$				
74 Γ_{6g}	2.975	711	53984	15.72	14 $^6T_{1g}$	11.25	6 ^6E_g	10.37	15 $^6T_{2g}$		
155 Γ_{8g}	2.952	311	53985								
156 Γ_{8g}	2.952	316	54007								
75 Γ_{6g}	2.975	784	54117	20.02	14 $^6T_{2g}$	19.00	13 $^6T_{2g}$	10.55	9 ^6E_g		
157 Γ_{8g}	2.953	299	54119	10.70	15 $^6T_{1g}$						
77 Γ_{7g}	2.975	797	54122	12.66	13 $^6T_{1g}$	10.04	16 $^6T_{1g}$				
158 Γ_{8g}	2.953	291	54173	46.91	5 $^8T_{2g}$	18.93	6 $^8T_{1g}$				
78 Γ_{7g}	2.975	845	54188								
76 Γ_{6g}	2.975	679	54237	15.67	15 $^6T_{2g}$						
159 Γ_{8g}	2.951	283	54255	13.31	14 $^6T_{2g}$	10.39	13 $^6T_{1g}$				
79 Γ_{7g}	2.975	753	54284	23.07	13 $^6T_{1g}$	13.81	5 ^6E_g	10.44	9 $^6T_{1g}$		
160 Γ_{8g}	2.950	284	54304	16.86	9 $^6T_{1g}$						
161 Γ_{8g}	2.951	299	54308	15.36	10 $^6T_{1g}$						
77 Γ_{6g}	2.975	643	54309	50.58	6 $^8T_{1g}$	45.81	5 $^8T_{2g}$				
162 Γ_{8g}	2.950	300	54323	16.47	7 $^6T_{2g}$	14.85	9 $^6T_{1g}$				
163 Γ_{8g}	2.953	300	54385	18.92	11 $^6T_{1g}$	11.94	11 $^6T_{2g}$	10.26	7 ^6E_g		
78 Γ_{6g}	2.975	706	54391	22.77	9 ^6E_g	10.96	4 $^6A_{2g}$				
80 Γ_{7g}	2.949	211	54419	36.83	5 $^8T_{2g}$	20.92	6 $^8T_{1g}$				
164 Γ_{8g}	2.952	298	54431	13.89	10 ^6E_g						
79 Γ_{6g}	2.975	616	54440	19.12	14 $^6T_{2g}$						
165 Γ_{8g}	2.950	291	54477	17.88	11 $^6T_{2g}$	15.48	12 $^6T_{1g}$	13.52	10 $^6T_{2g}$		
81 Γ_{7g}	2.942	224	54477	13.35	15 $^6T_{1g}$	10.09	5 $^8T_{2g}$				
166 Γ_{8g}	2.950	288	54507								
80 Γ_{6g}	2.975	665	54541	50.80	5 $^8T_{2g}$	14.97	6 $^8T_{1g}$				
167 Γ_{8g}	2.953	297	54554	31.40	16 $^6T_{2g}$	16.68	17 $^6T_{2g}$				
168 Γ_{8g}	2.954	313	54573	18.16	16 $^6T_{1g}$	10.60	17 $^6T_{2g}$				
82 Γ_{7g}	2.947	215	54578	15.14	14 $^6T_{1g}$	13.42	17 $^6T_{2g}$				
169 Γ_{8g}	2.954	293	54676	13.50	14 $^6T_{2g}$						
170 Γ_{8g}	2.955	322	54704	10.64	12 $^6T_{2g}$						
81 Γ_{6g}	2.975	775	54710	39.99	9 $^6T_{1g}$	21.47	7 $^6T_{2g}$				
83 Γ_{7g}	2.941	197	54711	15.62	10 $^6T_{1g}$	11.37	13 $^6T_{1g}$	11.33	7 ^6E_g	10.49	5 ^6E_g
171 Γ_{8g}	2.955	321	54734	15.83	12 $^6T_{2g}$						
82 Γ_{6g}	2.975	867	54842	14.01	12 $^6T_{2g}$	12.57	8 ^6E_g	10.80	13 $^6T_{2g}$		
84 Γ_{7g}	2.950	206	54858	14.47	10 ^6E_g	12.21	16 $^6T_{2g}$	10.99	15 $^6T_{1g}$		

85 Γ_{7g}	2.944	234	54911
83 Γ_{6g}	2.982	326	54932
172 Γ_{8g}	2.957	284	54943
173 Γ_{8g}	2.953	289	55008
84 Γ_{6g}	2.981	308	55057
174 Γ_{8g}	2.953	288	55062
86 Γ_{7g}	2.951	223	55131
175 Γ_{8g}	2.954	271	55144
176 Γ_{8g}	2.955	283	55158
177 Γ_{8g}	2.953	311	55175
87 Γ_{7g}	2.957	227	55216
85 Γ_{6g}	2.978	845	55244
178 Γ_{8g}	2.955	298	55273
88 Γ_{7g}	2.955	231	55299
179 Γ_{8g}	2.956	308	55307
86 Γ_{6g}	2.975	767	55309
87 Γ_{6g}	2.975	637	55329
89 Γ_{7g}	2.955	261	55369
180 Γ_{8g}	2.957	310	55404
88 Γ_{6g}	2.954	220	55468
89 Γ_{6g}	2.961	254	55531
181 Γ_{8g}	2.958	289	55536
182 Γ_{8g}	2.958	296	55563
90 Γ_{7g}	2.958	227	55572
90 Γ_{6g}	2.975	595	55648
91 Γ_{7g}	2.962	291	55661
92 Γ_{7g}	2.960	355	55664
93 Γ_{7g}	2.958	392	55669
183 Γ_{8g}	2.958	292	55762
91 Γ_{6g}	2.975	490	55783
94 Γ_{7g}	2.960	442	55791
184 Γ_{8g}	2.961	292	55834
185 Γ_{8g}	2.959	305	55868
186 Γ_{8g}	2.958	322	55934
92 Γ_{6g}	2.975	589	55985
95 Γ_{7g}	2.961	413	56094
187 Γ_{8g}	2.963	280	56139
188 Γ_{8g}	2.975	495	56213
93 Γ_{6g}	2.975	522	56221
189 Γ_{8g}	2.970	398	56270
94 Γ_{6g}	2.958	266	56302
190 Γ_{8g}	2.972	300	56465
95 Γ_{6g}	2.975	410	56483
191 Γ_{8g}	2.968	324	56498
192 Γ_{8g}	2.966	330	56579
96 Γ_{6g}	2.967	314	56587
96 Γ_{7g}	2.958	370	56615
193 Γ_{8g}	2.967	313	56701
97 Γ_{6g}	2.984	360	56830
194 Γ_{8g}	2.975	601	57034
98 Γ_{6g}	2.980	696	57039
195 Γ_{8g}	2.975	569	57146
97 Γ_{7g}	2.951	313	57220
98 Γ_{7g}	2.952	316	57296
196 Γ_{8g}	2.956	302	57311
99 Γ_{7g}	2.955	331	57408
197 Γ_{8g}	2.958	300	57424
198 Γ_{8g}	2.958	294	57503
100 Γ_{7g}	2.950	335	57545
199 Γ_{8g}	2.955	309	57547

11.82	5 $^6A_{1g}$	11.15	15 $^6T_{2g}$						
46.31	16 $^6T_{2g}$	13.70	17 $^6T_{2g}$						
17.18	13 $^6T_{1g}$	10.54	14 $^6T_{1g}$						
46.02	13 $^6T_{1g}$	19.07	12 $^6T_{2g}$						
25.02	15 $^6T_{2g}$	10.95	4 $^6A_{2g}$						
10.52	9 ^6E_g								
12.88	11 $^6T_{1g}$	10.77	12 $^6T_{2g}$	10.26	13 $^6T_{1g}$				
13.65	13 $^6T_{1g}$	12.68	14 $^6T_{2g}$	10.50	13 $^6T_{2g}$				
13.96	10 ^6E_g	10.73	17 $^6T_{2g}$						
28.54	12 $^6T_{1g}$	11.57	13 $^6T_{2g}$	10.53	8 ^6E_g				
16.52	15 $^6T_{1g}$	14.29	9 ^6E_g						
12.17	3 $^6A_{2g}$	11.65	11 $^6T_{2g}$	11.01	13 $^6T_{2g}$				
20.01	15 $^6T_{2g}$	13.98	14 $^6T_{1g}$						
26.59	13 $^6T_{2g}$	21.00	14 $^6T_{2g}$	19.84	13 $^6T_{1g}$				
12.10	15 $^6T_{2g}$	11.84	16 $^6T_{1g}$	11.54	17 $^6T_{2g}$				
14.63	11 $^6T_{2g}$	13.69	12 $^6T_{2g}$	13.15	13 $^6T_{2g}$				
22.57	17 $^6T_{2g}$	12.21	16 $^6T_{2g}$						
45.35	12 $^6T_{1g}$	12.16	8 ^6E_g						
23.49	14 $^6T_{2g}$	10.10	15 $^6T_{1g}$						
21.00	13 $^6T_{2g}$	16.42	8 ^6E_g	13.69	12 $^6T_{2g}$	12.52	11 $^6T_{2g}$		
20.32	14 $^6T_{2g}$	18.41	15 $^6T_{1g}$	12.03	17 $^6T_{2g}$	11.24	4 $^6A_{2g}$		
15.54	18 $^6T_{2g}$	15.20	11 ^6E_g	14.87	19 $^6T_{2g}$				
19.46	18 $^6T_{2g}$	15.00	11 ^6E_g	11.02	19 $^6T_{2g}$				
28.98	16 $^6T_{1g}$	17.74	10 ^6E_g						
24.98	19 $^6T_{2g}$	21.92	18 $^6T_{1g}$	19.08	5 $^6A_{2g}$				
37.26	16 $^6T_{1g}$	21.92	15 $^6T_{2g}$	19.95	5 $^6A_{1g}$				
37.22	16 $^6T_{2g}$	31.30	17 $^6T_{2g}$						
22.70	11 ^6E_g	12.36	19 $^6T_{1g}$	11.76	18 $^6T_{1g}$	10.85	19 $^6T_{2g}$		
10.78	17 $^6T_{1g}$								
29.60	16 $^6T_{1g}$	23.62	15 $^6T_{2g}$	13.61	5 $^6A_{1g}$				
28.05	16 $^6T_{2g}$	19.51	10 ^6E_g	13.50	15 $^6T_{2g}$				
27.68	11 ^6E_g	25.74	19 $^6T_{2g}$	10.01	18 $^6T_{1g}$				
23.87	17 $^6T_{2g}$	17.98	16 $^6T_{2g}$	17.24	10 ^6E_g	13.10	4 $^6A_{2g}$		
21.95	17 $^6T_{2g}$	16.73	16 $^6T_{2g}$	16.19	15 $^6T_{2g}$	10.89	10 ^6E_g		
42.89	17 $^6T_{2g}$	24.68	16 $^6T_{2g}$						
37.61	15 $^6T_{2g}$	22.63	16 $^6T_{1g}$	19.32	4 $^6A_{2g}$				
58.15	17 $^6T_{1g}$	13.14	11 ^6E_g						
18.71	19 $^6T_{2g}$	16.52	18 $^6T_{2g}$	14.59	5 $^6A_{2g}$	10.76	18 $^6T_{1g}$		
22.62	18 $^6T_{2g}$	15.98	18 $^6T_{1g}$	14.87	17 $^6T_{1g}$				
51.41	17 $^6T_{2g}$	14.24	16 $^6T_{2g}$	13.66	10 ^6E_g				
20.96	19 $^6T_{2g}$	16.20	17 $^6T_{1g}$	11.94	18 $^6T_{1g}$				
21.55	18 $^6T_{2g}$	20.64	11 ^6E_g	13.92	19 $^6T_{2g}$				
25.81	11 ^6E_g	22.36	6 $^6A_{1g}$	15.94	17 $^6T_{1g}$	12.83	12 ^6E_g		
18.36	18 $^6T_{2g}$	12.72	11 ^6E_g	11.80	19 $^6T_{2g}$	10.19	20 $^6T_{2g}$		
10.16	17 $^6T_{1g}$								
24.77	17 $^6T_{1g}$	11.00	19 $^6T_{1g}$	10.53	20 $^6T_{2g}$				
16.06	19 $^6T_{2g}$	13.35	17 $^6T_{1g}$	10.86	20 $^6T_{2g}$	10.13	11 ^6E_g		
23.92	11 ^6E_g	17.66	20 $^6T_{2g}$	10.96	13 ^6E_g	10.17	12 ^6E_g		
40.26	17 $^6T_{1g}$	11.97	18 $^6T_{1g}$						
15.88	17 $^6T_{1g}$	15.82	18 $^6T_{2g}$	11.18	11 ^6E_g				
17.91	18 $^6T_{2g}$	15.24	18 $^6T_{1g}$	13.09	5 $^6A_{2g}$				
23.62	17 $^6T_{1g}$	23.61	11 ^6E_g						
45.02	18 $^6T_{2g}$	14.84	19 $^6T_{2g}$	11.30	13 ^6E_g				
20.08	17 $^6T_{1g}$	17.22	18 $^6T_{2g}$	13.73	19 $^6T_{1g}$				
31.10	18 $^6T_{2g}$	13.41	19 $^6T_{1g}$	12.99	20 $^6T_{1g}$				
50.03	6 $^6A_{1g}$	20.75	17 $^6T_{1g}$						
27.22	18 $^6T_{2g}$	10.12	12 ^6E_g						
17.43	17 $^6T_{1g}$	16.43	6 $^6A_{1g}$	12.95	18 $^6T_{1g}$	12.80	12 ^6E_g		
12.76	18 $^6T_{2g}$	12.57	6 $^6A_{1g}$						
33.31	17 $^6T_{1g}$	12.50	18 $^6T_{2g}$						
20.56	18 $^6T_{1g}$	16.65	13 ^6E_g	13.94	19 $^6T_{1g}$	13.87	18 $^6T_{2g}$		
17.15	6 $^6A_{1g}$	12.85	18 $^6T_{1g}$						

99 Γ_{6g}	2.976	704	57598	23.61	20 $^6T_{2g}$	14.94	18 $^6T_{2g}$	13.72	19 $^6T_{2g}$		
101 Γ_{7g}	2.951	330	57629	17.79	18 $^6T_{1g}$	12.20	20 $^6T_{2g}$	11.51	12 ^6E_g	10.74	13 ^6E_g
200 Γ_{8g}	2.955	302	57656	19.89	19 $^6T_{1g}$	18.64	20 $^6T_{2g}$	11.63	13 ^6E_g		
100 Γ_{6g}	2.975	700	57710	31.77	19 $^6T_{2g}$	15.34	20 $^6T_{2g}$				
201 Γ_{8g}	2.956	291	57720	22.32	19 $^6T_{2g}$	14.94	18 $^6T_{2g}$	12.37	19 $^6T_{1g}$		
202 Γ_{8g}	2.954	304	57823	17.04	19 $^6T_{2g}$	13.31	19 $^6T_{1g}$	10.29	18 $^6T_{1g}$		
102 Γ_{7g}	2.951	311	57919	21.13	19 $^6T_{1g}$	15.24	13 ^6E_g	15.17	21 $^6T_{2g}$	11.05	20 $^6T_{1g}$
				10.40	20 $^6T_{2g}$						
203 Γ_{8g}	2.957	298	57929	19.44	12 ^6E_g	10.60	20 $^6T_{2g}$				
103 Γ_{7g}	2.956	365	57932	32.20	18 $^6T_{1g}$						
101 Γ_{6g}	2.952	263	57946	49.06	17 $^6T_{1g}$						
204 Γ_{8g}	2.957	319	57995	49.58	20 $^6T_{2g}$	14.51	13 ^6E_g				
205 Γ_{8g}	2.957	328	58029	20.82	19 $^6T_{1g}$	14.74	20 $^6T_{2g}$	10.54	21 $^6T_{2g}$	10.41	13 ^6E_g
206 Γ_{8g}	2.957	346	58047	20.67	13 ^6E_g	15.53	18 $^6T_{1g}$	11.11	19 $^6T_{2g}$		
104 Γ_{7g}	2.954	395	58074	23.50	19 $^6T_{1g}$	18.98	21 $^6T_{2g}$	10.19	20 $^6T_{1g}$		
102 Γ_{6g}	2.958	237	58131	41.19	12 ^6E_g	10.59	18 $^6T_{2g}$				
207 Γ_{8g}	2.955	347	58146	21.62	18 $^6T_{1g}$	14.18	21 $^6T_{2g}$	12.62	19 $^6T_{2g}$		
103 Γ_{6g}	2.954	303	58183	16.92	20 $^6T_{2g}$	15.86	21 $^6T_{2g}$				
105 Γ_{7g}	2.955	396	58249	54.72	19 $^6T_{1g}$	14.16	12 ^6E_g	10.87	18 $^6T_{1g}$		
208 Γ_{8g}	2.956	340	58276	17.29	18 $^6T_{1g}$	15.35	21 $^6T_{2g}$	14.07	13 ^6E_g		
106 Γ_{7g}	2.951	456	58328	32.27	21 $^6T_{2g}$	20.28	20 $^6T_{2g}$	15.77	18 $^6T_{1g}$	10.15	20 $^6T_{1g}$
209 Γ_{8g}	2.956	345	58363	36.16	19 $^6T_{1g}$	12.65	18 $^6T_{1g}$	10.08	20 $^6T_{1g}$	10.02	21 $^6T_{2g}$
104 Γ_{6g}	2.955	281	58375	19.38	18 $^6T_{1g}$	17.46	19 $^6T_{2g}$	15.80	6 $^6A_{2g}$		
210 Γ_{8g}	2.955	337	58498	25.05	19 $^6T_{1g}$	16.90	20 $^6T_{1g}$	11.23	6 $^6A_{2g}$	10.55	12 ^6E_g
105 Γ_{6g}	2.953	295	58524	51.37	19 $^6T_{1g}$	17.11	18 $^6T_{1g}$				
211 Γ_{8g}	2.953	333	58622	19.24	19 $^6T_{1g}$	15.75	20 $^6T_{1g}$	15.26	18 $^6T_{1g}$		
212 Γ_{8g}	2.954	347	58708	27.01	20 $^6T_{1g}$	20.41	19 $^6T_{1g}$	18.21	18 $^6T_{1g}$	10.76	21 $^6T_{2g}$
106 Γ_{6g}	2.958	268	58790	24.13	21 $^6T_{2g}$	21.96	13 ^6E_g				
107 Γ_{6g}	2.955	325	58829	41.84	20 $^6T_{1g}$	33.20	21 $^6T_{2g}$				
213 Γ_{8g}	2.953	338	58834	31.38	20 $^6T_{1g}$	18.44	21 $^6T_{2g}$	11.08	18 $^6T_{1g}$		
214 Γ_{8g}	2.952	352	58893	47.27	20 $^6T_{1g}$	12.95	20 $^6T_{2g}$				
108 Γ_{6g}	2.952	349	58942	34.37	6 $^6A_{2g}$	14.24	21 $^6T_{2g}$	11.56	20 $^6T_{2g}$	11.29	20 $^6T_{1g}$
215 Γ_{8g}	2.954	347	59006	36.89	20 $^6T_{1g}$	18.19	21 $^6T_{2g}$	11.97	13 ^6E_g		
109 Γ_{6g}	2.954	376	59015	32.50	21 $^6T_{2g}$	19.33	20 $^6T_{2g}$	14.06	13 ^6E_g		
110 Γ_{6g}	2.959	483	59039	52.25	21 $^6T_{1g}$	26.80	22 $^6T_{2g}$				
216 Γ_{8g}	2.953	354	59105	28.63	21 $^6T_{2g}$	21.25	20 $^6T_{1g}$	16.64	6 $^6A_{2g}$		
107 Γ_{7g}	2.954	327	59108	54.71	20 $^6T_{1g}$						
108 Γ_{7g}	2.955	338	59149	50.30	20 $^6T_{1g}$	20.14	13 ^6E_g				
217 Γ_{8g}	2.955	361	59167	69.72	21 $^6T_{2g}$						
218 Γ_{8g}	2.957	465	59287	44.77	22 $^6T_{2g}$	35.24	21 $^6T_{1g}$				
219 Γ_{8g}	2.959	497	59432	33.90	22 $^6T_{2g}$	23.95	21 $^6T_{1g}$	20.87	7 $^6A_{2g}$		
111 Γ_{6g}	2.961	507	59472	63.38	7 $^6A_{2g}$	14.46	20 $^6T_{2g}$				
109 Γ_{7g}	2.960	491	59493	68.66	21 $^6T_{1g}$						
220 Γ_{8g}	2.960	511	59507	58.09	7 $^6A_{2g}$	13.84	20 $^6T_{2g}$	11.59	22 $^6T_{2g}$		
110 Γ_{7g}	2.959	527	59593	69.19	21 $^6T_{1g}$						
221 Γ_{8g}	2.960	520	59612	62.76	21 $^6T_{1g}$	15.73	22 $^6T_{2g}$				
222 Γ_{8g}	2.961	496	59875	63.67	21 $^6T_{1g}$	21.11	22 $^6T_{2g}$				
111 Γ_{7g}	2.961	518	59887	74.46	22 $^6T_{2g}$	23.11	21 $^6T_{1g}$				
112 Γ_{6g}	2.962	510	59936	54.62	22 $^6T_{2g}$	23.82	21 $^6T_{1g}$				
223 Γ_{8g}	2.961	507	59960	43.92	22 $^6T_{2g}$	37.61	21 $^6T_{1g}$				
224 Γ_{8g}	2.961	518	59976	69.80	22 $^6T_{2g}$	18.47	21 $^6T_{1g}$				
113 Γ_{6g}	2.961	522	60005	78.08	22 $^6T_{2g}$						

$4f^7$ excited states

$4f^7(^6P_{3/2,5/2,7/2})$ [c]											
2 Γ_{7u}	2.969	267	30115	89.46	1 $^6T_{1u}$						
2 Γ_{8u}	2.969	267	30140	89.86	1 $^6T_{1u}$						
3 Γ_{8u}	2.969	267	30502	94.04	1 $^6T_{1u}$						
2 Γ_{6u}	2.969	267	30767	85.40	1 $^6T_{1u}$	11.97	3 $^6T_{2u}$				
4 Γ_{8u}	2.969	267	30783	85.64	1 $^6T_{1u}$						
3 Γ_{7u}	2.969	267	30807	85.97	1 $^6T_{1u}$	10.31	2 ^6E_u				

$4f^7(^6I_{7/2,9/2,11/2,13/2,15/2,17/2})$ [c]												
5 Γ_{8u}	2.969	266	34662	75.31	1 $^6T_{2u}$	13.77	1 ^6E_u					
3 Γ_{6u}	2.969	265	34663	75.20	1 $^6T_{2u}$	19.66	1 ^6E_u					
4 Γ_{7u}	2.969	266	34701	45.13	2 $^6T_{1u}$	24.63	2 $^6T_{2u}$	21.83	1 $^6A_{1u}$			
6 Γ_{8u}	2.969	265	34701	79.06	1 $^6T_{2u}$	11.54	1 ^6E_u					
4 Γ_{6u}	2.969	266	34707	84.83	1 $^6T_{2u}$							
7 Γ_{8u}	2.969	266	34729	91.58	1 $^6T_{2u}$							
8 Γ_{8u}	2.969	265	34743	39.27	2 $^6T_{1u}$	25.78	1 $^6A_{1u}$	23.97	2 $^6T_{2u}$			
5 Γ_{7u}	2.968	262	34750	85.94	1 $^6T_{2u}$							
9 Γ_{8u}	2.969	264	34794	43.91	2 $^6T_{1u}$	36.55	2 $^6T_{2u}$	15.93	1 $^6A_{1u}$			
5 Γ_{6u}	2.969	263	34817	52.44	2 $^6T_{2u}$	40.64	2 $^6T_{1u}$					
6 Γ_{7u}	2.969	265	34842	36.06	1 $^6A_{1u}$	31.52	2 $^6T_{2u}$	26.69	2 $^6T_{1u}$			
10 Γ_{8u}	2.969	264	34861	69.66	2 $^6T_{1u}$	21.43	2 $^6T_{2u}$					
6 Γ_{6u}	2.969	263	34892	84.76	2 $^6T_{2u}$	10.03	2 $^6T_{1u}$					
7 Γ_{7u}	2.969	265	34904	38.20	2 $^6T_{1u}$	34.71	1 ^6E_u	15.76	1 $^6A_{1u}$	11.20	2 $^6T_{2u}$	
11 Γ_{8u}	2.969	264	34936	44.95	2 $^6T_{2u}$	17.63	1 ^6E_u	16.79	2 $^6T_{1u}$	12.79	1 $^6A_{1u}$	
25 Γ_{7g}	2.937	263	34936	48.50	1 $^6A_{1g}$	40.93	3 $^6T_{1g}$					
12 Γ_{8u}	2.969	265	34945	37.00	2 $^6T_{1u}$	28.41	2 $^6T_{2u}$	14.78	1 ^6E_u	13.79	1 $^6A_{1u}$	
49 Γ_{8g}	2.937	263	34951	46.40	1 $^6A_{1g}$	41.99	3 $^6T_{1g}$					
13 Γ_{8u}	2.969	265	34960	68.50	1 ^6E_u	15.10	2 $^6T_{2u}$					
8 Γ_{7u}	2.969	265	34965	59.86	1 ^6E_u	35.11	2 $^6T_{1u}$					
14 Γ_{8u}	2.969	264	34988	56.38	1 ^6E_u	13.13	2 $^6T_{1u}$	12.15	2 $^6T_{2u}$			
7 Γ_{6u}	2.969	265	35000	59.73	1 ^6E_u	13.35	1 $^6T_{2u}$	10.87	1 $^6A_{2u}$			
9 Γ_{7u}	2.969	265	35044	53.10	2 $^6T_{1u}$	23.30	1 $^6A_{1u}$	22.27	2 $^6T_{2u}$			
8 Γ_{6u}	2.969	264	35048	30.67	2 $^6T_{2u}$	26.82	2 $^6T_{1u}$	18.43	1 ^6E_u	15.74	1 $^6A_{2u}$	
15 Γ_{8u}	2.969	264	35054	35.88	2 $^6T_{1u}$	27.22	2 $^6T_{2u}$	14.08	1 ^6E_u	12.78	1 $^6A_{1u}$	
16 Γ_{8u}	2.969	262	35078	69.86	2 $^6T_{2u}$	20.05	2 $^6T_{1u}$					
17 Γ_{8u}	2.969	267	35081	74.24	1 $^6A_{2u}$							
9 Γ_{6u}	2.969	266	35084	64.50	1 $^6A_{2u}$	18.15	2 $^6T_{2u}$	10.02	2 $^6T_{1u}$			
$4f^7(^6D_{1/2,3/2,5/2,7/2})$ [c]												
10 Γ_{6u}	2.968	265	37408	94.87	3 $^6T_{2u}$							
18 Γ_{8u}	2.968	266	37588	68.67	3 $^6T_{2u}$	31.05	2 ^6E_u					
19 Γ_{8u}	2.968	265	37625	76.86	3 $^6T_{2u}$	23.08	2 ^6E_u					
11 Γ_{6u}	2.968	268	37629	89.42	2 ^6E_u	10.54	3 $^6T_{2u}$					
20 Γ_{8u}	2.968	267	37910	47.49	3 $^6T_{2u}$	46.71	2 ^6E_u					
10 Γ_{7u}	2.968	265	38271	86.33	3 $^6T_{2u}$	10.66	1 $^6T_{1u}$					
21 Γ_{8u}	2.968	266	38363	50.60	3 $^6T_{2u}$	39.07	2 ^6E_u	10.29	1 $^6T_{1u}$			
12 Γ_{6u}	2.968	265	38473	82.55	3 $^6T_{2u}$	12.28	1 $^6T_{1u}$					
22 Γ_{8u}	2.968	267	38503	48.62	2 ^6E_u	39.45	3 $^6T_{2u}$	11.74	1 $^6T_{1u}$			
11 Γ_{7u}	2.968	268	38527	85.48	2 ^6E_u	11.57	1 $^6T_{1u}$					

Eu^{3+}-doped SrS

$4f^6(^7F_{0-6})$												
1 A_{1g}	2.800	286	0	47.13	1 $7T_{1g}$	36.92	1 $7T_{2g}$	10.12	1 $7A_{2g}$			
1 T_{1g}	2.800	286	373	49.18	1 $7T_{1g}$	36.47	1 $7T_{2g}$					
1 E_g	2.799	285	963	67.33	1 $7T_{1g}$	29.01	1 $7T_{2g}$					
1 T_{2g}	2.800	287	1137	42.70	1 $7T_{1g}$	39.80	1 $7T_{2g}$	13.86	1 $7A_{2g}$			
1 A_{2g}	2.799	285	1956	54.65	1 $7T_{1g}$	42.86	1 $7T_{2g}$					
2 T_{2g}	2.800	287	2017	46.15	1 $7T_{1g}$	32.05	1 $7T_{2g}$	19.23	1 $7A_{2g}$			
2 T_{1g}	2.800	287	2066	46.60	1 $7T_{2g}$	36.54	1 $7T_{1g}$	14.32	1 $7A_{2g}$			
3 T_{2g}	2.799	286	2951	70.46	1 $7T_{1g}$	23.92	1 $7T_{2g}$					
2 E_g	2.800	285	3170	74.60	1 $7T_{2g}$	23.36	1 $7T_{1g}$					
3 T_{1g}	2.800	288	3190	43.79	1 $7T_{2g}$	29.53	1 $7T_{1g}$	24.61	1 $7A_{2g}$			
2 A_{1g}	2.800	291	3211	50.44	1 $7A_{2g}$	37.56	1 $7T_{1g}$					
4 T_{1g}	2.799	286	4184	52.40	1 $7T_{1g}$	42.78	1 $7T_{2g}$					
3 E_g	2.799	285	4216	51.01	1 $7T_{2g}$	46.64	1 $7T_{1g}$					
4 T_{2g}	2.800	288	4247	62.26	1 $7T_{1g}$	25.79	1 $7A_{2g}$					
5 T_{1g}	2.800	287	4400	74.15	1 $7T_{2g}$	12.01	1 $7T_{1g}$	11.47	1 $7A_{2g}$			
4 E_g	2.799	285	5387	56.56	1 $7T_{1g}$	40.14	1 $7T_{2g}$					

5 T_{2g}	2.799	286	5407	52.28	1 $7T_{1g}$	43.48	1 $7T_{2g}$						
2 A_{2g}	2.799	285	5457	54.22	1 $7T_{2g}$	42.46	1 $7T_{1g}$						
6 T_{2g}	2.800	289	5619	45.05	1 $7T_{2g}$	33.67	1 $7A_{2g}$	17.99	1 $7T_{1g}$				
6 T_{1g}	2.800	289	5650	47.57	1 $7T_{2g}$	34.76	1 $7A_{2g}$	14.36	1 $7T_{1g}$				
3 A_{1g}	2.800	290	5676	48.77	1 $7T_{2g}$	36.45	1 $7A_{2g}$	11.47	1 $7T_{1g}$				
$4f^6(^5D_{0-3})$													
4 A_{1g}	2.798	285	19973	57.46	1 $5T_{2g}$	36.83	1 $5E_g$						
7 T_{1g}	2.798	285	20781	58.04	1 $5T_{2g}$	36.80	1 $5E_g$						
7 T_{2g}	2.797	285	22428	70.36	1 $5T_{2g}$	25.21	1 $5E_g$						
5 E_g	2.798	284	22521	54.04	1 $5E_g$	41.47	1 $5T_{2g}$						
8 T_{1g}	2.797	285	25111	85.65	1 $5T_{2g}$	10.04	1 $5E_g$						
8 T_{2g}	2.797	285	25153	49.90	1 $5E_g$	45.77	1 $5T_{2g}$						
3 A_{2g}	2.797	284	25190	95.44	1 $5E_g$								
$4f^6(^5D_4,^5L_{6-10},^5G_{2-6})$													
9 T_{2g}	2.797	285	28323	21.94	1 $5T_{1g}$	20.69	2 $5E_g$	16.46	4 $5T_{2g}$	14.24	2 $5T_{1g}$		
5 A_{1g}	2.797	284	28343	51.00	3 $5T_{2g}$	34.25	3 $5E_g$	11.53	4 $5T_{2g}$				
4 A_{2g}	2.797	285	28345	36.80	1 $5T_{1g}$	35.07	2 $5E_g$	14.96	2 $5T_{1g}$				
9 T_{1g}	2.797	284	28362	31.55	3 $5T_{2g}$	14.41	3 $5E_g$	13.19	2 $5T_{1g}$	11.83	1 $5T_{1g}$		
				10.75	4 $5T_{2g}$								
10 T_{2g}	2.797	284	28494	43.66	1 $5T_{1g}$	16.42	2 $5E_g$	10.07	4 $5T_{1g}$				
11 T_{2g}	2.797	285	28495	42.72	1 $5T_{1g}$	25.53	1 $5A_{1g}$						
6 E_g	2.797	285	28536	45.16	1 $5T_{1g}$	22.35	1 $5A_{1g}$	18.14	2 $5E_g$				
12 T_{2g}	2.797	285	28572	32.46	4 $5T_{2g}$	15.97	1 $5T_{1g}$	14.79	2 $5E_g$				
10 T_{1g}	2.797	285	28618	43.04	1 $5T_{1g}$	23.45	2 $5T_{2g}$						
7 E_g	2.797	284	28625	21.65	3 $5T_{2g}$	17.24	3 $5T_{1g}$	16.86	2 $5T_{1g}$	13.51	4 $5E_g$		
				13.26	4 $5T_{2g}$								
13 T_{2g}	2.797	283	28629	22.30	3 $5T_{2g}$	17.04	2 $5T_{1g}$	16.91	3 $5T_{1g}$	13.25	4 $5E_g$		
				12.24	4 $5T_{2g}$								
6 A_{1g}	2.797	281	28703	61.44	2 $5E_g$	14.13	2 $5T_{2g}$	13.04	5 $5T_{2g}$				
8 E_g	2.798	284	28706	32.23	3 $5T_{1g}$	17.07	4 $5T_{2g}$	17.02	4 $5E_g$	11.43	2 $5A_{1g}$		
5 A_{2g}	2.798	284	28715	42.37	2 $5T_{1g}$	20.16	4 $5E_g$	11.33	2 $5E_g$	10.61	3 $5E_g$		
14 T_{2g}	2.798	284	28825	75.92	2 $5T_{2g}$								
11 T_{1g}	2.797	285	28934	19.48	3 $5T_{2g}$	19.11	2 $5T_{1g}$	11.08	1 $5E_g$	10.83	1 $5T_{2g}$		
7 A_{1g}	2.797	284	28954	55.22	1 $5E_g$	35.33	1 $5T_{2g}$						
9 E_g	2.797	284	29001	29.36	3 $5E_g$	17.87	2 $5T_{2g}$	12.75	2 $5T_{1g}$	11.80	4 $5T_{2g}$		
12 T_{1g}	2.797	285	29015	30.02	1 $5E_g$	29.87	1 $5T_{2g}$	12.65	2 $5T_{2g}$				
15 T_{2g}	2.797	284	29029	28.53	3 $5T_{2g}$	14.21	2 $5T_{1g}$	12.61	4 $5T_{2g}$	11.17	4 $5E_g$		
10 E_g	2.797	284	29066	38.73	1 $5T_{2g}$	29.03	1 $5E_g$	12.20	2 $5E_g$				
16 T_{2g}	2.798	285	29110	51.85	1 $5T_{2g}$	13.39	1 $5E_g$	11.34	2 $5T_{2g}$				
17 T_{2g}	2.797	285	29122	33.57	2 $5E_g$	22.85	1 $5T_{1g}$	10.95	2 $5T_{2g}$	10.05	5 $5T_{2g}$		
18 T_{2g}	2.797	285	29131	21.75	1 $5T_{1g}$	20.33	1 $5A_{1g}$	15.08	2 $5T_{2g}$				
13 T_{1g}	2.797	283	29188	25.95	4 $5T_{2g}$	23.24	4 $5E_g$	19.51	3 $5T_{1g}$				
6 A_{2g}	2.797	285	29207	44.48	3 $5T_{1g}$	23.59	3 $5E_g$	22.51	4 $5E_g$				
11 E_g	2.797	284	29226	46.55	2 $5T_{2g}$	12.68	3 $5E_g$						
14 T_{1g}	2.798	285	29239	39.81	2 $5T_{2g}$	11.93	1 $5T_{1g}$						
19 T_{2g}	2.798	284	29250	29.67	3 $5T_{1g}$	19.79	2 $5A_{1g}$	19.09	2 $5T_{1g}$	10.73	3 $5E_g$		
12 E_g	2.797	285	29690	55.48	3 $5T_{2g}$	18.63	2 $5T_{1g}$	11.21	4 $5T_{2g}$				
20 T_{2g}	2.797	285	29716	30.57	2 $5T_{1g}$	29.09	3 $5E_g$	13.62	4 $5T_{2g}$				
15 T_{1g}	2.797	284	29792	25.37	3 $5T_{2g}$	21.47	4 $5T_{2g}$	13.16	2 $5T_{1g}$	12.96	3 $5E_g$		
				12.61	4 $5E_g$								
21 T_{2g}	2.797	285	29886	37.77	3 $5T_{1g}$	13.78	4 $5T_{2g}$	12.81	4 $5E_g$	10.21	3 $5T_{2g}$		
16 T_{1g}	2.798	284	29907	45.98	3 $5T_{1g}$	25.36	2 $5T_{1g}$	17.30	4 $5T_{2g}$				
8 A_{1g}	2.797	285	29956	55.57	4 $5E_g$	21.20	4 $5T_{2g}$	16.77	3 $5T_{2g}$				
13 E_g	2.797	283	30010	20.58	1 $5T_{1g}$	15.63	2 $5A_{1g}$	12.25	4 $5E_g$				
22 T_{2g}	2.797	284	30049	14.01	1 $5T_{1g}$	13.06	2 $5A_{1g}$	12.20	1 $5A_{1g}$	11.63	2 $5T_{1g}$		
14 E_g	2.797	285	30050	35.89	1 $5T_{1g}$	23.50	2 $5E_g$	13.78	1 $5A_{1g}$				
7 A_{2g}	2.797	285	30087	38.07	1 $5T_{1g}$	35.69	2 $5E_g$	12.27	4 $5T_{1g}$				
9 A_{1g}	2.797	284	30209	59.14	2 $5T_{2g}$	15.13	5 $5E_g$	14.91	2 $5E_g$				
17 T_{1g}	2.797	285	30209	53.06	2 $5T_{2g}$								
23 T_{2g}	2.798	284	30233	46.73	2 $5T_{2g}$	12.48	1 $5T_{1g}$	12.34	5 $5T_{1g}$				
8 A_{2g}	2.797	285	30652	42.03	3 $5T_{2g}$	24.71	4 $5T_{2g}$	22.18	2 $5T_{1g}$				

18 T_{1g}	2.797	285	30653	42.08	3 $5T_{2g}$	24.69	4 $5T_{2g}$	22.13	2 $5T_{1g}$		
24 T_{2g}	2.797	285	30656	28.86	2 $5T_{1g}$	27.16	3 $5T_{2g}$	22.27	4 $5T_{2g}$	10.84	3 $5E_g$
10 A_{1g}	2.797	284	30738	32.22	3 $5E_g$	29.71	4 $5E_g$	28.59	3 $5T_{2g}$		
19 T_{1g}	2.797	285	30751	40.27	3 $5T_{1g}$	21.82	4 $5T_{2g}$	13.84	3 $5E_g$	10.86	3 $5T_{2g}$
15 E_g	2.797	285	30819	28.81	4 $5E_g$	25.41	4 $5T_{2g}$	18.20	2 $5A_{1g}$		
25 T_{2g}	2.798	284	30895	27.89	2 $5A_{1g}$	23.94	2 $5T_{1g}$	18.43	4 $5T_{2g}$	12.98	4 $5E_g$
				10.47	3 $5T_{1g}$						
20 T_{1g}	2.798	284	30926	42.40	3 $5T_{1g}$	38.25	4 $5E_g$				
21 T_{1g}	2.797	285	31709	56.79	3 $5T_{2g}$	20.63	3 $5E_g$	11.73	2 $5T_{1g}$		
16 E_g	2.797	285	31757	30.99	3 $5T_{2g}$	29.07	2 $5T_{1g}$	28.90	3 $5E_g$		
22 T_{1g}	2.797	285	31772	35.81	2 $5T_{1g}$	26.96	3 $5E_g$	17.68	3 $5T_{2g}$	10.42	4 $5T_{2g}$
11 A_{1g}	2.797	285	31812	61.93	4 $5T_{2g}$	26.16	3 $5E_g$	10.33	4 $5E_g$		
23 T_{1g}	2.797	285	31856	38.21	4 $5T_{2g}$	24.23	2 $5T_{1g}$	14.89	4 $5E_g$	13.27	3 $5T_{1g}$
26 T_{2g}	2.797	285	31897	34.64	4 $5T_{2g}$	29.53	3 $5T_{1g}$	11.77	4 $5E_g$		
9 A_{2g}	2.798	284	32058	51.10	4 $5E_g$	36.67	3 $5T_{1g}$	11.99	2 $5T_{1g}$		
27 T_{2g}	2.798	284	32094	40.56	3 $5T_{1g}$	26.56	4 $5E_g$	24.33	2 $5A_{1g}$		
17 E_g	2.798	284	32106	40.50	3 $5T_{1g}$	30.54	2 $5A_{1g}$	21.63	4 $5E_g$		

[a] Absorption oscillator strengths for 1 $\Gamma_{6u,8u,7u} \rightarrow i$ transitions are calculated at $d_{\mathrm{Eu-F}}$= 2.950 Å; the reference value is f_{ref} = 1.906×10^{-3}. Emission oscillator strengths for 1 $\Gamma_{8g} \rightarrow$1 Γ_{6u},1 Γ_{8u},1 Γ_{7u} and radiative emission lifetime are calculated at $d_{\mathrm{Eu-F}}$= 2.900 Å; the reference value is f_{ref} = 9.517×10^{-4}.
[b] The analyses of the wave functions have been done at $d_{\mathrm{Eu-F}}$= 2.900 Å ($4f^7$), 2.900 Å ($4f^6(5d^1 + 6sa^1_{1g})$), 2.800 Å ($4f^6$).
[c] C.f. Table S7.
[d] C.f. Table S8.

TABLE S14: Spectroscopic constants and analyses of the spin-orbit wave functions of the ground and lowest lying excited states of Eu^{2+} and Eu^{3+} -doped BaS octahedral defects. Eu–S bond distances ($d_{\mathrm{Eu-S},e}$ in Å), EuS_6 breathing mode harmonic vibrational frequencies ($\omega_{a_{1g}}$ in cm^{-1}), minimum-to-minimum energy differences (T_e in cm^{-1}), and relative absorption and emission oscillator strengths (f_i^{abs}/f_{ref} and f_i^{emi}/f_{ref}) are given. Calculated radiative emission lifetime for the $4f^6(^7F_J)5de_g^1$ – 1 Γ_{8g} excited state is 0.263 μs. Local distortion around the Eu^{2+}impurity, relative to experimental crystal structure d_{Ba-F}= 3.187 Å, is $d_{\mathrm{Eu-S},e}(1\Gamma_{6u}) - d_{\mathrm{Ba-S}} = -0.100$; ionic radii mismatch is +0.17 Å[31]. See Fig. 3, S3 and text for details.

State	$d_{\mathrm{Eu-S},e}$	$\omega_{a_{1g}}$	T_e	f_i^{abs}/f_{ref} [a]	f_i^{emi}/f_{ref} [a]	weights of terms larger than 10% [b]							
Eu^{2+}-doped BaS													
$4f^7(^8S_{7/2})$ [c]													
1 Γ_{6u}	3.087	204	0		1.00	97.73	1 $^8A_{1u}$						
1 Γ_{8u}	3.087	204	0		0.42	97.73	1 $^8A_{1u}$						
1 Γ_{7u}	3.087	204	0		0.07	97.74	1 $^8A_{1u}$						
$4f^6(5d + ITE_{a_{1g}})^1$ excited states													
$4f^6(^7F_J)5dt_{2g}^1$ High-Spin coupling [d]													
1 Γ_{8g}	3.037	196	20356	1.00		37.31	1 $^8T_{1g}$	24.88	1 $^8T_{2g}$	22.01	1 ^8E_g	12.70	2 $^8T_{1g}$
2 Γ_{8g}	3.036	196	20624	0.64		34.34	1 $^8T_{2g}$	32.70	1 $^8T_{1g}$	20.38	1 ^8E_g		
1 Γ_{7g}	3.035	196	20837	1.28		55.81	1 $^8T_{2g}$	30.04	2 $^8T_{1g}$				
3 Γ_{8g}	3.035	196	21115	1.52		40.40	1 $^8T_{2g}$	22.77	1 ^8E_g	19.82	1 $^8T_{1g}$	12.55	2 $^8T_{1g}$
1 Γ_{6g}	3.035	196	21144	0.36		51.49	1 $^8T_{1g}$	22.58	1 ^8E_g	11.58	1 $^8T_{2g}$	10.33	2 $^8T_{1g}$
2 Γ_{7g}	3.035	196	21381	2.41		40.89	2 $^8T_{1g}$	33.02	1 $^8T_{2g}$	15.13	1 ^8E_g		
4 Γ_{8g}	3.035	196	21689	1.60		33.38	1 $^8T_{2g}$	31.69	1 $^8T_{1g}$	15.40	2 $^8T_{1g}$	14.06	1 ^8E_g
2 Γ_{6g}	3.035	196	21760	0.53		49.72	1 $^8T_{1g}$	26.38	1 ^8E_g				
5 Γ_{8g}	3.034	196	21963	5.61		44.20	2 $^8T_{1g}$	27.44	1 $^8T_{2g}$	21.53	1 $^8T_{1g}$		
6 Γ_{8g}	3.034	195	22410	2.07		49.45	1 $^8T_{1g}$	19.11	1 ^8E_g	13.63	2 $^8T_{1g}$	10.14	1 $^8T_{2g}$
3 Γ_{7g}	3.034	196	22529	2.82		39.36	2 $^8T_{1g}$	22.32	1 ^8E_g	14.85	1 $^8T_{2g}$	10.80	1 $^8T_{1g}$
7 Γ_{8g}	3.034	196	22543	3.79		48.22	1 $^8T_{2g}$	20.41	2 $^8T_{1g}$	16.72	1 $^8T_{1g}$		
3 Γ_{6g}	3.034	196	22749	1.81		40.39	2 $^8T_{1g}$	36.97	1 $^8T_{2g}$	18.16	1 $^8T_{1g}$		
4 Γ_{6g}	3.032	196	23081	0.08		23.12	2 $^8T_{2g}$	22.39	3 $^8T_{1g}$	20.54	2 ^8E_g	10.38	2 $^8T_{1g}$
4 Γ_{7g}	3.033	195	23112	1.13		51.47	1 $^8T_{1g}$	17.70	1 $^8T_{2g}$	12.72	2 ^8E_g		
8 Γ_{8g}	3.032	195	23119	0.87		24.36	2 $^8T_{2g}$	18.70	2 ^8E_g	13.50	3 $^8T_{1g}$	12.41	2 $^8T_{1g}$
9 Γ_{8g}	3.034	197	23192	1.15		21.52	1 $^8T_{2g}$	19.85	1 ^8E_g	15.93	2 $^8T_{1g}$	13.62	1 $^8T_{1g}$
						12.48	2 $^8T_{2g}$						
5 Γ_{7g}	3.031	195	23269	0.76		30.43	2 $^8T_{2g}$	16.47	3 $^8T_{1g}$	11.26	1 $^8T_{2g}$	10.34	1 $^8T_{1g}$
5 Γ_{6g}	3.033	195	23417	1.34		40.00	1 $^8T_{2g}$	15.36	2 $^8T_{1g}$	13.54	2 $^8T_{2g}$	10.80	2 ^8E_g
6 Γ_{7g}	3.034	196	23578	2.45		34.98	1 $^8T_{1g}$	22.56	1 ^8E_g	22.50	2 $^8T_{1g}$	12.17	1 $^8T_{2g}$
10 Γ_{8g}	3.033	195	23669	3.68		23.93	2 $^8T_{2g}$	18.59	2 ^8E_g	13.95	2 $^8T_{1g}$	11.50	1 $^8T_{2g}$
						11.04	3 $^8T_{1g}$	10.13	1 ^8E_g				
11 Γ_{8g}	3.034	197	23735	0.85		22.13	2 $^8T_{1g}$	21.50	1 ^8E_g	17.69	2 ^8E_g	17.62	2 $^8T_{2g}$
12 Γ_{8g}	3.032	196	23894	0.77		33.80	2 ^8E_g	27.70	3 $^8T_{1g}$	13.67	2 $^8T_{2g}$		
6 Γ_{6g}	3.032	195	23899	0.50		33.11	2 $^8T_{2g}$	19.09	1 $^8T_{1g}$	10.58	3 $^8T_{1g}$		
7 Γ_{7g}	3.032	196	23957	0.88		23.37	2 $^8T_{1g}$	23.19	1 $^8T_{2g}$	17.70	3 $^8T_{1g}$	15.97	2 $^8T_{2g}$
7 Γ_{6g}	3.033	196	24213	4.43		28.21	2 $^8T_{1g}$	24.98	1 $^8T_{2g}$	18.07	1 $^8T_{1g}$	13.46	1 ^8E_g
						11.13	3 $^8T_{1g}$						
13 Γ_{8g}	3.032	196	24271	5.78		24.45	1 $^8T_{2g}$	24.07	2 $^8T_{1g}$	17.79	1 $^8T_{1g}$	13.05	3 $^8T_{1g}$
14 Γ_{8g}	3.034	196	24400	0.77		30.15	2 $^8T_{2g}$	25.16	1 $^8T_{2g}$	13.30	1 ^8E_g	13.18	2 ^8E_g
15 Γ_{8g}	3.034	197	24511	3.43		21.04	1 ^8E_g	19.68	2 $^8T_{1g}$	18.92	2 ^8E_g	17.57	1 $^8T_{1g}$
8 Γ_{7g}	3.033	196	24722	1.37		29.60	3 $^8T_{1g}$	10.02	2 $^8T_{1g}$				
16 Γ_{8g}	3.034	196	24746	1.34		21.68	1 ^8E_g	13.70	1 $^8T_{1g}$	13.44	2 ^8E_g	10.95	2 $^8T_{2g}$
						10.91	1 $^8T_{2g}$						
9 Γ_{7g}	3.033	196	24943	0.91		24.61	3 $^8T_{1g}$	14.64	2 ^8E_g	14.10	2 $^8T_{1g}$	11.41	1 $^8T_{1g}$
17 Γ_{8g}	3.033	196	24985	1.13		23.16	2 $^8T_{2g}$	18.93	3 $^8T_{1g}$	10.93	2 $^8T_{1g}$		
8 Γ_{6g}	3.032	196	25047	0.16		48.99	2 $^8T_{2g}$	10.36	3 $^8T_{1g}$				
18 Γ_{8g}	3.033	196	25072	2.94		25.49	3 $^8T_{1g}$	24.37	2 $^8T_{1g}$	17.09	1 $^8T_{1g}$	14.69	2 $^8T_{2g}$
9 Γ_{6g}	3.034	196	25425	0.04		34.63	1 $^8T_{2g}$	25.84	2 ^8E_g	14.80	1 ^8E_g		

19 Γ_{8g}	3.034	196	25443	0.60	27.62	1 $^8T_{2g}$	19.11	2 ^8E_g	16.06	1 $^8T_{1g}$	15.70	1 ^8E_g
					11.65	3 $^8T_{1g}$						
10 Γ_{7g}	3.034	196	25550	0.13	27.27	1 $^8T_{1g}$	20.18	1 $^8T_{2g}$	17.45	2 ^8E_g	15.75	1 ^8E_g
10 Γ_{6g}	3.033	196	25755	5.45	63.77	2 $^8T_{1g}$	21.50	1 $^8T_{2g}$				
20 Γ_{8g}	3.033	196	25784	11.17	51.65	2 $^8T_{1g}$	15.11	1 $^8T_{2g}$	10.92	1 $^8T_{1g}$		
21 Γ_{8g}	3.033	196	25803	10.07	42.34	2 $^8T_{1g}$	18.96	1 $^8T_{1g}$				
22 Γ_{8g}	3.031	195	25989	0.25	51.27	2 $^8T_{2g}$	22.50	3 $^8T_{1g}$				
11 Γ_{7g}	3.031	195	25997	0.03	64.46	2 $^8T_{2g}$						
23 Γ_{8g}	3.032	196	26054	0.37	35.77	2 $^8T_{2g}$	14.84	2 ^8E_g	12.82	3 $^8T_{1g}$		
11 Γ_{6g}	3.032	195	26165	0.41	32.05	3 $^8T_{1g}$	20.58	2 $^8T_{2g}$	10.04	1 $^8T_{1g}$		
12 Γ_{6g}	3.033	196	26223	0.91	21.92	3 $^8T_{1g}$	15.94	2 ^8E_g				
24 Γ_{8g}	3.033	195	26370	0.94	43.60	3 $^8T_{1g}$	17.22	1 $^8T_{1g}$				
12 Γ_{7g}	3.034	195	26451	0.44	46.21	3 $^8T_{1g}$	17.93	1 $^8T_{1g}$				
25 Γ_{8g}	3.034	194	26802		85.62	1 $^6T_{1g}$						
26 Γ_{8g}	3.032	196	27106	0.39	39.30	2 $^8T_{2g}$	25.68	2 ^8E_g	13.08	3 $^8T_{1g}$		
13 Γ_{7g}	3.032	196	27284	0.01	43.71	2 $^8T_{2g}$	15.44	2 ^8E_g				
27 Γ_{8g}	3.032	195	27415	0.71	38.94	3 $^8T_{1g}$	28.45	2 $^8T_{2g}$	15.74	2 ^8E_g		
13 Γ_{6g}	3.030	195	27487	0.21	38.95	2 $^8T_{2g}$	30.56	3 $^8T_{1g}$				
28 Γ_{8g}	3.032	195	27538	0.87	49.13	3 $^8T_{1g}$	20.70	2 ^8E_g	17.22	2 $^8T_{2g}$		
14 Γ_{7g}	3.032	196	27926	0.42	40.25	3 $^8T_{1g}$						
29 Γ_{8g}	3.032	196	28010	0.88	44.19	3 $^8T_{1g}$						
14 Γ_{6g}	3.032	196	28036	0.45	44.72	3 $^8T_{1g}$						
$4f^6(^7F_J)5dt^1_{2g}$ Low-Spin coupling [d]												
30 Γ_{8g}	3.033	194	28106	0.01	80.13	1 $^6T_{1g}$						
15 Γ_{7g}	3.033	194	28146	0.01	79.76	1 $^6T_{1g}$						
16 Γ_{7g}	3.026	192	29697	0.03	37.16	2 $^6T_{1g}$	34.73	1 ^6E_g	22.40	1 $^6T_{1g}$		
31 Γ_{8g}	3.030	194	29946	0.19	54.36	1 $^6T_{1g}$	27.52	1 $^6T_{2g}$				
15 Γ_{6g}	3.027	190	29952	0.11	53.76	1 $^6T_{1g}$	27.27	1 $^6T_{2g}$				
32 Γ_{8g}	3.025	193	30088	0.03	50.25	2 $^6T_{1g}$	24.68	1 ^6E_g	10.15	1 $^6T_{2g}$		
17 Γ_{7g}	3.027	192	30182	0.07	29.22	1 $^6T_{2g}$	28.62	1 $^6T_{1g}$	26.56	2 $^6T_{1g}$		
16 Γ_{6g}	3.025	192	30263	0.01	28.32	2 $^6T_{1g}$	19.53	1 $^6T_{2g}$	16.57	1 ^6E_g	15.18	2 $^6T_{2g}$
33 Γ_{8g}	3.024	191	30617	0.05	23.56	2 $^6T_{1g}$	21.26	2 $^6T_{2g}$	20.97	1 ^6E_g	15.47	1 $^6A_{2g}$
18 Γ_{7g}	3.028	193	30810	0.06	37.62	1 $^6T_{1g}$	25.99	2 $^6T_{1g}$	17.14	1 $^6T_{2g}$		
17 Γ_{6g}	3.025	191	30924	0.04	36.91	1 $^6T_{2g}$	35.72	2 $^6T_{1g}$	11.79	1 ^6E_g		
34 Γ_{8g}	3.024	191	31133	0.04	19.32	1 $^6A_{2g}$	18.05	2 $^6T_{2g}$	12.92	1 $^6T_{2g}$	12.10	2 $^6T_{1g}$
					11.36	1 $^6T_{1g}$	10.12	1 ^6E_g				
18 Γ_{6g}	3.023	191	31327	0.01	38.08	1 $^6A_{2g}$	25.02	2 $^6T_{2g}$	10.90	2 $^6T_{1g}$		
35 Γ_{8g}	3.026	192	31397	0.20	33.91	2 $^6T_{1g}$	29.00	1 $^6T_{2g}$	20.01	1 ^6E_g		
36 Γ_{8g}	3.024	191	31520	0.17	25.27	1 ^6E_g	23.29	1 $^6T_{2g}$	21.36	2 $^6T_{1g}$		
19 Γ_{6g}	3.026	191	31949	0.16	34.03	1 ^6E_g	33.10	1 $^6T_{2g}$	19.87	2 $^6T_{2g}$		
37 Γ_{8g}	3.021	190	32023	0.24	21.47	3 $^6T_{1g}$	19.56	1 ^6E_g	16.32	2 $^6T_{1g}$	15.58	2 $^6T_{2g}$
					10.79	2 ^6E_g						
38 Γ_{8g}	3.023	192	32143	0.10	24.60	2 $^6T_{2g}$	21.38	1 $^6T_{2g}$	14.87	2 ^6E_g	12.11	2 $^6T_{1g}$
					11.50	3 $^6T_{1g}$						
19 Γ_{7g}	3.026	190	32389		52.06	2 $^6T_{1g}$	29.74	1 $^6T_{2g}$				
20 Γ_{7g}	3.020	192	32540	0.16	36.93	3 $^6T_{1g}$	16.60	2 ^6E_g	14.26	1 $^6A_{1g}$	12.84	2 $^6T_{1g}$
20 Γ_{6g}	3.022	190	32565	0.02	35.76	2 ^6E_g	24.27	2 $^6T_{2g}$	20.02	1 ^6E_g		
39 Γ_{8g}	3.021	191	32827	0.05	24.09	2 ^6E_g	19.59	2 $^6T_{2g}$	15.85	1 $^6A_{2g}$	15.59	3 $^6T_{1g}$
21 Γ_{6g}	3.026	192	32932	0.17	48.13	1 $^6T_{2g}$	13.18	3 $^6T_{1g}$	10.38	2 $^6T_{1g}$		
40 Γ_{8g}	3.026	191	33040	0.13	39.50	2 $^6T_{1g}$	22.71	1 $^6T_{2g}$	12.30	2 $^6T_{2g}$		
21 Γ_{7g}	3.025	190	33195	0.04	37.62	2 $^6T_{1g}$	29.05	1 ^6E_g	13.94	3 $^6T_{1g}$	12.82	2 $^6T_{2g}$
41 Γ_{8g}	3.021	191	33197	0.19	33.80	2 $^6T_{2g}$	22.44	3 $^6T_{1g}$	14.91	1 $^6T_{2g}$	13.35	1 $^6A_{1g}$
42 Γ_{8g}	3.026	191	33442	0.26	34.88	2 $^6T_{1g}$	31.20	1 $^6T_{2g}$	16.99	1 ^6E_g		
22 Γ_{7g}	3.021	191	33499	0.06	33.03	2 ^6E_g	29.63	3 $^6T_{1g}$	13.08	1 ^6E_g		
43 Γ_{8g}	3.026	191	33772	0.51	57.85	1 $^6T_{2g}$	16.17	1 ^6E_g	13.22	2 $^6T_{1g}$		
23 Γ_{7g}	3.021	191	34051	0.10	57.39	2 $^6T_{2g}$	22.75	1 $^6A_{1g}$				
44 Γ_{8g}	3.021	190	34173	0.15	25.73	2 $^6T_{2g}$	20.05	1 $^6A_{1g}$	15.19	2 ^6E_g	12.24	1 $^6A_{2g}$
					11.23	3 $^6T_{1g}$						
22 Γ_{6g}	3.021	191	34240	0.02	28.58	3 $^6T_{1g}$	24.74	1 $^6A_{2g}$	22.61	2 $^6T_{2g}$	16.44	1 $^6T_{2g}$
45 Γ_{8g}	3.022	189	34357	0.01	59.49	3 $^6T_{1g}$	10.92	2 $^6T_{2g}$				
46 Γ_{8g}	3.021	192	34385	0.09	32.73	3 $^6T_{1g}$	26.42	2 ^6E_g	18.79	2 $^6T_{2g}$	10.75	1 $^6T_{2g}$

23 Γ_{6g}	3.021	190	35443	0.10	38.85	3 $^6T_{1g}$	36.07	2 $^6T_{2g}$	13.46	1 $^6A_{2g}$		
47 Γ_{8g}	3.021	190	35494	0.07	41.46	2 $^6T_{2g}$	25.71	2 ^6E_g	15.23	1 $^6A_{2g}$		
24 Γ_{7g}	3.020	190	35665	0.12	51.29	3 $^6T_{1g}$	34.07	2 ^6E_g				
48 Γ_{8g}	3.020	190	35668	0.13	34.46	3 $^6T_{1g}$	33.72	2 ^6E_g	23.18	2 $^6T_{2g}$		
24 Γ_{6g}	3.020	190	35701	0.02	44.25	2 ^6E_g	39.55	2 $^6T_{2g}$				
25 Γ_{7g}	3.019	189	35974	0.13	47.51	1 $^6A_{1g}$	40.03	3 $^6T_{1g}$				
49 Γ_{8g}	3.019	188	35997	1.97	45.03	1 $^6A_{1g}$	40.05	3 $^6T_{1g}$				
$4f^6(^7F_J)(5de^1_g + ITE^1_{a_{1g}})$ High-Spin coupling [d]												
50 Γ_{8g}	3.054	164	36508	5.73	55.73	3 $^8T_{2g}$	34.05	4 $^8T_{1g}$				
26 Γ_{7g}	3.057	172	36598	3.24	63.36	3 $^8T_{2g}$	30.82	4 $^8T_{1g}$				
51 Γ_{8g}	3.054	162	36834	1.30	78.38	3 $^8T_{2g}$						
27 Γ_{7g}	3.050	172	37166	6.84	59.11	4 $^8T_{1g}$	29.74	3 $^8T_{2g}$				
52 Γ_{8g}	3.051	176	37524	9.53	42.93	3 $^8T_{2g}$	42.07	4 $^8T_{1g}$				
25 Γ_{6g}	3.051	172	37614	2.80	48.32	3 $^8T_{2g}$	28.76	4 $^8T_{1g}$	11.01	5 $^8T_{1g}$		
53 Γ_{8g}	3.051	171	38009	10.16	45.98	4 $^8T_{1g}$	38.45	3 $^8T_{2g}$				
26 Γ_{6g}	3.051	182	38176	3.92	32.89	4 $^8T_{1g}$	29.22	3 $^8T_{2g}$	14.74	3 ^8E_g	11.11	4 $^8T_{2g}$
28 Γ_{7g}	3.052	175	38422	3.75	48.89	3 $^8T_{2g}$	33.66	4 $^8T_{1g}$	12.48	3 ^8E_g		
54 Γ_{8g}	3.050	182	38573	4.13	31.72	4 $^8T_{2g}$	30.73	3 $^8T_{2g}$	16.50	3 ^8E_g	14.60	4 $^8T_{1g}$
55 Γ_{8g}	3.048	164	38835	4.52	28.88	4 $^8T_{2g}$	25.83	4 $^8T_{1g}$	24.82	5 $^8T_{1g}$	14.91	3 $^8T_{2g}$
27 Γ_{6g}	3.046	158	38836	2.45	49.01	4 $^8T_{2g}$	29.89	4 $^8T_{1g}$	12.78	5 $^8T_{1g}$		
56 Γ_{8g}	3.053	193	39036	1.18	48.62	5 $^8T_{1g}$	40.97	3 ^8E_g				
57 Γ_{8g}	3.051	169	39311	9.59	47.91	4 $^8T_{1g}$	30.63	3 $^8T_{2g}$	15.67	5 $^8T_{1g}$		
29 Γ_{7g}	3.051	164	39399	7.58	64.54	4 $^8T_{1g}$	24.85	3 $^8T_{2g}$				
28 Γ_{6g}	3.045	156	39590	1.08	35.23	4 $^8T_{2g}$	30.27	5 $^8T_{1g}$	18.23	3 $^8T_{2g}$	10.69	4 $^8T_{1g}$
58 Γ_{8g}	3.050	182	39626	1.50	36.78	4 $^8T_{2g}$	21.03	5 $^8T_{1g}$	16.58	3 ^8E_g	12.67	4 $^8T_{1g}$
					11.07	3 $^8T_{2g}$						
30 Γ_{7g}	3.051	194	39691	0.02	41.02	4 $^8T_{2g}$	23.94	3 ^8E_g	19.10	5 $^8T_{1g}$	13.16	3 $^8T_{2g}$
29 Γ_{6g}	3.054	164	39817	1.85	62.86	3 $^8T_{2g}$	19.45	5 $^8T_{1g}$	11.09	4 $^8T_{1g}$		
59 Γ_{8g}	3.052	180	40123	9.44	48.20	4 $^8T_{1g}$	18.20	3 $^8T_{2g}$	16.02	3 ^8E_g	10.41	5 $^8T_{1g}$
30 Γ_{6g}	3.051	236	40215	0.72	37.70	4 $^8T_{2g}$	32.61	3 ^8E_g	16.76	5 $^8T_{1g}$		
60 Γ_{8g}	3.051	204	40237	2.46	32.11	4 $^8T_{2g}$	29.70	3 ^8E_g	22.28	5 $^8T_{1g}$	10.31	4 $^8T_{1g}$
61 Γ_{8g}	3.052	229	40726	3.50	39.03	3 $^8T_{2g}$	22.22	4 $^8T_{1g}$	15.62	3 ^8E_g	12.49	4 $^8T_{2g}$
31 Γ_{7g}	3.047	163	40807	0.01	57.72	5 $^8T_{1g}$	24.83	4 $^8T_{2g}$				
31 Γ_{6g}	2.954	228	40866	7.45	70.37	4 $^8T_{1g}$	23.13	3 $^8T_{2g}$				
62 Γ_{8g}	3.051	232	40923	4.65	30.09	5 $^8T_{1g}$	24.25	3 ^8E_g	21.33	4 $^8T_{2g}$	16.81	4 $^8T_{1g}$
63 Γ_{8g}	3.051	229	41035	10.86	43.91	4 $^8T_{1g}$	21.34	5 $^8T_{1g}$	14.93	4 $^8T_{2g}$	13.98	3 ^8E_g
32 Γ_{6g}	3.000	464	41101	0.87	48.91	6 $^8T_{1g}$	41.16	5 $^8T_{2g}$				
64 Γ_{8g}	3.000	295	41349	1.09	53.28	4 $^8T_{2g}$	23.08	5 $^8T_{1g}$	17.29	3 ^8E_g		
32 Γ_{7g}	3.050	295	41479	0.01	54.24	4 $^8T_{2g}$	33.19	3 ^8E_g				
33 Γ_{6g}	3.044	171	41658	0.01	51.39	4 $^8T_{2g}$	39.22	5 $^8T_{1g}$				
65 Γ_{8g}	2.969	151	41681	0.03	51.80	6 $^8T_{1g}$	39.99	5 $^8T_{2g}$				
66 Γ_{8g}	3.000	491	41810	3.37	59.53	6 $^8T_{1g}$	35.55	5 $^8T_{2g}$				
33 Γ_{7g}	2.992	163	42004	0.04	55.10	5 $^8T_{2g}$	24.75	6 $^8T_{1g}$				
67 Γ_{8g}	3.050	489	42222	0.63	47.11	5 $^8T_{1g}$	37.01	3 ^8E_g				
34 Γ_{6g}	3.052	271	42281	0.29	56.82	5 $^8T_{1g}$	32.17	3 ^8E_g				
34 Γ_{7g}	2.943	236	42325	0.01	73.80	5 $^8T_{1g}$	14.06	3 ^8E_g				
68 Γ_{8g}	3.047	143	42521	0.10	60.86	5 $^8T_{1g}$	23.02	3 ^8E_g				
35 Γ_{6g}	3.000	453	42604	0.01	60.16	5 $^8T_{2g}$	34.48	6 $^8T_{1g}$				
69 Γ_{8g}	3.000	518	42722	0.18	47.44	6 $^8T_{1g}$	37.13	5 $^8T_{2g}$				
35 Γ_{7g}	3.006	202	42806	0.02	54.03	5 $^8T_{2g}$	33.26	6 $^8T_{1g}$				
70 Γ_{8g}	3.049	337	43072	0.10	75.37	4 $^8T_{2g}$	12.16	3 ^8E_g				
71 Γ_{8g}	3.050	299	43233	0.03	67.40	4 $^8T_{2g}$	28.43	5 $^8T_{1g}$				
36 Γ_{7g}	3.042	161	43245	0.01	70.53	4 $^8T_{2g}$	26.37	5 $^8T_{1g}$				
72 Γ_{8g}	2.990	188	43446	0.05	58.07	6 $^8T_{1g}$	40.93	5 $^8T_{2g}$				
36 Γ_{6g}	2.938	187	43495	0.02	38.54	6 $^8T_{1g}$	18.85	5 $^8T_{2g}$				
73 Γ_{8g}	2.993	187	43573	0.02	65.66	5 $^8T_{2g}$	22.06	6 $^8T_{1g}$				
37 Γ_{6g}	2.900	196	44146	0.03	64.00	6 $^8T_{1g}$	33.66	5 $^8T_{2g}$				
74 Γ_{8g}	2.923	165	44269	0.05	51.39	5 $^8T_{2g}$	48.21	6 $^8T_{1g}$				
75 Γ_{8g}	2.900	196	44366	0.03	47.21	5 $^8T_{2g}$	30.26	6 $^8T_{1g}$				
37 Γ_{7g}	2.900	196	44393	0.03	62.84	6 $^8T_{1g}$						
76 Γ_{8g}	2.900	196	45483	0.07	63.24	6 $^8T_{1g}$	36.74	5 $^8T_{2g}$				

38 Γ_{7g}	2.900	196	45497	0.03	54.77	6 $^8T_{1g}$	45.16	5 $^8T_{2g}$						
39 Γ_{7g}	2.900	196	45767	0.01	39.37	5 $^8T_{2g}$	24.16	6 $^8T_{1g}$						
77 Γ_{8g}	2.900	196	45796	0.02	44.11	5 $^8T_{2g}$	17.93	6 $^8T_{1g}$						
38 Γ_{6g}	2.900	196	45833	0.01	45.67	5 $^8T_{2g}$	13.52	6 $^8T_{1g}$						

$4f^7$ excited states

$4f^7(^6P_{3/2,5/2,7/2})$ [c]

2 Γ_{7u}	3.080	203	30281		88.99	1 $^6T_{1u}$								
2 Γ_{8u}	3.080	203	30304		89.34	1 $^6T_{1u}$								
3 Γ_{8u}	3.080	203	30683		93.91	1 $^6T_{1u}$								
2 Γ_{6u}	3.080	203	30916		84.52	1 $^6T_{1u}$	12.66	3 $^6T_{2u}$						
4 Γ_{8u}	3.080	203	30932		84.77	1 $^6T_{1u}$								
3 Γ_{7u}	3.080	203	30956		85.07	1 $^6T_{1u}$	10.96	2 ^6E_u						

$4f^7(^6I_{7/2,9/2,11/2,13/2,15/2,17/2})$ [c]

5 Γ_{8u}	3.079	202	34795		79.07	1 $^6T_{2u}$	14.66	1 ^6E_u						
3 Γ_{6u}	3.079	202	34796		78.81	1 $^6T_{2u}$	19.44	1 ^6E_u						
6 Γ_{8u}	3.078	202	34800		86.14	1 $^6T_{2u}$								
4 Γ_{6u}	3.078	202	34809		87.45	1 $^6T_{2u}$								
7 Γ_{8u}	3.078	202	34812		91.39	1 $^6T_{2u}$								
4 Γ_{7u}	3.079	202	34812		87.59	1 $^6T_{2u}$								
8 Γ_{8u}	3.080	202	34873		48.84	2 $^6T_{1u}$	38.40	1 $^6A_{1u}$						
5 Γ_{7u}	3.080	202	34874		42.19	2 $^6T_{1u}$	27.53	1 $^6A_{1u}$	23.10	2 $^6T_{2u}$				
9 Γ_{8u}	3.080	202	34909		51.85	2 $^6T_{1u}$	41.96	2 $^6T_{2u}$						
5 Γ_{6u}	3.080	202	34924		49.82	2 $^6T_{1u}$	46.61	2 $^6T_{2u}$						
6 Γ_{7u}	3.080	202	34949		41.27	2 $^6T_{1u}$	30.98	2 $^6T_{2u}$	20.89	1 $^6A_{1u}$				
10 Γ_{8u}	3.080	202	34952		74.30	2 $^6T_{1u}$	19.06	2 $^6T_{2u}$						
6 Γ_{6u}	3.080	202	34997		87.52	2 $^6T_{2u}$								
7 Γ_{7u}	3.080	202	35009		29.47	2 $^6T_{1u}$	26.55	1 ^6E_u	22.48	2 $^6T_{2u}$	21.05	1 $^6A_{1u}$		
11 Γ_{8u}	3.080	202	35042		40.56	2 $^6T_{2u}$	32.44	1 ^6E_u	11.37	1 $^6A_{2u}$				
12 Γ_{8u}	3.080	202	35068		39.72	2 $^6T_{2u}$	37.93	2 $^6T_{1u}$	16.69	1 $^6A_{1u}$				
13 Γ_{8u}	3.080	202	35083		63.09	1 ^6E_u	15.91	2 $^6T_{2u}$						
8 Γ_{7u}	3.080	202	35084		65.14	1 ^6E_u	28.57	2 $^6T_{1u}$						
14 Γ_{8u}	3.080	202	35125		35.50	1 ^6E_u	21.02	2 $^6T_{2u}$	15.35	2 $^6T_{1u}$	15.26	1 $^6A_{2u}$		
					10.54	1 $^6A_{1u}$								
7 Γ_{6u}	3.080	202	35141		33.24	1 $^6A_{2u}$	29.30	1 ^6E_u	20.11	2 $^6T_{2u}$	11.18	2 $^6T_{1u}$		
8 Γ_{6u}	3.080	202	35223		48.83	1 ^6E_u	16.17	2 $^6T_{2u}$	15.26	1 $^6T_{2u}$	12.43	1 $^6A_{2u}$		
9 Γ_{7u}	3.080	202	35223		49.12	2 $^6T_{1u}$	26.67	1 $^6A_{1u}$	21.63	2 $^6T_{2u}$				
15 Γ_{8u}	3.080	202	35238		27.75	2 $^6T_{2u}$	26.53	1 ^6E_u	21.60	2 $^6T_{1u}$				
16 Γ_{8u}	3.080	202	35258		46.18	1 $^6A_{2u}$	20.46	2 $^6T_{2u}$	13.35	2 $^6T_{1u}$				
17 Γ_{8u}	3.080	202	35266		61.08	2 $^6T_{2u}$	13.43	2 $^6T_{1u}$	11.62	1 $^6A_{2u}$				
9 Γ_{6u}	3.080	202	35268		44.97	1 $^6A_{2u}$	28.13	2 $^6T_{2u}$	19.32	2 $^6T_{1u}$				

$4f^7(^6D_{1/2,3/2,5/2,7/2})$ [c]

10 Γ_{6u}	3.079	202	37397		72.40	3 $^6T_{2u}$	24.72	2 ^6E_u						
18 Γ_{8u}	3.079	202	37421		59.19	3 $^6T_{2u}$	37.52	2 ^6E_u						
19 Γ_{8u}	3.079	202	37454		73.35	3 $^6T_{2u}$	23.51	2 ^6E_u						
11 Γ_{6u}	3.079	202	37659		67.62	2 ^6E_u	31.65	3 $^6T_{2u}$						
20 Γ_{8u}	3.079	202	37956		55.24	3 $^6T_{2u}$	37.08	2 ^6E_u						
10 Γ_{7u}	3.079	202	38180		85.12	3 $^6T_{2u}$	11.22	1 $^6T_{1u}$						
21 Γ_{8u}	3.079	202	38239		57.43	3 $^6T_{2u}$	28.25	2 ^6E_u	11.22	1 $^6T_{1u}$				
12 Γ_{6u}	3.079	202	38262		78.00	3 $^6T_{2u}$	13.11	1 $^6T_{1u}$						
22 Γ_{8u}	3.079	202	38307		55.71	2 ^6E_u	28.60	3 $^6T_{2u}$	12.09	1 $^6T_{1u}$				
11 Γ_{7u}	3.079	202	38317		83.13	2 ^6E_u	12.32	1 $^6T_{1u}$						

Eu^{3+}-doped BaS

$4f^6(^7F_{0-6})$

1 A_{1g}	2.800	286	0		47.13	1 $^7T_{1g}$	36.92	1 $^7T_{2g}$	10.12	1 $^7A_{2g}$				
1 T_{1g}	2.800	286	373		49.18	1 $^7T_{1g}$	36.47	1 $^7T_{2g}$						
1 E_g	2.799	285	963		67.33	1 $^7T_{1g}$	29.01	1 $^7T_{2g}$						

1 T_{2g}	2.800	287	1137	42.70	1 $7T_{1g}$	39.80	1 $7T_{2g}$	13.86	1 $7A_{2g}$			
1 A_{2g}	2.799	285	1956	54.65	1 $7T_{1g}$	42.86	1 $7T_{2g}$					
2 T_{2g}	2.800	287	2017	46.15	1 $7T_{1g}$	32.05	1 $7T_{2g}$	19.23	1 $7A_{2g}$			
2 T_{1g}	2.800	287	2066	46.60	1 $7T_{2g}$	36.54	1 $7T_{1g}$	14.32	1 $7A_{2g}$			
3 T_{2g}	2.799	286	2951	70.46	1 $7T_{1g}$	23.92	1 $7T_{2g}$					
2 E_g	2.800	285	3170	74.60	1 $7T_{2g}$	23.36	1 $7T_{1g}$					
3 T_{1g}	2.800	288	3190	43.79	1 $7T_{2g}$	29.53	1 $7T_{1g}$	24.61	1 $7A_{2g}$			
2 A_{1g}	2.800	291	3211	50.44	1 $7A_{2g}$	37.56	1 $7T_{1g}$					
4 T_{1g}	2.799	286	4184	52.40	1 $7T_{1g}$	42.78	1 $7T_{2g}$					
3 E_g	2.799	285	4216	51.01	1 $7T_{2g}$	46.64	1 $7T_{1g}$					
4 T_{2g}	2.800	288	4247	62.26	1 $7T_{1g}$	25.79	1 $7A_{2g}$					
5 T_{1g}	2.800	287	4400	74.15	1 $7T_{2g}$	12.01	1 $7T_{1g}$	11.47	1 $7A_{2g}$			
4 E_g	2.799	285	5387	56.56	1 $7T_{1g}$	40.14	1 $7T_{2g}$					
5 T_{2g}	2.799	286	5407	52.28	1 $7T_{1g}$	43.48	1 $7T_{2g}$					
2 A_{2g}	2.799	285	5457	54.22	1 $7T_{2g}$	42.46	1 $7T_{1g}$					
6 T_{2g}	2.800	289	5619	45.05	1 $7T_{2g}$	33.67	1 $7A_{2g}$	17.99	1 $7T_{1g}$			
6 T_{1g}	2.800	289	5650	47.57	1 $7T_{2g}$	34.76	1 $7A_{2g}$	14.36	1 $7T_{1g}$			
3 A_{1g}	2.800	290	5676	48.77	1 $7T_{2g}$	36.45	1 $7A_{2g}$	11.47	1 $7T_{1g}$			
$4f^6(^5D_{0-3})$												
4 A_{1g}	2.798	285	19973	57.46	1 $5T_{2g}$	36.83	1 $5E_g$					
7 T_{1g}	2.798	285	20781	58.04	1 $5T_{2g}$	36.80	1 $5E_g$					
7 T_{2g}	2.797	285	22428	70.36	1 $5T_{2g}$	25.21	1 $5E_g$					
5 E_g	2.798	284	22521	54.04	1 $5E_g$	41.47	1 $5T_{2g}$					
8 T_{1g}	2.797	285	25111	85.65	1 $5T_{2g}$	10.04	1 $5E_g$					
8 T_{2g}	2.797	285	25153	49.90	1 $5E_g$	45.77	1 $5T_{2g}$					
3 A_{2g}	2.797	284	25190	95.44	1 $5E_g$							
$4f^6(^5D_4,^5L_{6-10},^5G_{2-6})$												
9 T_{2g}	2.797	285	28323	21.94	1 $5T_{1g}$	20.69	2 $5E_g$	16.46	4 $5T_{2g}$	14.24	2 $5T_{1g}$	
5 A_{1g}	2.797	284	28343	51.00	3 $5T_{2g}$	34.25	3 $5E_g$	11.53	4 $5T_{2g}$			
4 A_{2g}	2.797	285	28345	36.80	1 $5T_{1g}$	35.07	2 $5E_g$	14.96	2 $5T_{1g}$			
9 T_{1g}	2.797	284	28362	31.55	3 $5T_{2g}$	14.41	3 $5E_g$	13.19	2 $5T_{1g}$	11.83	1 $5T_{1g}$	
				10.75	4 $5T_{2g}$							
10 T_{2g}	2.797	284	28494	43.66	1 $5T_{1g}$	16.42	2 $5E_g$	10.07	4 $5T_{1g}$			
11 T_{2g}	2.797	285	28495	42.72	1 $5T_{1g}$	25.53	1 $5A_{1g}$					
6 E_g	2.797	285	28536	45.16	1 $5T_{1g}$	22.35	1 $5A_{1g}$	18.14	2 $5E_g$			
12 T_{2g}	2.797	285	28572	32.46	4 $5T_{2g}$	15.97	1 $5T_{1g}$	14.79	2 $5E_g$			
10 T_{1g}	2.797	285	28618	43.04	1 $5T_{1g}$	23.45	2 $5T_{2g}$					
7 E_g	2.797	284	28625	21.65	3 $5T_{2g}$	17.24	3 $5T_{1g}$	16.86	2 $5T_{1g}$	13.51	4 $5E_g$	
				13.26	4 $5T_{2g}$							
13 T_{2g}	2.797	283	28629	22.30	3 $5T_{2g}$	17.04	2 $5T_{1g}$	16.91	3 $5T_{1g}$	13.25	4 $5E_g$	
				12.24	4 $5T_{2g}$							
6 A_{1g}	2.797	281	28703	61.44	2 $5E_g$	14.13	2 $5T_{2g}$	13.04	5 $5T_{2g}$			
8 E_g	2.798	284	28706	32.23	3 $5T_{1g}$	17.07	4 $5T_{2g}$	17.02	4 $5E_g$	11.43	2 $5A_{1g}$	
5 A_{2g}	2.798	284	28715	42.37	2 $5T_{1g}$	20.16	4 $5E_g$	11.33	2 $5E_g$	10.61	3 $5E_g$	
14 T_{2g}	2.798	284	28825	75.92	2 $5T_{2g}$							
11 T_{1g}	2.797	285	28934	19.48	3 $5T_{2g}$	19.11	2 $5T_{1g}$	11.08	1 $5E_g$	10.83	1 $5T_{2g}$	
7 A_{1g}	2.797	284	28954	55.22	1 $5E_g$	35.33	1 $5T_{2g}$					
9 E_g	2.797	284	29001	29.36	3 $5E_g$	17.87	2 $5T_{2g}$	12.75	2 $5T_{1g}$	11.80	4 $5T_{2g}$	
12 T_{1g}	2.797	285	29015	30.02	1 $5E_g$	29.87	1 $5T_{2g}$	12.65	2 $5T_{2g}$			
15 T_{2g}	2.797	284	29029	28.53	3 $5T_{2g}$	14.21	2 $5T_{1g}$	12.61	4 $5T_{2g}$	11.17	4 $5E_g$	
10 E_g	2.797	284	29066	38.73	1 $5T_{2g}$	29.03	1 $5E_g$	12.20	2 $5E_g$			
16 T_{2g}	2.798	285	29110	51.85	1 $5T_{2g}$	13.39	1 $5E_g$	11.34	2 $5T_{2g}$			
17 T_{2g}	2.797	285	29122	33.57	2 $5E_g$	22.85	1 $5T_{1g}$	10.95	2 $5T_{2g}$	10.05	5 $5T_{2g}$	
18 T_{2g}	2.797	285	29131	21.75	1 $5T_{1g}$	20.33	1 $5A_{1g}$	15.08	2 $5T_{2g}$			
13 T_{1g}	2.797	283	29188	25.95	4 $5T_{2g}$	23.24	4 $5E_g$	19.51	3 $5T_{1g}$			
6 A_{2g}	2.797	285	29207	44.48	3 $5T_{1g}$	23.59	3 $5E_g$	22.51	4 $5E_g$			
11 E_g	2.797	284	29226	46.55	2 $5T_{2g}$	12.68	3 $5E_g$					
14 T_{1g}	2.798	285	29239	39.81	2 $5T_{2g}$	11.93	1 $5T_{1g}$					
19 T_{2g}	2.798	284	29250	29.67	3 $5T_{1g}$	19.79	2 $5A_{1g}$	19.09	2 $5T_{1g}$	10.73	3 $5E_g$	
12 E_g	2.797	285	29690	55.48	3 $5T_{2g}$	18.63	2 $5T_{1g}$	11.21	4 $5T_{2g}$			
20 T_{2g}	2.797	285	29716	30.57	2 $5T_{1g}$	29.09	3 $5E_g$	13.62	4 $5T_{2g}$			

15 T_{1g}	2.797	284	29792	25.37	3 $5T_{2g}$	21.47	4 $5T_{2g}$	13.16	2 $5T_{1g}$	12.96	3 $5E_g$
				12.61	4 $5E_g$						
21 T_{2g}	2.797	285	29886	37.77	3 $5T_{1g}$	13.78	4 $5T_{2g}$	12.81	4 $5E_g$	10.21	3 $5T_{2g}$
16 T_{1g}	2.798	284	29907	45.98	3 $5T_{1g}$	25.36	2 $5T_{1g}$	17.30	4 $5T_{2g}$		
8 A_{1g}	2.797	285	29956	55.57	4 $5E_g$	21.20	4 $5T_{2g}$	16.77	3 $5T_{2g}$		
13 E_g	2.797	283	30010	20.58	1 $5T_{1g}$	15.63	2 $5A_{1g}$	12.25	4 $5E_g$		
22 T_{2g}	2.797	284	30049	14.01	1 $5T_{1g}$	13.06	2 $5A_{1g}$	12.20	1 $5A_{1g}$	11.63	2 $5T_{1g}$
14 E_g	2.797	285	30050	35.89	1 $5T_{1g}$	23.50	2 $5E_g$	13.78	1 $5A_{1g}$		
7 A_{2g}	2.797	285	30087	38.07	1 $5T_{1g}$	35.69	2 $5E_g$	12.27	4 $5T_{1g}$		
9 A_{1g}	2.797	284	30209	59.14	2 $5T_{2g}$	15.13	5 $5E_g$	14.91	2 $5E_g$		
17 T_{1g}	2.797	285	30209	53.06	2 $5T_{2g}$						
23 T_{2g}	2.798	284	30233	46.73	2 $5T_{2g}$	12.48	1 $5T_{1g}$	12.34	5 $5T_{1g}$		
8 A_{2g}	2.797	285	30652	42.03	3 $5T_{2g}$	24.71	4 $5T_{2g}$	22.18	2 $5T_{1g}$		
18 T_{1g}	2.797	285	30653	42.08	3 $5T_{2g}$	24.69	4 $5T_{2g}$	22.13	2 $5T_{1g}$		
24 T_{2g}	2.797	285	30656	28.86	2 $5T_{1g}$	27.16	3 $5T_{2g}$	22.27	4 $5T_{2g}$	10.84	3 $5E_g$
10 A_{1g}	2.797	284	30738	32.22	3 $5E_g$	29.71	4 $5E_g$	28.59	3 $5T_{2g}$		
19 T_{1g}	2.797	285	30751	40.27	3 $5T_{1g}$	21.82	4 $5T_{2g}$	13.84	3 $5E_g$	10.86	3 $5T_{2g}$
15 E_g	2.797	285	30819	28.81	4 $5E_g$	25.41	4 $5T_{2g}$	18.20	2 $5A_{1g}$		
25 T_{2g}	2.798	284	30895	27.89	2 $5A_{1g}$	23.94	2 $5T_{1g}$	18.43	4 $5T_{2g}$	12.98	4 $5E_g$
				10.47	3 $5T_{1g}$						
20 T_{1g}	2.798	284	30926	42.40	3 $5T_{1g}$	38.25	4 $5E_g$				
21 T_{1g}	2.797	285	31709	56.79	3 $5T_{2g}$	20.63	3 $5E_g$	11.73	2 $5T_{1g}$		
16 E_g	2.797	285	31757	30.99	3 $5T_{2g}$	29.07	2 $5T_{1g}$	28.90	3 $5E_g$		
22 T_{1g}	2.797	285	31772	35.81	2 $5T_{1g}$	26.96	3 $5E_g$	17.68	3 $5T_{2g}$	10.42	4 $5T_{2g}$
11 A_{1g}	2.797	285	31812	61.93	4 $5T_{2g}$	26.16	3 $5E_g$	10.33	4 $5E_g$		
23 T_{1g}	2.797	285	31856	38.21	4 $5T_{2g}$	24.23	2 $5T_{1g}$	14.89	4 $5E_g$	13.27	3 $5T_{1g}$
26 T_{2g}	2.797	285	31897	34.64	4 $5T_{2g}$	29.53	3 $5T_{1g}$	11.77	4 $5E_g$		
9 A_{2g}	2.798	284	32058	51.10	4 $5E_g$	36.67	3 $5T_{1g}$	11.99	2 $5T_{1g}$		
27 T_{2g}	2.798	284	32094	40.56	3 $5T_{1g}$	26.56	4 $5E_g$	24.33	2 $5A_{1g}$		
17 E_g	2.798	284	32106	40.50	3 $5T_{1g}$	30.54	2 $5A_{1g}$	21.63	4 $5E_g$		

[a] Absorption oscillator strengths for 1 $\Gamma_{6u,8u,7u} \rightarrow i$ transitions are calculated at $d_{\mathrm{Eu-F}}$= 3.100 Å; the reference value is f_{ref} = 1.906×10^{-3}. Emission oscillator strengths for 1 $\Gamma_{8g} \rightarrow$1 Γ_{6u},1 Γ_{8u},1 Γ_{7u} and radiative emission lifetime are calculated at $d_{\mathrm{Eu-F}}$= 3.050 Å; the reference value is f_{ref} = 8.969×10^{-4}.

[b] The analyses of the wave functions have been done at $d_{\mathrm{Eu-F}}$= 3.100 Å ($4f^7$), 3.100 Å ($4f^6(5d^1 + 6sa^1_{1g})$), 2.850 Å ($4f^6$).

[c] C.f. Table S7.

[d] C.f. Table S8.

TABLE S15: Comparison between calculated and experimental exciations energies. For the lowest $4f^6 5d^1$ state of Eu^{2+}, zero-phonon lines (ZPL) were visible in low temperature emission or excitation spectra in most cases, except for the BaF_2 and BaS hosts. In the latter two cases, the ZPL location was estimated (shown in italic). Energies given in cm^{-1}.

		E_{calc}	E_{exp}	diff.			E_{calc}	E_{exp}	diff.			E_{calc}	E_{exp}	diff.
			CaF_2:Eu^{2+}					SrF_2:Eu^{2+}					BaF_2:Eu^{2+}	
$4f^7$			Ref. 32		$4f^7$			Ref. 32		$4f^7$			Ref. 33	
^8S		0	0	0	^8S		0	0	0	^8S		0	0	0
^6P	2 Γ_{8u}	30442	27558	2884	^6P	2 Γ_{8u}	30577	27654	2923	^6P	2 Γ_{8u}	30809	27727	3082
	2 Γ_{7u}	30453	27564	2889		2 Γ_{7u}	30585	27658	2927		2 Γ_{7u}	30815	27729	3086
	3 Γ_{8u}	30826	27588	3238		3 Γ_{8u}	30962	27672	3290		3 Γ_{8u}	31194	27738	3456
	2 Γ_{6u}	31053	27959	3094		2 Γ_{6u}	31194	28066	3128					
	4 Γ_{8u}	31065	27999	3066		4 Γ_{8u}	31205	28098	3107					
^6I	3 Γ_{6u}	34758	30760	3998	^6I	3 Γ_{6u}	34938	30887	4051					
	5 Γ_{8u}	34766	30880	3886		5 Γ_{8u}	34945	31000	3945					
	6 Γ_{8u}	34798	31057	3741		4 Γ_{6u}	34989	31210	3779					
	7 Γ_{8u}	34807	31107	3700		5 Γ_{6u}	35261	31407	3854					
	8 Γ_{8u}	35033	31296	3737		6 Γ_{7u}	35315	31450	3865					
	10 Γ_{8u}	35172	31318	3854		6 Γ_{6u}	35317	31479	3838					
	5 Γ_{7u}	35182	31371	3811		2 Γ_{8u}	35356	31526	3830					
	6 Γ_{7u}	35210	31433	3777		7 Γ_{6u}	35362	31561	3801					
	12 Γ_{8u}	35213	31446	3767		7 Γ_{7u}	35382	31590	3792					
	7 Γ_{7u}	35242	31485	3757		3 Γ_{8u}	35405	31610	3795					
	8 Γ_{6u}	35265	31513	3752		8 Γ_{6u}	35414	31632	3782					
	14 Γ_{8u}	35315	31540	3775		8 Γ_{7u}	35442	31647	3795					
	15 Γ_{8u}	35376	31653	3723		5 Γ_{8u}	35499	31749	3750					
	17 Γ_{8u}	35496	31710	3786		9 Γ_{6u}	35590	31766	3824					
	9 Γ_{7u}	35510	31748	3762		9 Γ_{6u}	35590	31766	3824					
^6D	10 Γ_{6u}	37633	33890	3743		9 Γ_{7u}	35633	31828	3805					
	19 Γ_{8u}	37672	34010	3662	^6D	10 Γ_{6u}	37811	33990	3821					
	11 Γ_{6u}	37925	34503	3422		19 Γ_{8u}	37829	34115	3714					
	20 Γ_{8u}	38099	34620	3479		20 Γ_{8u}	38276	34650	3626					
	21 Γ_{8u}	38311	34685	3626		21 Γ_{8u}	38489	34740	3749					
	12 Γ_{6u}	38515	34785	3730		10 Γ_{7u}	38557	34770	3787					
	22 Γ_{8u}	38609	34950	3659		12 Γ_{6u}	38667	34860	3807					
$4f^6 5d^1$			Ref. 34		$4f^6 5d^1$			Ref. 33		$4f^6 5d^1$			Ref. 33	
	1 Γ_{8g}	25720	24215	1505		1 Γ_{8g}	26828	24925	1903		1 Γ_{8g}	28044	*25636*	*2408*
			CaF_2:Eu^{3+}											
$4f^6$			Ref. 35											
$^7F_0$	1 A_{1g}	0	0	0										
$^7F_1$	1 T_{1g}	345	337	8										
$^7F_2$	1 T_{2g}	803	811	-8										
	1 E_g	1406	1342	64										
$^7F_3$	2 T_{1g}	1971	1857	114										
	2 T_{2g}	2111	1968	143										
	1 A_{2g}	2352	2107	245										
$^7F_4$	2 A_{1g}	2501	2845	-344										
	3 T_{1g}	3114	2879	235										
	3 T_{2g}	3361	3021	340										
	2 E_g	3472	3233	239										
$^7F_5$	4 T_{2g}	4132	3793	339										
	4 T_{1g}	4404	3933	471										
	3 E_g	4600	4028	572										
	5 T_{1g}	4602	4438	164										
$^7F_6$	3 A_{1g}	5524	4920	604										
	6 T_{1g}	5580	4946	634										
	5 T_{2g}	5603	5044	559										

	4 E_g	5806	5062	744
	6 T_{2g}	5813	5184	629
	2 A_{2g}	5827	5411	416
$^5D_0$	4 A_{1g}	20023	17274	2749
$^5D_1$	7 T_{1g}	20828	19030	1798

	CaS:Eu^{2+}				SrS:Eu^{2+}				BaS:Eu^{2+}			
$4f^6$5d^1			Ref. 36		$4f^6$5d^1		Ref. 37		$4f^6$5d^1		Ref. 38	
	1 Γ_{8g}	17309	15995	1314	1 Γ_{8g}	18978	17191	1787	1 Γ_{8g}	20356	*18729*	*1627*

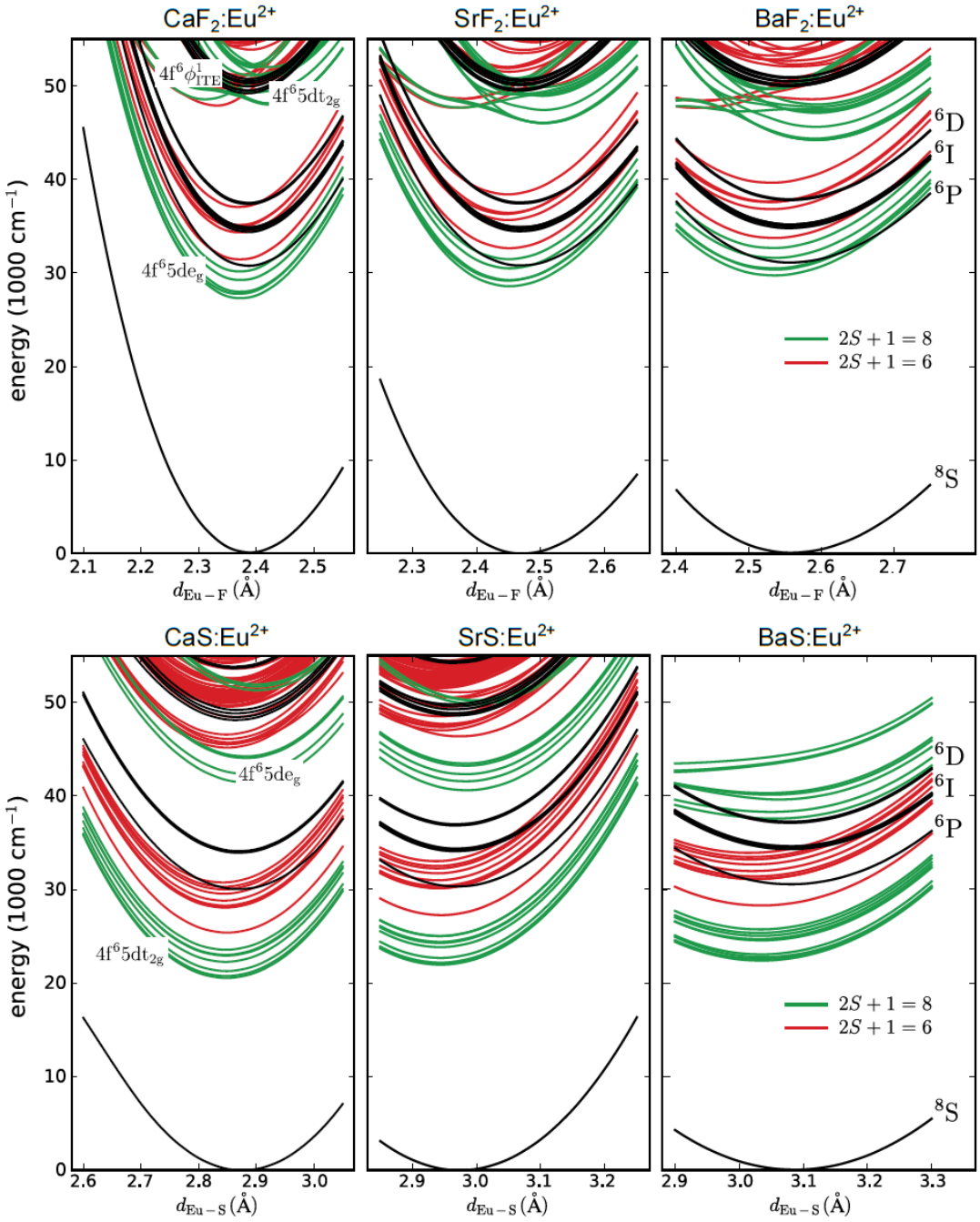

FIG. S1. Potential energy curves at spin-orbit-free MS-RASPT2 level for the Eu^{2+} impurity in the alkaline earth fluorides CaF_2, SrF_2 and BaF_2 and alkaline earth sulfides CaS, SrS and BaS. The black curves show the levels that correspond to the $4f^7$ configuration, while green and red curves originate from the excited states with $4f^6(5d,ITE_{a_{1g}}/6s)^1$ configurations, indicating spin-octet and spin-sextet levels respectively. Fig. 3 from the main text shows the potential energy curves after spin-orbit coupling is included.

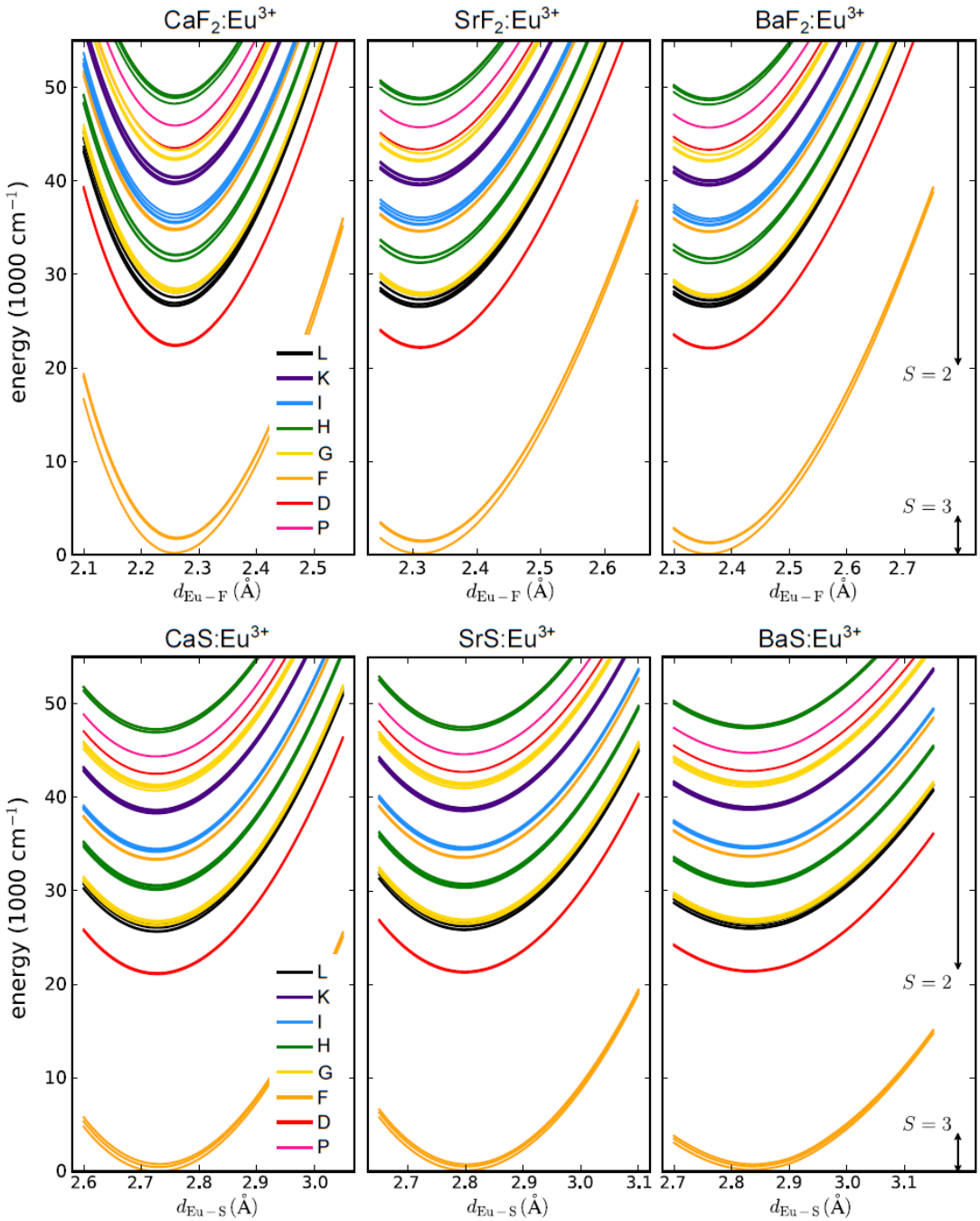

FIG. S2. Potential energy curves at spin-orbit-free MS-RASPT2 level for states of the $4f^6$ configuration of the Eu^{3+} impurity in the alkaline earth fluorides CaF_2, SrF_2 and BaF_2 and alkaline earth sulfides CaS, SrS and BaS. The color of the curves denotes the main L value of the associated ^{2S+1}L term.

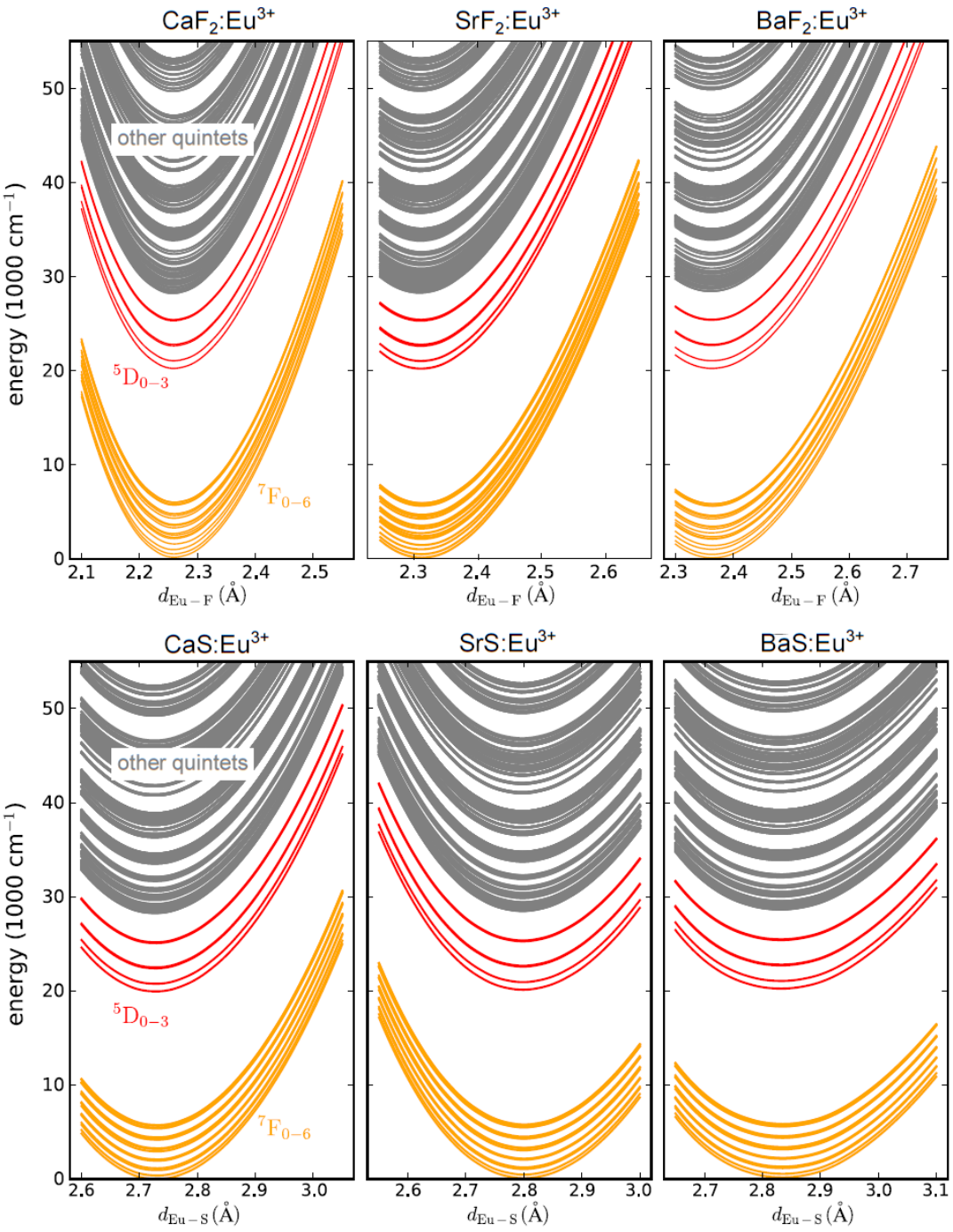

FIG. S3. Potential energy curves after spin-orbit coupling (at RASSI-SO level) for states of the $4f^6$ configuration of the Eu^{3+} impurity in the alkaline earth fluorides CaF_2, SrF_2 and BaF_2 and alkaline earth sulfides CaS, SrS and BaS. The orange and red curves correspond to the low-lying ^7F and ^5D multiplets respectively, while the grey curves show higher levels originating from other spin-quintet multiplets.