

Supplementary Information
for
Natural van der Waals silicates as hosts for telecom quantum
emitters: the case of erbium-doped talc

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S1. SUPPLEMENTARY RESULTS

S1.1. Comparison of R2SCAN and HSE06 functionals

In order to evaluate the performance of the R2SCAN functional relative to the more expensive hybrid alternative, HSE06, we ran comparative test calculations. In particular, the formation energy (E^f) and M-O bond lengths (where M stands for Mg or Er) were determined using identical VASP settings (as described under section S2) apart from functional choice. The results are summarized in Tab. S1. Overall, formation energies (herein omitting the E_{corr} term) agree within an error range of 1 eV, while bond distances are essentially identical.

Table S1. Comparison of R2SCAN and HSE06 results.

Defect	E^f (eV)		$r(\text{M-O})$ (Å)	
	R2SCAN	HSE06	R2SCAN	HSE06
Bulk talc (Mg_1)	-	-	2.05-2.06	2.04-2.07
Bulk talc (Mg_2)	-	-	2.04-2.07	2.05-2.08
Er _{Mg1}	(optimization failed)	-1.5	(optimization failed)	2.29-2.31
Er _{Mg2}	-1.6	-2.4	2.20-2.29	2.20-2.29
V _H Er _{Mg1}	-3.3	-4.3	2.02-2.34	2.02-2.33
V _H Er _{Mg2}	-3.3	-4.3	2.02-2.33	2.02-2.33
2V _H Er _{Mg1}	-0.8	-1.4	2.04-2.22	2.04-2.22
2V _H Er _{Mg2}	-0.3	-1.2	2.06-2.25	2.09-2.24

S1.2. Interstitial erbium defects in talc

In this section, we investigate bilayer talc represented by a 3x2x2 supercell. A positively charged erbium ion is introduced between the layers to examine whether erbium preferentially incorporates into the talc lattice (as described in the main text) or tends to occupy an interstitial position, see S1.

The presence of Er³⁺ does not alter the interlayer oxygen-oxygen distances significantly (pristine: 4.27Å; with Er³⁺: 4.16Å), however, significant changes in the orientation of nearby

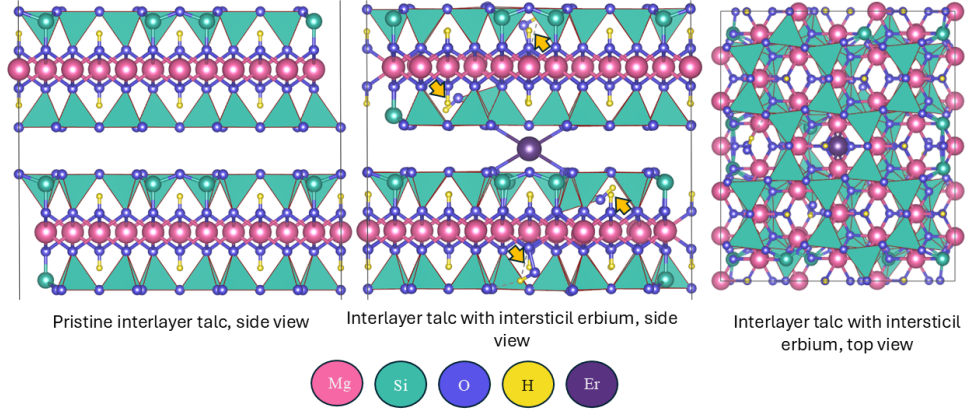


Fig. S1. The structure of a two layer pristine talc and with an interstitial Er atom. Purple, turquoise, mauve, blue, and yellow spheres indicate the positions of erbium, silicon, magnesium, oxygen, and hydrogen atoms.

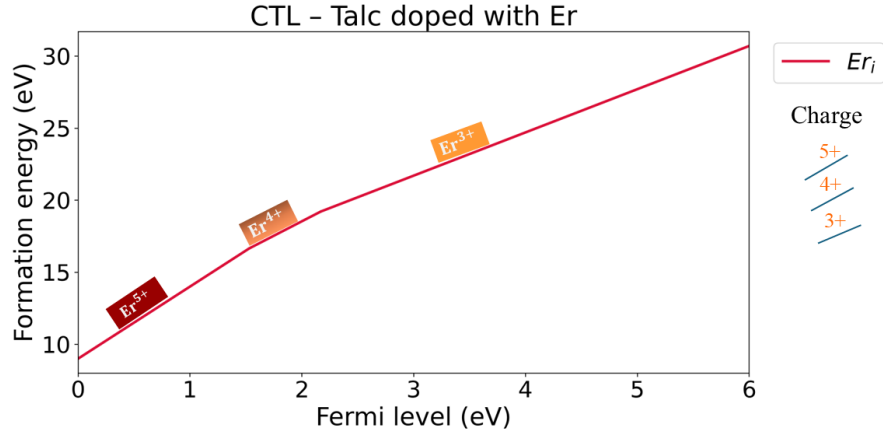


Fig. S2. Formation energy of the interstitial erbium centers in talc as a function of the Fermi level.

OH groups can be observed, see yellow arrows in Fig.S1.

The calculated formation energy of interstitial Er^{n+} ($n=3-5$ in the relevant Fermi level range) is high: 9.0 eV is calculated even at the most favorable p-type conditions (Fig. S2), indicating that erbium preferentially occupies the Mg^{2+} sites.

S1.3. Construction of cluster models

The cluster model for each species of Tab. 1 was prepared as follows. The starting point is the DFT-optimized supercell geometry (specific to the given defect), from which the position of $274 - n_{V_H}$ atoms were cut, where n_{V_H} is the number of hydrogen vacancy sites (V_H) in the studied defect. The 274 atoms would correspond to Si, O, Mg, and yellow-labeled structural H atoms, as shown in Fig. S3, in the case of bulk talc; for a given erbium-containing defect, however, an Er atom is selected in lieu of Mg at site "1" or "2" (for Er_{Mg1} and Er_{Mg2} substitutionals, respectively), and one or two hydrogen atoms from the OH group(s) closest to Er is absent for " V_H " and " $2V_H$ " type defects, respectively. Finally, 24 terminal H atoms (labeled by orange in Fig. S1) were added to the outer oxygen atoms of the two tetrahedral silicate sheets, at which the Si-O bonds were cut to create the finite-size cluster. These terminal atoms were placed at the position of the missing Si neighbors, but the O-H distance was reduced to 1.01 Å, without changing angles or dihedral angles.

The geometries for all cluster models in xyz format can be found in section S3.

The above described process of cluster model construction was motivated by the work of Tunega and Turi Nagy [1], where the 298-atom cluster of Fig. S1 was presented as a charge-neutral molecular model for bulk talc. It was also demonstrated that the electronic properties of the central part of the cluster (i.e. the vicinity of centers "1" and "2") closely resemble those of infinite monolayer talc.

S1.4. Comparison of supercell and cluster models

To validate our cluster model, we assessed whether it is sufficiently large to reproduce the electrostatic environment of the embedded Er center in the investigated systems. For this purpose, we compared the coordinate-dependence of the local potential energy of electrons near Er, as obtained from two periodic VASP calculations, i.e. (1) cluster model within a 25 Å vacuum box and (2) the corresponding reference supercell model, as described under Methods in the main text. Both calculations were performed using the R2SCAN functional, with identical settings (see section S2.)

The VASP LOCPOT file stores the local potential on a uniform real-space grid, which is to be compared for the two models. Herein, this comparison is provided for the plane of Er

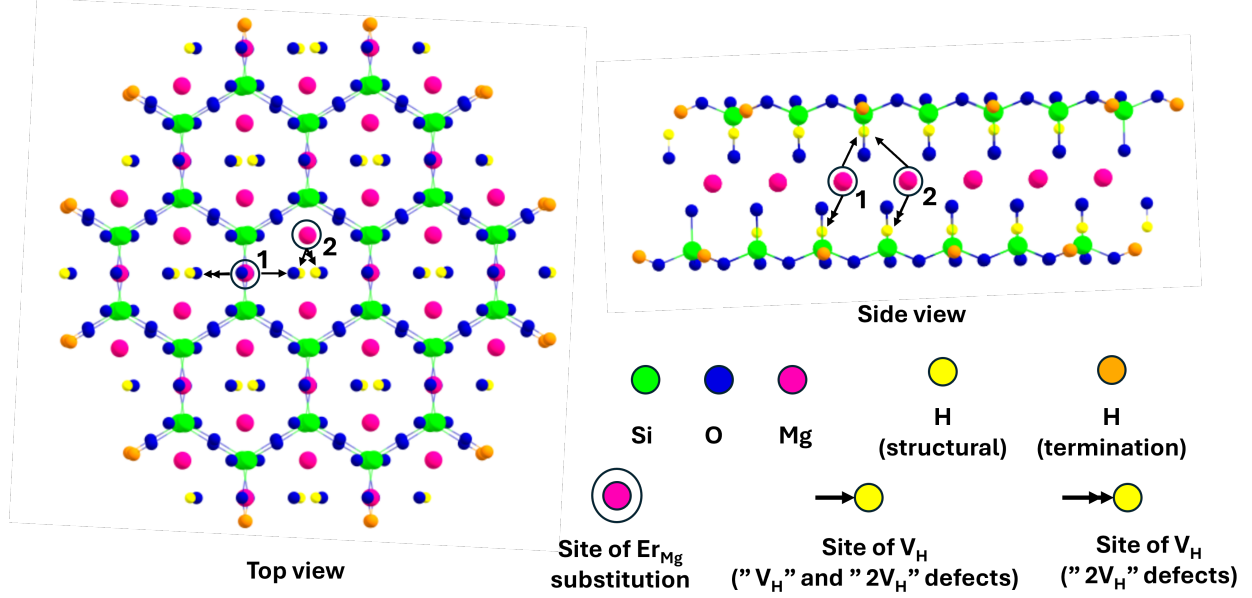


Fig. S3. Visualization of the 298-atom cluster model used to study the erbium-containing defects in talc.

and Mg atoms, in the vicinity of Er (Fig. S4).

Since the absolute zero of the potential is set independently in the calculations, the two LOCPOT maps were compared only after removal of the constant offset, following the usual potential-alignment logic employed in supercell defect calculations [2]. The latter was determined by minimizing the mean absolute difference between the local potentials. Furthermore, near-core regions (shown in white in Fig. S4) were excluded from both the visual comparison and all numerical diagnostics, as the local potential close to the nuclei is dominated by steep atomic-scale features, the frozen-core/projector-augmented-wave representation, and grid interpolation details rather than by the varying embedding field of interest [3, 4]. Specifically, circular masks of radius 1.2 Å around Er and 0.8 Å around Mg were applied to conservatively exclude the PAW near-core regions from the comparison.

A cluster model that is too small is expected to show artificial boundary effects in the potential map, because the electrostatic response of the real periodic environment is replaced by vacuum and by the finite termination of the cluster. In practice this may appear as an unphysical long-range gradient or curvature of the offset-corrected LOCPOT toward the edges of the plotted region, even if the immediate coordination shell is geometrically identical. Accordingly, as the measure of cluster model quality, we plot the deviation between the

two offset-corrected potentials over the chemically relevant region (Fig. S4, right column). In Tab. S2, we also report a scalar similarity index (S_{LOCPOT}), computed from the mean absolute error of local potential energies as

$$S_{LOCPOT} = 1 - \frac{\langle |V_{cluster}(x, y) - V_{supercell}(x, y)| \rangle}{\max(V_{cluster}, V_{supercell}) - \min(V_{cluster}, V_{supercell})} \quad (S1)$$

The value of S_{LOCPOT} approaches 1 in the case of essentially identical potential energy maps, while reduces nearly to zero if the model-related variation of data becomes commensurable to the maximal potential energy difference observed within one LOCPOT map.

Fig. S4 and Tab. S2 clearly indicate that the local potential energy maps sampled from cluster models properly reflect those sampled from corresponding supercells. No visually detectable effect of cluster termination can be observed, and all S_{LOCPOT} values remain above 0.98, showing perfect similarity.

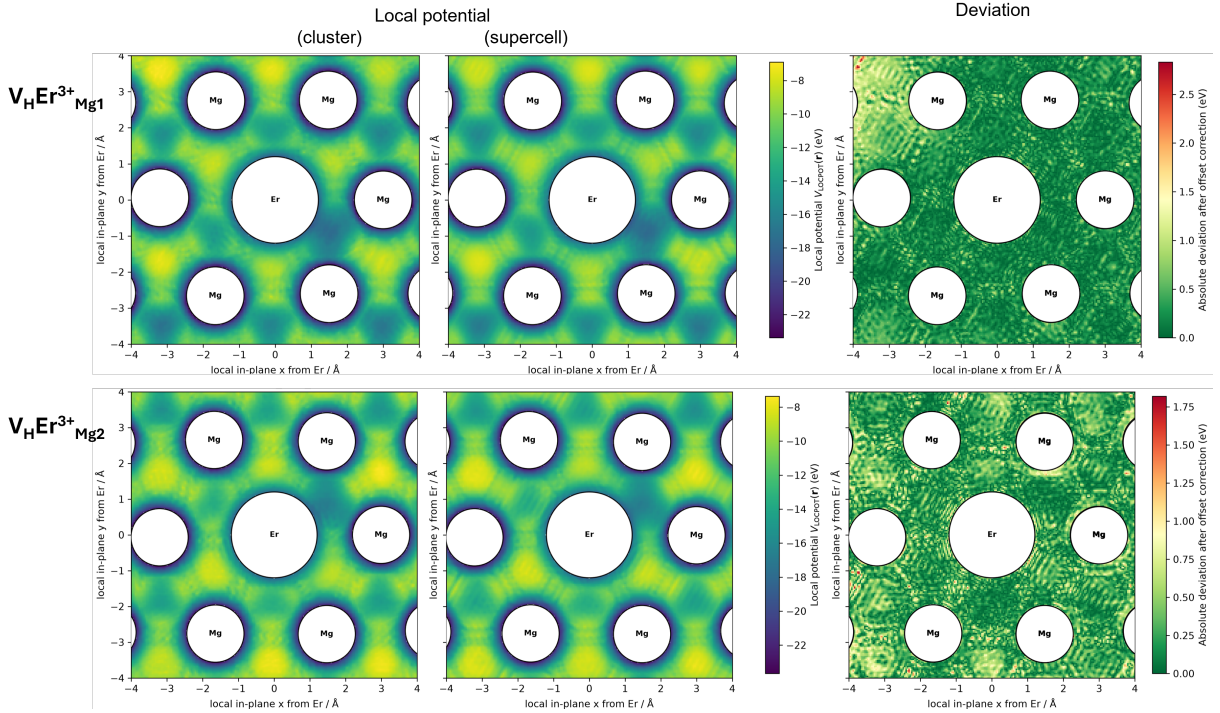


Fig. S4. Comparison of local potential energies of electrons in cluster models (left column) and supercells (middle column) in the vicinity of the Er center. Plots of the right column indicate coordinate-dependent deviations.

Table S2. Similarity index (S_{LOCPOT}) calculated from cluster-model and supercell-model local potential energy maps.

Defect	S_{LOCPOT}
$V_H Er_{Mg1}^{3+}$	0.982
$V_H Er_{Mg2}^{3+}$	0.982

S1.5. Boltzmann statistics of ${}^4I_{13/2} \rightarrow {}^4I_{15/2}$ and ${}^4I_7 \rightarrow {}^4I_8$ emissions

The radiative photoluminescence (PL) rates were obtained by post-processing the SOC-corrected ORCA one-photon spectroscopy output by an in-house developed script. In the first step, two parts of the ORCA output are parsed: the SOC-corrected combined electric-dipole/magnetic-dipole/electric-quadrupole absorption table and the ORCA Boltzmann population block. Each row of the ORCA spectrum has the form $f \rightarrow i$ where (f) is the final state of PL, i.e. the lower-energy state and (i) is the initial state of PL, i.e. the upper-energy state. The same transition is interpreted as an emission channel in the reverse direction ($i \rightarrow f$). Only transitions for which the f state belongs to the selected lower manifold and i state belongs to the selected emitting manifold are retained. For Er^{3+} the default lower manifold is taken as states (0,...,15), corresponding to the (${}^4I_{15/2}$) multiplet, and the default emitting manifold is taken as states (16,...,29), corresponding to the (${}^4I_{13/2}$) multiplet. For Er^{4+} , the corresponding default windows are states (0,...,16) for the (5I_8) lower manifold and states (17,...,31) for the (5I_7) emitting manifold. The transition energy (ΔE_{if}), as well as magnetic and electric dipole induced oscillator strengths (f_{if}^M, f_{if}^E) are extracted for all individual $i \rightarrow f$ transitions separately. We note here that oscillator strengths printed by ORCA are population-weighted absorption oscillator strengths. Therefore, before using them to calculate emission rates, the population weighing needs to be removed. We further note that electric and magnetic transition dipole moments (μ_M, μ_E) can be obtained from the oscillator strength using the general formula of

$$\mu_{if} = \left(\frac{3f_{if}}{2\Delta E_{if}} \right)^{1/2} \quad (S2)$$

The electric-dipole and magnetic-dipole spontaneous-emission rates are then computed from the corresponding oscillator strengths as

$$k_{if}^M = \frac{2\alpha^3}{t_{au}} n^3 (\Delta E_{if})^2 f_{if}^M. \quad (S3)$$

and

$$k_{if}^E = \frac{2\alpha^3}{t_{\text{au}}} n (\Delta E_{if})^2 f_{if}^E. \quad (\text{S4})$$

where n is the refractive index of the host medium, t_{au} is the atomic unit of time, and α is the fine-structure constant. Thus, we apply an n -scaling to the electric-dipole contribution and an n^3 -scaling to the magnetic-dipole contribution. Finally, the rate of a given individual Stark transition is obtained as

$$k_{if} = \frac{1}{\tau_{if}} = k_{if}^M + k_{if}^E \quad (\text{S5})$$

From the point of view of quantum applications, these individual rates determine the brightness of a selected, well-defined optical transition that can be enhanced by the Purcell effect. Therefore, the highest obtained k_{if} values are provided in Tab. 4 of the main text.

General optoelectronic applications, on the other hand, do not require single-photon emission and can utilize all Stark transitions. In this case, the brightness is related to the total rate (k^{total}) of all available ZPLs. To investigate this total rate, we prepared a Boltzmann averaging as follows.

When investigating overall brightness from multiple ZPLs, k_{if} is not equal to the expected rate of photon emission, as the relative Boltzmann population of the initial Stark state ($0 < p_i < 1$) also has to be accounted for by a prefactor. In the case of non-Kramers ions, such as Er^{4+} , the radiative rate belonging to individual ZPLs (k_{if}^{eff}) corresponds simply to

$$k_{if}^{eff} = \frac{1}{\tau_{if}^{eff}} = p_i k_{if} \quad (\text{S6})$$

For Kramers ions, such as Er^{3+} , however, a single ZPL arises from four individual rates, as two initial ($i1, i2$) and two final ($f1, f2$) states are degenerate. Therefore, the PL rate observable in experiments ($k_{if}^{eff, Kramers}$) is

$$k_{if}^{eff, Kramers} = \frac{1}{\tau_{if}^{eff, Kramers}} = \sum_{i=1,2} \sum_{f=1,2} p_i k_{if} \quad (\text{S7})$$

For a given emitting Stark state (i), the total electric- and magnetic-dipole rates are obtained by summing over all selected lower-manifold final states:

$$k_i^E = \sum_{f \in \mathcal{F}} k_{if}^E \quad (\text{S8})$$

$$k_i^{\text{M}} = \sum_{f \in \mathcal{F}} k_{if}^{\text{M}} \quad (\text{S9})$$

$$k_i = k_i^{\text{M}} + k_i^{\text{E}} \quad (\text{S10})$$

Here, $\mathcal{F}$ denotes the selected final-state manifold. The thermal averaging is then performed on the initial side of PL, as also indicated in equations (3) and (4) in the main text:

$$k^{\text{total}} = \sum_i p_i k_i \quad (\text{S11})$$

For the compact characterization of the overall transition strength (which is presented in Tab. 3 of the main text), we define a representative emission energy as the Boltzmann-weighted average over all retained emission lines,

$$\Delta E_{\text{rep}} = \frac{\sum_i p_i \sum_{f \in \mathcal{F}} \Delta E_{if}}{\sum_i p_i \sum_{f \in \mathcal{F}} 1}. \quad (\text{S12})$$

Using this representative energy, effective electric and magnetic transition moments are back-calculated from the thermally averaged rates. The effective electric transition dipole is obtained as

$$\mu_{\text{E}}^{\text{eff}} = \left[\frac{3t_{\text{au}} \sum_i p_i k_i^{\text{E}}}{4\alpha^3 n (\Delta E_{\text{rep}})^3} \right]^{1/2}. \quad (\text{S13})$$

and is reported in Debye. The effective magnetic transition dipole is obtained as

$$\mu_{\text{M}}^{\text{eff}} = \left[\frac{3t_{\text{au}} \sum_i p_i k_i^{\text{M}}}{4\alpha^3 n^3 (\Delta E_{\text{rep}})^3} \right]^{1/2}. \quad (\text{S14})$$

and is reported in units of (μ_{B}) .

Finally, we provide a characteristic emission-energy interval for all defects, which was determined from the transition-resolved PL intensity. For each $i \rightarrow f$ transition, the intensity can be defined as k^{eff} , and one can sort all transitions by their emission energies. Based on the gathered data, we report the narrowest contiguous energy interval for which the summed intensity reaches at least 95% of the total PL intensity.

Table S3. Detailed Kramers-pair-resolved PL rates for **free** Er^{3+} **ion**. "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.75	1.00×10^0	0	6.03×10^0	1.66×10^2	1.43×10^{-1}	8.61×10^{-1}	1.16×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	5.10×10^{-1}	0	1.57×10^0	6.37×10^2	1.43×10^{-1}	2.24×10^{-1}	4.46×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.75	2.52×10^{-1}	0	3.85×10^{-1}	2.60×10^3	1.43×10^{-1}	5.50×10^{-2}	1.82×10^4	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.75	1.41×10^{-1}	0	1.20×10^{-1}	8.34×10^3	1.43×10^{-1}	1.71×10^{-2}	5.84×10^4	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.75	1.44×10^{-2}	0	1.25×10^{-3}	8.00×10^5	1.43×10^{-1}	1.79×10^{-4}	5.60×10^6	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.75	1.65×10^{-1}	0	1.64×10^{-1}	6.08×10^3	1.43×10^{-1}	2.35×10^{-2}	4.26×10^4	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.75	3.52×10^{-2}	0	7.46×10^{-3}	1.34×10^5	1.43×10^{-1}	1.07×10^{-3}	9.38×10^5	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.75	7.91×10^{-3}	1.86×10^{-7}	3.78×10^{-4}	2.65×10^6	1.43×10^{-1}	5.39×10^{-5}	1.85×10^7	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.75	3.77×10^{-2}	0	8.58×10^{-3}	1.16×10^5	1.43×10^{-1}	1.23×10^{-3}	8.15×10^5	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.75	7.30×10^{-1}	0	3.22×10^0	3.11×10^2	1.43×10^{-1}	4.60×10^{-1}	2.18×10^3	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.75	8.35×10^{-1}	0	4.21×10^0	2.38×10^2	1.43×10^{-1}	6.01×10^{-1}	1.66×10^3	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.75	1.67×10^{-1}	0	1.68×10^{-1}	5.96×10^3	1.43×10^{-1}	2.40×10^{-2}	4.17×10^4	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.75	1.06×10^{-1}	0	6.79×10^{-2}	1.47×10^4	1.43×10^{-1}	9.70×10^{-3}	1.03×10^5	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.75	2.48×10^{-1}	0	3.73×10^{-1}	2.68×10^3	1.43×10^{-1}	5.32×10^{-2}	1.88×10^4	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.75	1.33×10^{-1}	0	1.07×10^{-1}	9.33×10^3	1.43×10^{-1}	1.53×10^{-2}	6.53×10^4	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.75	1.46×10^{-1}	0	1.29×10^{-1}	7.77×10^3	1.43×10^{-1}	1.84×10^{-2}	5.44×10^4	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.75	4.27×10^{-1}	0	1.10×10^0	9.08×10^2	1.43×10^{-1}	1.57×10^{-1}	6.36×10^3	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.75	1.82×10^{-1}	0	2.00×10^{-1}	5.00×10^3	1.43×10^{-1}	2.86×10^{-2}	3.50×10^4	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.75	1.19×10^{-1}	0	8.54×10^{-2}	1.17×10^4	1.43×10^{-1}	1.22×10^{-2}	8.20×10^4	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	1.67×10^{-1}	0	1.68×10^{-1}	5.94×10^3	1.43×10^{-1}	2.41×10^{-2}	4.15×10^4	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.75	1.02×10^0	0	6.24×10^0	1.60×10^2	1.43×10^{-1}	8.92×10^{-1}	1.12×10^3	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.75	4.26×10^{-2}	0	1.09×10^{-2}	9.14×10^4	1.43×10^{-1}	1.56×10^{-3}	6.40×10^5	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.75	1.84×10^{-1}	0	2.04×10^{-1}	4.91×10^3	1.43×10^{-1}	2.91×10^{-2}	3.44×10^4	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.75	2.10×10^{-1}	0	2.65×10^{-1}	3.77×10^3	1.43×10^{-1}	3.79×10^{-2}	2.64×10^4	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.75	3.17×10^{-2}	0	6.06×10^{-3}	1.65×10^5	1.43×10^{-1}	8.66×10^{-4}	1.16×10^6	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.75	4.74×10^{-1}	0	1.36×10^0	7.37×10^2	1.43×10^{-1}	1.94×10^{-1}	5.15×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.75	4.68×10^{-1}	0	1.32×10^0	7.57×10^2	1.43×10^{-1}	1.89×10^{-1}	5.30×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.75	7.05×10^{-1}	0	3.00×10^0	3.34×10^2	1.43×10^{-1}	4.28×10^{-1}	2.34×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.75	1.34×10^{-1}	0	1.08×10^{-1}	9.24×10^3	1.43×10^{-1}	1.55×10^{-2}	6.47×10^4	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.75	5.85×10^{-1}	0	2.06×10^0	4.84×10^2	1.43×10^{-1}	2.95×10^{-1}	3.39×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.75	1.87×10^{-1}	0	2.11×10^{-1}	4.73×10^3	1.43×10^{-1}	3.02×10^{-2}	3.31×10^4	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.75	1.87×10^{-1}	0	2.12×10^{-1}	4.71×10^3	1.43×10^{-1}	3.03×10^{-2}	3.30×10^4	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.75	9.63×10^{-2}	0	5.59×10^{-2}	1.79×10^4	1.43×10^{-1}	7.99×10^{-3}	1.25×10^5	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.75	3.50×10^{-1}	0	7.41×10^{-1}	1.35×10^3	1.43×10^{-1}	1.06×10^{-1}	9.45×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.75	4.37×10^{-1}	0	1.15×10^0	8.67×10^2	1.43×10^{-1}	1.65×10^{-1}	6.07×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.75	7.22×10^{-1}	0	3.14×10^0	3.18×10^2	1.43×10^{-1}	4.49×10^{-1}	2.23×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.75	1.37×10^{-1}	0	1.13×10^{-1}	8.84×10^3	1.43×10^{-1}	1.62×10^{-2}	6.19×10^4	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.75	1.36×10^{-1}	0	1.11×10^{-1}	9.00×10^3	1.43×10^{-1}	1.59×10^{-2}	6.30×10^4	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.75	6.90×10^{-1}	0	2.87×10^0	3.48×10^2	1.43×10^{-1}	4.10×10^{-1}	2.44×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.75	1.20×10^{-1}	0	8.69×10^{-2}	1.15×10^4	1.43×10^{-1}	1.24×10^{-2}	8.05×10^4	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.75	8.04×10^{-2}	0	3.90×10^{-2}	2.56×10^4	1.43×10^{-1}	5.57×10^{-3}	1.80×10^5	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.75	4.99×10^{-2}	0	1.50×10^{-2}	6.65×10^4	1.43×10^{-1}	2.15×10^{-3}	4.65×10^5	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.75	9.54×10^{-2}	0	5.50×10^{-2}	1.82×10^4	1.43×10^{-1}	7.85×10^{-3}	1.27×10^5	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.75	1.22×10^{-1}	0	8.97×10^{-2}	1.11×10^4	1.43×10^{-1}	1.28×10^{-2}	7.81×10^4	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.75	3.41×10^{-1}	0	7.02×10^{-1}	1.42×10^3	1.43×10^{-1}	1.00×10^{-1}	9.97×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.75	8.59×10^{-1}	0	4.45×10^0	2.25×10^2	1.43×10^{-1}	6.35×10^{-1}	1.57×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.75	3.22×10^{-1}	0	6.25×10^{-1}	1.60×10^3	1.43×10^{-1}	8.92×10^{-2}	1.12×10^4	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.75	6.18×10^{-1}	0	2.30×10^0	4.34×10^2	1.43×10^{-1}	3.29×10^{-1}	3.04×10^3	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.75	2.51×10^{-2}	0	3.79×10^{-3}	2.64×10^5	1.43×10^{-1}	5.41×10^{-4}	1.85×10^6	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.75	1.53×10^{-1}	0	1.40×10^{-1}	7.12×10^3	1.43×10^{-1}	2.01×10^{-2}	4.99×10^4	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.75	7.75×10^{-2}	0	3.62×10^{-2}	2.76×10^4	1.43×10^{-1}	5.17×10^{-3}	1.93×10^5	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.75	3.04×10^{-1}	0	5.56×10^{-1}	1.80×10^3	1.43×10^{-1}	7.94×10^{-2}	1.26×10^4	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.75	3.43×10^{-2}	0	7.09×10^{-3}	1.41×10^5	1.43×10^{-1}	1.01×10^{-3}	9.87×10^5	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.75	1.07×10^{-1}	0	6.97×10^{-2}	1.44×10^4	1.43×10^{-1}	9.95×10^{-3}	1.00×10^5	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.75	7.30×10^{-1}	0	3.22×10^0	3.11×10^2	1.43×10^{-1}	4.59×10^{-1}	2.18×10^3	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.75	8.39×10^{-1}	0	4.25×10^0	2.36×10^2	1.43×10^{-1}	6.06×10^{-1}	1.65×10^3	0.0	100.0

We note that due to the limitations of the QDPT treatment, theoretically exact degeneracies might break in numerical results. This effect, however, has negligible influence on the rates that determine practical applications.

Table S4. Detailed Kramers-pair-resolved PL rates for Er_{Mg1}^{3+} . "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.76	4.71×10^{-1}	2.63×10^{-4}	5.07×10^0	1.97×10^2	2.43×10^{-1}	1.23×10^0	8.11×10^2	0.2	99.8
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	3.03×10^{-1}	6.25×10^{-5}	2.06×10^0	4.85×10^2	2.43×10^{-1}	5.01×10^{-1}	2.00×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.75	9.13×10^{-1}	1.64×10^{-4}	1.84×10^1	54.438	2.43×10^{-1}	4.47×10^0	2.24×10^2	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.74	3.74×10^{-1}	1.42×10^{-4}	3.02×10^0	3.31×10^2	2.43×10^{-1}	7.35×10^{-1}	1.36×10^3	0.1	99.9
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.74	2.94×10^{-1}	2.52×10^{-4}	1.86×10^0	5.38×10^2	2.43×10^{-1}	4.52×10^{-1}	2.21×10^3	0.4	99.6
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.71	7.35×10^{-2}	9.11×10^{-5}	1.01×10^{-1}	9.85×10^3	2.43×10^{-1}	2.47×10^{-2}	4.05×10^4	0.7	99.3
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.70	4.79×10^{-2}	1.05×10^{-4}	4.24×10^{-2}	2.36×10^4	2.43×10^{-1}	1.03×10^{-2}	9.71×10^4	2.3	97.7
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.70	7.12×10^{-2}	4.32×10^{-5}	9.09×10^{-2}	1.10×10^4	2.43×10^{-1}	2.21×10^{-2}	4.53×10^4	0.2	99.8
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.76	8.38×10^{-1}	1.67×10^{-4}	1.63×10^1	61.333	2.08×10^{-1}	3.39×10^0	2.95×10^2	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.76	4.72×10^{-1}	9.35×10^{-5}	5.10×10^0	1.96×10^2	2.08×10^{-1}	1.06×10^0	9.42×10^2	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.75	2.44×10^{-1}	2.17×10^{-4}	1.33×10^0	7.50×10^2	2.08×10^{-1}	2.78×10^{-1}	3.60×10^3	0.4	99.6
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.75	4.33×10^{-1}	1.03×10^{-4}	4.12×10^0	2.43×10^2	2.08×10^{-1}	8.57×10^{-1}	1.17×10^3	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.75	5.58×10^{-1}	1.39×10^{-4}	6.79×10^0	1.47×10^2	2.08×10^{-1}	1.41×10^0	7.07×10^2	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.71	1.98×10^{-2}	2.22×10^{-4}	1.20×10^{-2}	8.34×10^4	2.08×10^{-1}	2.50×10^{-3}	4.01×10^5	37.7	62.3
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.70	7.65×10^{-2}	1.11×10^{-4}	1.09×10^{-1}	9.21×10^3	2.08×10^{-1}	2.26×10^{-2}	4.42×10^4	1.0	99.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.70	6.64×10^{-2}	1.64×10^{-4}	8.28×10^{-2}	1.21×10^4	2.08×10^{-1}	1.72×10^{-2}	5.80×10^4	2.9	97.1
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.76	5.91×10^{-1}	5.64×10^{-5}	8.18×10^0	1.22×10^2	1.87×10^{-1}	1.53×10^0	6.53×10^2	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.76	8.08×10^{-1}	2.72×10^{-4}	1.51×10^1	66.307	1.87×10^{-1}	2.82×10^0	3.54×10^2	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.75	2.62×10^{-1}	1.32×10^{-4}	1.56×10^0	6.43×10^2	1.87×10^{-1}	2.91×10^{-1}	3.44×10^3	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	5.10×10^{-1}	1.33×10^{-4}	5.77×10^0	1.73×10^2	1.87×10^{-1}	1.08×10^0	9.26×10^2	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.75	4.65×10^{-1}	1.59×10^{-4}	4.78×10^0	2.09×10^2	1.87×10^{-1}	8.94×10^{-1}	1.12×10^3	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.71	5.30×10^{-2}	1.77×10^{-4}	5.67×10^{-2}	1.76×10^4	1.87×10^{-1}	1.06×10^{-2}	9.42×10^4	5.1	94.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.71	4.89×10^{-2}	1.51×10^{-4}	4.66×10^{-2}	2.15×10^4	1.87×10^{-1}	8.72×10^{-3}	1.15×10^5	4.4	95.6
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.70	5.12×10^{-2}	1.72×10^{-4}	5.09×10^{-2}	1.96×10^4	1.87×10^{-1}	9.53×10^{-3}	1.05×10^5	5.2	94.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.77	9.19×10^{-2}	1.46×10^{-4}	2.02×10^{-1}	4.96×10^3	1.75×10^{-1}	3.54×10^{-2}	2.83×10^4	1.2	98.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.76	5.21×10^{-1}	2.64×10^{-4}	6.33×10^0	1.58×10^2	1.75×10^{-1}	1.11×10^0	9.01×10^2	0.1	99.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.76	4.60×10^{-1}	1.14×10^{-4}	4.82×10^0	2.07×10^2	1.75×10^{-1}	8.46×10^{-1}	1.18×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.75	7.09×10^{-1}	2.01×10^{-4}	1.12×10^1	89.170	1.75×10^{-1}	1.97×10^0	5.08×10^2	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.75	6.76×10^{-1}	5.26×10^{-5}	1.02×10^1	98.499	1.75×10^{-1}	1.78×10^0	5.61×10^2	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.72	3.79×10^{-2}	6.26×10^{-5}	2.81×10^{-2}	3.56×10^4	1.75×10^{-1}	4.92×10^{-3}	2.03×10^5	1.3	98.7
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.71	1.10×10^{-1}	1.66×10^{-4}	2.28×10^{-1}	4.38×10^3	1.75×10^{-1}	4.01×10^{-2}	2.50×10^4	1.1	98.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.71	9.92×10^{-2}	1.48×10^{-4}	1.85×10^{-1}	5.41×10^3	1.75×10^{-1}	3.24×10^{-2}	3.09×10^4	1.1	98.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.79	2.26×10^{-1}	2.60×10^{-4}	1.34×10^0	7.45×10^2	6.50×10^{-2}	8.72×10^{-2}	1.15×10^4	0.6	99.4
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.79	2.13×10^{-1}	1.12×10^{-4}	1.17×10^0	8.55×10^2	6.50×10^{-2}	7.60×10^{-2}	1.32×10^4	0.1	99.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.78	1.50×10^{-1}	1.59×10^{-4}	5.71×10^{-1}	1.75×10^3	6.50×10^{-2}	3.71×10^{-2}	2.70×10^4	0.5	99.5
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.78	2.94×10^{-1}	1.39×10^{-4}	2.13×10^0	4.69×10^2	6.50×10^{-2}	1.39×10^{-1}	7.21×10^3	0.1	99.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.78	2.76×10^{-1}	1.98×10^{-4}	1.88×10^0	5.32×10^2	6.50×10^{-2}	1.22×10^{-1}	8.18×10^3	0.2	99.8
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.74	7.50×10^{-1}	1.04×10^{-4}	1.21×10^1	82.865	6.50×10^{-2}	7.84×10^{-1}	1.28×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.73	4.05×10^{-1}	1.13×10^{-4}	3.41×10^0	2.93×10^2	6.50×10^{-2}	2.22×10^{-1}	4.51×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.73	5.20×10^{-1}	1.21×10^{-4}	5.60×10^0	1.79×10^2	6.50×10^{-2}	3.64×10^{-1}	2.75×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.79	1.79×10^{-1}	2.17×10^{-4}	8.41×10^{-1}	1.19×10^3	6.34×10^{-2}	5.33×10^{-2}	1.88×10^4	0.7	99.3
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.79	2.16×10^{-1}	6.79×10^{-5}	1.20×10^0	8.31×10^2	6.34×10^{-2}	7.62×10^{-2}	1.31×10^4	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.78	1.73×10^{-1}	2.50×10^{-4}	7.66×10^{-1}	1.31×10^3	6.34×10^{-2}	4.85×10^{-2}	2.06×10^4	1.0	99.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.78	2.56×10^{-1}	2.29×10^{-4}	1.63×10^0	6.15×10^2	6.34×10^{-2}	1.03×10^{-1}	9.71×10^3	0.4	99.6
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.78	2.85×10^{-1}	1.76×10^{-4}	2.00×10^0	5.01×10^2	6.34×10^{-2}	1.27×10^{-1}	7.90×10^3	0.2	99.8
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.74	6.78×10^{-1}	1.50×10^{-4}	9.90×10^0	1.01×10^2	6.34×10^{-2}	6.27×10^{-1}	1.59×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.73	5.39×10^{-1}	1.36×10^{-4}	6.07×10^0	1.65×10^3	6.34×10^{-2}	3.85×10^{-1}	2.60×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.73	5.07×10^{-1}	1.10×10^{-4}	5.34×10^0	1.87×10^2	6.34×10^{-2}	3.38×10^{-1}	2.96×10^3	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.79	1.43×10^{-1}	6.50×10^{-5}	5.41×10^{-1}	1.85×10^3	5.79×10^{-2}	3.13×10^{-2}	3.19×10^4	0.1	99.9
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.79	2.00×10^{-1}	1.35×10^{-4}	1.04×10^0	9.62×10^2	5.79×10^{-2}	6.02×10^{-2}	1.66×10^4	0.2	99.8
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.78	5.51×10^{-2}	1.78×10^{-4}	8.12×10^{-2}	1.23×10^4	5.79×10^{-2}	4.70×10^{-3}	2.13×10^5	4.8	95.2
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.78	1.16×10^{-1}	2.28×10^{-4}	3.41×10^{-1}	2.93×10^3	5.79×10^{-2}	1.97×10^{-2}	5.06×10^4	1.8	98.2
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.78	1.12×10^{-1}	2.14×10^{-4}	3.19×10^{-1}	3.13×10^3	5.79×10^{-2}	1.85×10^{-2}	5.41×10^4	1.7	98.3
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.74	2.83×10^{-1}	8.19×10^{-5}	1.74×10^0	5.75×10^2	5.79×10^{-2}	1.01×10^{-1}	9.93×10^3	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.74	7.40×10^{-1}	1.56×10^{-4}	1.15×10^1	86.604	5.79×10^{-2}	6.68×10^{-1}	1.50×10^3	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.73	6.69×10^{-1}	5.83×10^{-5}	9.36×10^0	1.07×10^2	5.79×10^{-2}	5.42×10^{-1}	1.85×10^3	0.0	100.0

Table S5. Detailed Kramers-pair-resolved PL rates for Er_{Mg2}^{3+} . "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.76	4.54×10^{-1}	4.66×10^{-4}	4.72×10^0	2.12×10^2	2.42×10^{-1}	1.15×10^0	8.73×10^2	0.5	99.5
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	2.81×10^{-1}	1.41×10^{-4}	1.78×10^0	5.62×10^2	2.42×10^{-1}	4.31×10^{-1}	2.32×10^3	0.1	99.9
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.75	9.33×10^{-1}	1.82×10^{-4}	1.92×10^1	52.202	2.42×10^{-1}	4.65×10^0	2.15×10^2	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.74	3.77×10^{-1}	9.80×10^{-5}	3.07×10^0	3.26×10^2	2.42×10^{-1}	7.45×10^{-1}	1.34×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.74	2.72×10^{-1}	8.15×10^{-5}	1.59×10^0	6.30×10^2	2.42×10^{-1}	3.85×10^{-1}	2.60×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.71	7.00×10^{-2}	4.01×10^{-4}	1.06×10^{-1}	9.42×10^3	2.42×10^{-1}	2.58×10^{-2}	3.88×10^4	13.7	86.3
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.70	4.15×10^{-2}	4.45×10^{-4}	4.87×10^{-2}	2.05×10^4	2.42×10^{-1}	1.18×10^{-2}	8.47×10^4	35.7	64.3
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.70	6.74×10^{-2}	3.32×10^{-4}	9.13×10^{-2}	1.10×10^4	2.42×10^{-1}	2.21×10^{-2}	4.52×10^4	10.5	89.5
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.76	8.86×10^{-1}	2.77×10^{-4}	1.82×10^1	55.027	2.06×10^{-1}	3.75×10^0	2.67×10^2	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.76	4.48×10^{-1}	2.31×10^{-4}	4.58×10^0	2.18×10^2	2.06×10^{-1}	9.45×10^{-1}	1.06×10^3	0.1	99.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.75	1.23×10^{-1}	4.92×10^{-4}	3.67×10^{-1}	2.72×10^3	2.06×10^{-1}	7.56×10^{-2}	1.32×10^4	7.1	92.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.75	4.48×10^{-1}	2.03×10^{-4}	4.40×10^0	2.27×10^2	2.06×10^{-1}	9.08×10^{-1}	1.10×10^3	0.1	99.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.75	5.35×10^{-1}	2.65×10^{-4}	6.25×10^0	1.60×10^2	2.06×10^{-1}	1.29×10^0	7.76×10^2	0.1	99.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.71	1.76×10^{-2}	4.61×10^{-4}	2.55×10^{-2}	3.93×10^4	2.06×10^{-1}	5.25×10^{-3}	1.90×10^5	76.9	23.1
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.70	7.67×10^{-2}	2.21×10^{-4}	1.13×10^{-1}	8.87×10^3	2.06×10^{-1}	2.32×10^{-2}	4.30×10^4	3.9	96.1
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.70	6.87×10^{-2}	4.93×10^{-4}	1.08×10^{-1}	9.28×10^3	2.06×10^{-1}	2.22×10^{-2}	4.50×10^4	20.0	80.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.76	5.05×10^{-1}	4.08×10^{-4}	5.97×10^0	1.67×10^2	1.86×10^{-1}	1.11×10^0	8.99×10^2	0.3	99.7
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.76	8.34×10^{-1}	2.91×10^{-4}	1.60×10^1	62.330	1.86×10^{-1}	2.99×10^0	3.35×10^2	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.75	2.54×10^{-1}	2.42×10^{-4}	1.47×10^0	6.81×10^2	1.86×10^{-1}	2.73×10^{-1}	3.66×10^3	0.4	99.6
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	5.80×10^{-1}	2.94×10^{-4}	7.49×10^0	1.34×10^2	1.86×10^{-1}	1.39×10^0	7.17×10^2	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.75	4.24×10^{-1}	4.39×10^{-4}	4.00×10^0	2.50×10^2	1.86×10^{-1}	7.44×10^{-1}	1.34×10^3	0.5	99.5
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.71	4.75×10^{-2}	5.88×10^{-4}	7.55×10^{-2}	1.32×10^4	1.86×10^{-1}	1.41×10^{-2}	7.11×10^4	42.6	57.4
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.71	5.28×10^{-2}	3.83×10^{-4}	6.53×10^{-2}	1.53×10^4	1.86×10^{-1}	1.22×10^{-2}	8.23×10^4	20.3	79.7
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.71	5.75×10^{-2}	2.05×10^{-4}	6.50×10^{-2}	1.54×10^4	1.86×10^{-1}	1.21×10^{-2}	8.26×10^4	5.8	94.2
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.76	1.56×10^{-1}	2.03×10^{-4}	5.80×10^{-1}	1.72×10^3	1.77×10^{-1}	1.02×10^{-1}	9.77×10^3	0.8	99.2
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.76	5.08×10^{-1}	2.32×10^{-4}	5.99×10^0	1.67×10^2	1.77×10^{-1}	1.06×10^0	9.45×10^2	0.1	99.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.76	4.74×10^{-1}	3.35×10^{-4}	5.12×10^0	1.95×10^2	1.77×10^{-1}	9.04×10^{-1}	1.11×10^3	0.2	99.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.75	6.42×10^{-1}	2.98×10^{-4}	9.22×10^0	1.08×10^2	1.77×10^{-1}	1.63×10^0	6.14×10^2	0.1	99.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.75	7.27×10^{-1}	3.41×10^{-4}	1.17×10^1	85.109	1.77×10^{-1}	2.07×10^0	4.82×10^2	0.1	99.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.72	3.79×10^{-2}	3.07×10^{-4}	3.66×10^{-2}	2.73×10^4	1.77×10^{-1}	6.47×10^{-3}	1.55×10^5	24.1	75.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.71	1.07×10^{-1}	6.07×10^{-4}	2.48×10^{-1}	4.03×10^3	1.77×10^{-1}	4.38×10^{-2}	2.28×10^4	13.5	86.5
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.71	9.55×10^{-2}	3.08×10^{-4}	1.78×10^{-1}	5.61×10^3	1.77×10^{-1}	3.14×10^{-2}	3.18×10^4	4.8	95.2
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.79	2.32×10^{-1}	4.25×10^{-4}	1.42×10^0	7.04×10^2	6.58×10^{-2}	9.35×10^{-2}	1.07×10^4	1.6	98.4
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.79	2.11×10^{-1}	6.37×10^{-4}	1.19×10^0	8.41×10^2	6.58×10^{-2}	7.82×10^{-2}	1.28×10^4	4.2	95.8
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.78	1.41×10^{-1}	3.78×10^{-4}	5.14×10^{-1}	1.94×10^3	6.58×10^{-2}	3.38×10^{-2}	2.96×10^4	3.4	96.6
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.78	3.02×10^{-1}	4.15×10^{-4}	2.27×10^0	4.41×10^2	6.58×10^{-2}	1.49×10^{-1}	6.71×10^3	0.9	99.1
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.77	2.42×10^{-1}	4.67×10^{-4}	1.47×10^0	6.82×10^2	6.58×10^{-2}	9.65×10^{-2}	1.04×10^4	1.8	98.2
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.74	7.43×10^{-1}	2.08×10^{-4}	1.19×10^1	84.346	6.58×10^{-2}	7.80×10^{-1}	1.28×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.73	4.31×10^{-1}	2.61×10^{-4}	3.88×10^0	2.58×10^2	6.58×10^{-2}	2.55×10^{-1}	3.92×10^3	0.2	99.8
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.73	5.16×10^{-1}	3.44×10^{-4}	5.51×10^0	1.81×10^2	6.58×10^{-2}	3.63×10^{-1}	2.76×10^3	0.2	99.8
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.79	1.69×10^{-1}	3.11×10^{-4}	7.53×10^{-1}	1.33×10^3	6.40×10^{-2}	4.82×10^{-2}	2.07×10^4	1.6	98.4
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.79	2.23×10^{-1}	4.70×10^{-4}	1.30×10^0	7.67×10^2	6.40×10^{-2}	8.35×10^{-2}	1.20×10^4	2.1	97.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.78	1.68×10^{-1}	4.64×10^{-4}	7.34×10^{-1}	1.36×10^3	6.40×10^{-2}	4.70×10^{-2}	2.13×10^4	3.6	96.4
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.78	2.43×10^{-1}	4.26×10^{-4}	1.48×10^0	6.74×10^2	6.40×10^{-2}	9.50×10^{-2}	1.05×10^4	1.5	98.5
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.78	3.05×10^{-1}	3.65×10^{-4}	2.30×10^0	4.35×10^2	6.40×10^{-2}	1.47×10^{-1}	6.79×10^3	0.7	99.3
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.74	6.82×10^{-1}	1.75×10^{-4}	1.00×10^1	99.863	6.40×10^{-2}	6.41×10^{-1}	1.56×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.74	5.40×10^{-1}	2.45×10^{-4}	6.10×10^0	1.64×10^2	6.40×10^{-2}	3.91×10^{-1}	2.56×10^3	0.1	99.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.73	5.04×10^{-1}	2.73×10^{-4}	5.27×10^0	1.90×10^2	6.40×10^{-2}	3.38×10^{-1}	2.96×10^3	0.1	99.9
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.79	1.43×10^{-1}	2.37×10^{-4}	5.45×10^{-1}	1.84×10^3	5.88×10^{-2}	3.20×10^{-2}	3.12×10^4	1.3	98.7
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.79	1.99×10^{-1}	1.98×10^{-4}	1.03×10^0	9.68×10^2	5.88×10^{-2}	6.07×10^{-2}	1.65×10^4	0.5	99.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.78	6.09×10^{-2}	1.55×10^{-4}	9.71×10^{-2}	1.03×10^4	5.88×10^{-2}	5.70×10^{-3}	1.75×10^5	3.0	97.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.78	1.05×10^{-1}	4.95×10^{-4}	3.03×10^{-1}	3.31×10^3	5.88×10^{-2}	1.78×10^{-2}	5.63×10^4	9.8	90.2
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.78	1.46×10^{-1}	5.89×10^{-4}	5.73×10^{-1}	1.75×10^3	5.88×10^{-2}	3.37×10^{-2}	2.97×10^4	7.3	92.7
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.74	2.89×10^{-1}	2.53×10^{-4}	1.82×10^0	5.49×10^2	5.88×10^{-2}	1.07×10^{-1}	9.34×10^3	0.4	99.6
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.74	7.28×10^{-1}	2.07×10^{-4}	1.12×10^1	89.369	5.88×10^{-2}	6.57×10^{-1}	1.52×10^3	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.74	6.80×10^{-1}	3.46×10^{-4}	9.70×10^0	1.03×10^2	5.88×10^{-2}	5.70×10^{-1}	1.75×10^3	0.1	99.9

Table S6. Detailed Kramers-pair-resolved PL rates for $V_H Er_{Mg1}^{3+}$. "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.75	8.98×10^{-1}	3.00×10^{-3}	1.92×10^1	51.996	2.66×10^{-1}	5.11×10^0	1.96×10^2	5.1	94.9
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	3.17×10^{-1}	1.65×10^{-3}	2.53×10^0	3.95×10^2	2.66×10^{-1}	6.72×10^{-1}	1.49×10^3	11.6	88.4
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.74	6.38×10^{-1}	1.76×10^{-3}	9.11×10^0	1.10×10^2	2.66×10^{-1}	2.42×10^0	4.13×10^2	3.6	96.4
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.74	2.28×10^{-1}	3.34×10^{-3}	2.26×10^0	4.42×10^2	2.66×10^{-1}	6.02×10^{-1}	1.66×10^3	50.8	49.2
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.73	1.28×10^{-1}	2.42×10^{-3}	9.17×10^{-1}	1.09×10^3	2.66×10^{-1}	2.44×10^{-1}	4.11×10^3	63.3	36.7
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.71	5.73×10^{-2}	2.85×10^{-3}	8.18×10^{-1}	1.22×10^3	2.66×10^{-1}	2.17×10^{-1}	4.60×10^3	92.3	7.7
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.71	5.00×10^{-2}	2.36×10^{-3}	5.55×10^{-1}	1.80×10^3	2.66×10^{-1}	1.47×10^{-1}	6.78×10^3	91.5	8.5
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.67	2.34×10^{-2}	1.47×10^{-3}	1.77×10^{-1}	5.66×10^3	2.66×10^{-1}	4.70×10^{-2}	2.13×10^4	95.0	5.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.76	5.12×10^{-1}	2.78×10^{-3}	6.92×10^0	1.44×10^2	2.17×10^{-1}	1.50×10^0	6.66×10^2	12.5	87.5
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.76	9.04×10^{-1}	2.51×10^{-3}	1.92×10^1	51.999	2.17×10^{-1}	4.17×10^0	2.40×10^2	3.6	96.4
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.75	4.90×10^{-1}	1.94×10^{-3}	5.69×10^0	1.76×10^2	2.17×10^{-1}	1.24×10^0	8.09×10^2	7.1	92.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.74	3.38×10^{-1}	1.82×10^{-3}	2.84×10^0	3.52×10^2	2.17×10^{-1}	6.16×10^{-1}	1.62×10^3	12.3	87.7
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.73	1.18×10^{-1}	1.89×10^{-3}	6.51×10^{-1}	1.54×10^3	2.17×10^{-1}	1.41×10^{-1}	7.08×10^3	55.5	44.5
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.72	7.55×10^{-2}	2.22×10^{-3}	5.82×10^{-1}	1.72×10^3	2.17×10^{-1}	1.26×10^{-1}	7.92×10^3	80.8	19.2
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.71	1.16×10^{-1}	1.96×10^{-3}	6.18×10^{-1}	1.62×10^3	2.17×10^{-1}	1.34×10^{-1}	7.45×10^3	58.0	42.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.68	2.94×10^{-2}	2.11×10^{-3}	3.71×10^{-1}	2.69×10^3	2.17×10^{-1}	8.06×10^{-2}	1.24×10^4	96.2	3.8
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.76	3.49×10^{-1}	2.74×10^{-3}	3.71×10^0	2.69×10^2	1.86×10^{-1}	6.91×10^{-1}	1.45×10^3	22.9	77.1
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.76	4.94×10^{-1}	3.32×10^{-3}	6.86×10^0	1.46×10^2	1.86×10^{-1}	1.28×10^0	7.84×10^2	17.9	82.1
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.75	6.55×10^{-1}	1.80×10^{-3}	9.97×10^0	1.00×10^2	1.86×10^{-1}	1.85×10^0	5.39×10^2	3.5	96.5
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	7.86×10^{-1}	2.02×10^{-3}	1.41×10^1	70.805	1.86×10^{-1}	2.63×10^0	3.81×10^2	3.1	96.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.74	9.48×10^{-2}	2.08×10^{-3}	6.37×10^{-1}	1.57×10^3	1.86×10^{-1}	1.18×10^{-1}	8.44×10^3	70.0	30.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.72	5.01×10^{-2}	3.14×10^{-3}	1.00×10^0	1.00×10^3	1.86×10^{-1}	1.86×10^{-1}	5.38×10^3	95.0	5.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.72	1.09×10^{-1}	1.95×10^{-3}	5.93×10^{-1}	1.69×10^3	1.86×10^{-1}	1.10×10^{-1}	9.06×10^3	60.6	39.4
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.68	4.34×10^{-2}	2.06×10^{-3}	3.78×10^{-1}	2.65×10^3	1.86×10^{-1}	7.02×10^{-2}	1.42×10^4	91.6	8.4
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.77	2.13×10^{-1}	1.92×10^{-3}	1.55×10^0	6.46×10^2	1.23×10^{-1}	1.90×10^{-1}	5.26×10^3	28.1	71.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.77	2.09×10^{-1}	2.82×10^{-3}	1.98×10^0	5.06×10^2	1.23×10^{-1}	2.43×10^{-1}	4.12×10^3	47.0	53.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.76	2.68×10^{-1}	1.63×10^{-3}	1.99×10^0	5.03×10^2	1.23×10^{-1}	2.44×10^{-1}	4.10×10^3	15.2	84.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.76	5.34×10^{-1}	3.85×10^{-3}	8.23×10^0	1.21×10^2	1.23×10^{-1}	1.01×10^0	9.89×10^2	20.1	79.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.75	9.29×10^{-1}	3.49×10^{-3}	2.05×10^1	48.865	1.23×10^{-1}	2.51×10^0	3.98×10^2	6.4	93.6
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.73	2.02×10^{-1}	1.65×10^{-3}	1.12×10^0	8.90×10^2	1.23×10^{-1}	1.38×10^{-1}	7.25×10^3	24.4	75.6
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.73	2.58×10^{-1}	1.98×10^{-3}	1.74×10^0	5.73×10^2	1.23×10^{-1}	2.14×10^{-1}	4.67×10^3	22.3	77.7
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.69	3.73×10^{-2}	3.67×10^{-3}	1.18×10^0	8.50×10^2	1.23×10^{-1}	1.45×10^{-1}	6.92×10^3	97.9	2.1
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.78	1.83×10^{-1}	3.03×10^{-3}	1.96×10^0	5.09×10^2	9.29×10^{-2}	1.82×10^{-1}	5.48×10^3	57.1	42.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.78	1.97×10^{-1}	4.55×10^{-3}	3.44×10^0	2.91×10^2	9.29×10^{-2}	3.19×10^{-1}	3.13×10^3	72.0	28.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.77	1.66×10^{-1}	2.28×10^{-3}	1.27×10^0	7.87×10^2	9.29×10^{-2}	1.18×10^{-1}	8.47×10^2	47.6	52.4
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.77	3.49×10^{-1}	4.58×10^{-3}	5.31×10^0	1.88×10^2	9.29×10^{-2}	4.93×10^{-1}	2.03×10^3	45.3	54.7
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.76	3.36×10^{-1}	1.33×10^{-3}	2.78×10^0	3.60×10^2	9.29×10^{-2}	2.58×10^{-1}	3.88×10^3	7.1	92.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.74	8.28×10^{-1}	1.74×10^{-3}	1.50×10^1	66.475	9.29×10^{-2}	1.40×10^0	7.16×10^2	2.1	97.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.74	5.13×10^{-1}	1.72×10^{-3}	5.84×10^0	1.71×10^2	9.29×10^{-2}	5.43×10^{-1}	1.84×10^3	5.2	94.8
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.70	5.94×10^{-2}	2.73×10^{-3}	7.19×10^{-1}	1.39×10^3	9.29×10^{-2}	6.68×10^{-2}	1.50×10^4	91.1	8.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.78	1.82×10^{-1}	4.23×10^{-3}	3.02×10^0	3.31×10^2	8.99×10^{-2}	2.72×10^{-1}	3.68×10^3	72.3	27.7
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.78	2.21×10^{-1}	3.50×10^{-3}	2.68×10^0	3.73×10^2	8.99×10^{-2}	2.41×10^{-1}	4.15×10^3	54.9	45.1
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.77	8.51×10^{-2}	8.55×10^{-4}	2.60×10^{-1}	3.84×10^3	8.99×10^{-2}	2.34×10^{-2}	4.28×10^4	32.8	67.2
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.77	1.80×10^{-1}	1.80×10^{-3}	1.15×10^0	8.73×10^2	8.99×10^{-2}	1.03×10^{-1}	9.71×10^3	32.5	67.5
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.76	3.16×10^{-1}	3.71×10^{-3}	3.81×10^0	2.62×10^2	8.99×10^{-2}	3.43×10^{-1}	2.92×10^3	40.1	59.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.74	5.87×10^{-1}	1.45×10^{-3}	7.65×10^0	1.31×10^2	8.99×10^{-2}	6.88×10^{-1}	1.45×10^3	2.9	97.1
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.74	8.17×10^{-1}	2.21×10^{-3}	1.46×10^1	68.476	8.99×10^{-2}	1.31×10^0	7.62×10^2	3.4	96.6
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.70	3.59×10^{-2}	1.20×10^{-3}	1.51×10^{-1}	6.64×10^3	8.99×10^{-2}	1.35×10^{-2}	7.38×10^4	84.3	15.7
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.81	7.96×10^{-2}	1.74×10^{-3}	5.97×10^{-1}	1.67×10^3	2.57×10^{-2}	1.53×10^{-2}	6.52×10^4	69.7	30.3
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.81	8.30×10^{-2}	1.64×10^{-3}	5.56×10^{-1}	1.80×10^3	2.57×10^{-2}	1.43×10^{-2}	7.00×10^4	65.3	34.7
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.80	9.50×10^{-2}	3.03×10^{-3}	1.46×10^0	6.83×10^2	2.57×10^{-2}	3.76×10^{-2}	2.66×10^4	83.2	16.8
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.80	1.54×10^{-1}	4.64×10^{-3}	3.46×10^0	2.89×10^2	2.57×10^{-2}	8.89×10^{-2}	1.13×10^4	81.4	18.6
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.79	3.62×10^{-1}	4.74×10^{-3}	6.23×10^0	1.60×10^2	2.57×10^{-2}	1.60×10^{-1}	6.25×10^3	45.3	54.7
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.77	1.03×10^{-1}	2.10×10^{-3}	7.82×10^{-1}	1.28×10^3	2.57×10^{-2}	2.01×10^{-2}	4.98×10^4	67.0	33.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.77	7.65×10^{-2}	1.88×10^{-3}	5.52×10^{-1}	1.81×10^3	2.57×10^{-2}	1.42×10^{-2}	7.05×10^4	74.5	25.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.73	9.78×10^{-1}	3.42×10^{-3}	2.12×10^1	47.168	2.57×10^{-2}	5.44×10^{-1}	1.84×10^3	5.6	94.4

Table S7. Detailed Kramers-pair-resolved PL rates for $V_H Er_{Mg2}^{3+}$. "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.75	8.23×10^{-1}	3.11×10^{-3}	1.64×10^1	61.138	2.56×10^{-1}	4.19×10^0	2.39×10^2	6.5	93.5
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	4.36×10^{-1}	1.50×10^{-3}	4.48×10^0	2.23×10^2	2.56×10^{-1}	1.15×10^0	8.71×10^2	5.4	94.6
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.74	6.75×10^{-1}	1.52×10^{-3}	1.01×10^1	98.691	2.56×10^{-1}	2.60×10^0	3.85×10^2	2.4	97.6
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.74	2.14×10^{-1}	2.98×10^{-3}	1.90×10^0	5.27×10^2	2.56×10^{-1}	4.86×10^{-1}	2.06×10^3	48.4	51.6
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.73	1.52×10^{-1}	2.10×10^{-3}	9.15×10^{-1}	1.09×10^3	2.56×10^{-1}	2.35×10^{-1}	4.26×10^3	48.0	52.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.72	5.54×10^{-2}	2.19×10^{-3}	5.06×10^{-1}	1.98×10^3	2.56×10^{-1}	1.30×10^{-1}	7.71×10^3	88.3	11.7
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.71	4.40×10^{-2}	1.86×10^{-3}	3.53×10^{-1}	2.83×10^3	2.56×10^{-1}	9.06×10^{-2}	1.10×10^4	89.7	10.3
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.68	2.88×10^{-2}	1.53×10^{-3}	1.99×10^{-1}	5.04×10^3	2.56×10^{-1}	5.09×10^{-2}	1.97×10^4	93.2	6.8
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.76	5.96×10^{-1}	2.21×10^{-3}	8.68×10^0	1.15×10^2	2.22×10^{-1}	1.92×10^0	5.20×10^2	6.2	93.8
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.75	8.82×10^{-1}	2.11×10^{-3}	1.81×10^1	55.192	2.22×10^{-1}	4.02×10^0	2.49×10^2	2.7	97.3
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.75	4.15×10^{-1}	1.62×10^{-3}	4.07×10^0	2.46×10^2	2.22×10^{-1}	9.02×10^{-1}	1.11×10^3	6.9	93.1
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.74	3.63×10^{-1}	1.74×10^{-3}	3.18×10^0	3.15×10^2	2.22×10^{-1}	7.04×10^{-1}	1.42×10^3	10.0	90.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.73	1.30×10^{-1}	2.13×10^{-3}	8.11×10^{-1}	1.23×10^3	2.22×10^{-1}	1.80×10^{-1}	5.56×10^3	56.5	43.5
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.72	8.05×10^{-2}	2.12×10^{-3}	5.53×10^{-1}	1.81×10^3	2.22×10^{-1}	1.23×10^{-1}	8.15×10^3	77.0	23.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.71	1.27×10^{-1}	1.73×10^{-3}	5.86×10^{-1}	1.71×10^3	2.22×10^{-1}	1.30×10^{-1}	7.70×10^3	46.7	52.4
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.68	2.81×10^{-2}	1.93×10^{-3}	3.10×10^{-1}	3.23×10^3	2.22×10^{-1}	6.87×10^{-2}	1.46×10^4	95.8	4.2
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.76	3.85×10^{-1}	2.31×10^{-3}	4.06×10^0	2.46×10^2	1.87×10^{-1}	7.58×10^{-1}	1.32×10^3	14.8	85.2
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.76	4.62×10^{-1}	3.35×10^{-3}	6.18×10^0	1.62×10^2	1.87×10^{-1}	1.15×10^0	8.67×10^2	20.3	79.7
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.75	6.68×10^{-1}	1.69×10^{-3}	1.03×10^1	96.909	1.87×10^{-1}	1.93×10^0	5.19×10^2	3.0	97.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	7.87×10^{-1}	2.02×10^{-3}	1.42×10^1	70.668	1.87×10^{-1}	2.64×10^0	3.79×10^2	3.1	96.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.74	9.71×10^{-2}	1.65×10^{-3}	4.83×10^{-1}	2.07×10^3	1.87×10^{-1}	9.01×10^{-2}	1.11×10^4	58.4	41.6
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.72	6.03×10^{-2}	3.16×10^{-3}	1.04×10^0	9.65×10^2	1.87×10^{-1}	1.93×10^{-1}	5.17×10^3	93.0	7.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.72	1.01×10^{-1}	1.99×10^{-3}	5.74×10^{-1}	1.74×10^3	1.87×10^{-1}	1.07×10^{-1}	9.32×10^3	65.3	34.7
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.68	4.51×10^{-2}	1.94×10^{-3}	3.42×10^{-1}	2.92×10^3	1.87×10^{-1}	6.39×10^{-2}	1.57×10^4	90.0	10.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.77	2.31×10^{-1}	1.88×10^{-3}	1.72×10^0	5.83×10^2	1.25×10^{-1}	2.14×10^{-1}	4.67×10^3	24.3	75.7
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.77	2.11×10^{-1}	2.53×10^{-3}	1.82×10^0	5.51×10^2	1.25×10^{-1}	2.27×10^{-1}	4.41×10^3	40.9	59.1
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.76	2.99×10^{-1}	1.71×10^{-3}	2.42×10^0	4.13×10^2	1.25×10^{-1}	3.02×10^{-1}	3.31×10^3	13.6	86.4
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.76	5.19×10^{-1}	3.58×10^{-3}	7.64×10^0	1.31×10^2	1.25×10^{-1}	9.54×10^{-1}	1.05×10^3	18.7	81.3
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.75	9.40×10^{-1}	3.13×10^{-3}	2.07×10^1	48.338	1.25×10^{-1}	2.58×10^0	3.87×10^2	5.1	94.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.73	2.00×10^{-1}	1.65×10^{-3}	1.11×10^0	9.03×10^2	1.25×10^{-1}	1.38×10^{-1}	7.23×10^3	24.8	75.2
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.73	2.41×10^{-1}	1.88×10^{-3}	1.53×10^0	6.54×10^2	1.25×10^{-1}	1.91×10^{-1}	5.24×10^3	22.7	77.3
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.69	3.27×10^{-2}	2.91×10^{-3}	7.41×10^{-1}	1.35×10^3	1.25×10^{-1}	9.26×10^{-2}	1.08×10^4	97.5	2.5
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.78	1.74×10^{-1}	2.85×10^{-3}	1.74×10^0	5.76×10^2	9.49×10^{-2}	1.65×10^{-1}	6.07×10^3	56.7	43.3
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.78	1.84×10^{-1}	4.46×10^{-3}	3.22×10^0	3.11×10^2	9.49×10^{-2}	3.05×10^{-1}	3.28×10^3	74.0	26.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.77	1.71×10^{-1}	2.22×10^{-3}	1.28×10^0	7.80×10^2	9.49×10^{-2}	1.22×10^{-1}	8.22×10^3	44.9	55.1
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.77	3.45×10^{-1}	3.81×10^{-3}	4.49×10^0	2.23×10^2	9.49×10^{-2}	4.26×10^{-1}	2.35×10^3	37.1	62.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.76	3.42×10^{-1}	1.88×10^{-3}	3.05×10^0	3.27×10^2	9.49×10^{-2}	2.90×10^{-1}	3.45×10^3	12.8	87.2
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.74	8.61×10^{-1}	1.64×10^{-3}	1.62×10^1	61.644	9.49×10^{-2}	1.54×10^0	6.50×10^2	1.7	98.3
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.74	4.68×10^{-1}	1.59×10^{-3}	4.87×10^0	2.05×10^2	9.49×10^{-2}	4.62×10^{-1}	2.17×10^3	5.3	94.7
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.70	5.42×10^{-2}	2.12×10^{-3}	4.51×10^{-1}	2.22×10^3	9.49×10^{-2}	4.27×10^{-2}	2.34×10^4	88.1	11.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.78	2.14×10^{-1}	3.43×10^{-3}	2.58×10^0	3.88×10^2	8.97×10^{-2}	2.31×10^{-1}	4.32×10^3	55.5	44.5
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.78	1.93×10^{-1}	3.49×10^{-3}	2.39×10^0	4.18×10^2	8.97×10^{-2}	2.15×10^{-1}	4.66×10^3	61.2	38.8
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.77	9.54×10^{-2}	1.14×10^{-3}	3.73×10^{-1}	2.68×10^3	8.97×10^{-2}	3.35×10^{-2}	2.99×10^4	41.0	59.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.77	2.20×10^{-1}	2.17×10^{-3}	1.70×10^0	5.90×10^2	8.97×10^{-2}	1.52×10^{-1}	6.57×10^3	32.0	68.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.76	2.82×10^{-1}	3.04×10^{-3}	2.85×10^0	3.51×10^2	8.97×10^{-2}	2.56×10^{-1}	3.91×10^3	36.1	63.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.74	5.46×10^{-1}	1.20×10^{-3}	6.59×10^0	1.52×10^2	8.97×10^{-2}	5.91×10^{-1}	1.69×10^3	2.3	97.7
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.74	8.50×10^{-1}	1.92×10^{-3}	1.56×10^1	63.969	8.97×10^{-2}	1.40×10^0	7.13×10^2	2.4	97.6
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.70	3.68×10^{-2}	1.73×10^{-3}	2.91×10^{-1}	3.43×10^3	8.97×10^{-2}	2.61×10^{-2}	3.83×10^4	91.5	8.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.81	8.58×10^{-2}	1.59×10^{-3}	5.57×10^{-1}	1.79×10^3	2.60×10^{-2}	1.45×10^{-2}	6.91×10^4	62.6	37.4
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.81	8.23×10^{-2}	1.47×10^{-3}	4.83×10^{-1}	2.07×10^3	2.60×10^{-2}	1.26×10^{-2}	7.97×10^4	60.7	39.3
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.80	1.07×10^{-1}	2.86×10^{-3}	1.40×10^0	7.16×10^2	2.60×10^{-2}	3.63×10^{-2}	2.76×10^4	77.4	22.6
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.80	1.53×10^{-1}	3.89×10^{-3}	2.60×10^0	3.84×10^2	2.60×10^{-2}	6.76×10^{-2}	1.48×10^4	75.7	24.3
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.79	3.62×10^{-1}	4.03×10^{-3}	5.44×10^0	1.84×10^2	2.60×10^{-2}	1.41×10^{-1}	7.07×10^3	37.5	62.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.77	9.84×10^{-2}	1.52×10^{-3}	5.13×10^{-1}	1.95×10^3	2.60×10^{-2}	1.33×10^{-2}	7.51×10^4	53.7	46.3
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.77	7.62×10^{-2}	1.87×10^{-3}	5.48×10^{-1}	1.83×10^3	2.60×10^{-2}	1.42×10^{-2}	7.03×10^4	74.5	25.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.73	9.92×10^{-1}	3.15×10^{-3}	2.16×10^1	46.342	2.60×10^{-2}	5.60×10^{-1}	1.78×10^3	4.7	95.3

Table S8. Detailed Kramers-pair-resolved PL rates for $2V_H Er_{Mg1}^{3+}$. "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.76	1.04×10^0	7.34×10^{-5}	2.47×10^1	40.474	3.12×10^{-1}	7.70×10^0	1.30×10^2	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	4.61×10^{-1}	8.88×10^{-5}	4.74×10^0	2.11×10^2	3.12×10^{-1}	1.48×10^0	6.77×10^2	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.74	3.62×10^{-1}	9.95×10^{-5}	2.77×10^0	3.61×10^2	3.12×10^{-1}	8.65×10^{-1}	1.16×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.73	1.67×10^{-1}	3.59×10^{-5}	5.70×10^{-1}	1.75×10^3	3.12×10^{-1}	1.78×10^{-1}	5.62×10^3	0.0	100.0
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.72	8.43×10^{-2}	6.21×10^{-5}	1.38×10^{-1}	7.26×10^3	3.12×10^{-1}	4.29×10^{-2}	2.33×10^4	0.3	99.7
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.71	5.98×10^{-2}	1.02×10^{-4}	6.89×10^{-2}	1.45×10^4	3.12×10^{-1}	2.15×10^{-2}	4.66×10^4	1.4	98.6
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.70	7.31×10^{-2}	6.00×10^{-5}	9.90×10^{-2}	1.01×10^4	3.12×10^{-1}	3.09×10^{-2}	3.24×10^4	0.3	99.7
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.63	1.36×10^{-2}	4.41×10^{-5}	2.61×10^{-3}	3.84×10^5	3.12×10^{-1}	8.13×10^{-4}	1.23×10^6	4.8	95.2
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.76	3.82×10^{-1}	9.17×10^{-5}	3.43×10^0	2.91×10^2	2.36×10^{-1}	8.10×10^{-1}	1.23×10^3	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.76	9.74×10^{-1}	1.16×10^{-4}	2.17×10^1	46.039	2.36×10^{-1}	5.13×10^0	1.95×10^2	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.74	5.69×10^{-1}	8.80×10^{-5}	7.04×10^0	1.42×10^2	2.36×10^{-1}	1.66×10^0	6.02×10^2	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.74	1.79×10^{-1}	9.52×10^{-5}	6.74×10^{-1}	1.48×10^3	2.36×10^{-1}	1.59×10^{-1}	6.29×10^3	0.1	99.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.72	5.54×10^{-2}	8.86×10^{-5}	6.18×10^{-2}	1.62×10^4	2.36×10^{-1}	1.46×10^{-2}	6.85×10^4	1.2	98.8
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.72	1.78×10^{-1}	4.39×10^{-5}	6.20×10^{-1}	1.61×10^3	2.36×10^{-1}	1.46×10^{-1}	6.83×10^3	0.0	100.0
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.71	1.06×10^{-1}	7.16×10^{-5}	2.14×10^{-1}	4.68×10^3	2.36×10^{-1}	5.04×10^{-2}	1.98×10^4	0.2	99.8
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.64	1.47×10^{-2}	4.35×10^{-5}	3.14×10^{-3}	3.18×10^5	2.36×10^{-1}	7.42×10^{-4}	1.35×10^6	4.0	96.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.77	1.56×10^{-1}	5.79×10^{-5}	5.92×10^{-1}	1.69×10^3	1.62×10^{-1}	9.59×10^{-2}	1.04×10^4	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.77	3.18×10^{-1}	1.52×10^{-4}	2.40×10^0	4.16×10^2	1.62×10^{-1}	3.89×10^{-1}	2.57×10^3	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.75	7.73×10^{-1}	1.48×10^{-4}	1.35×10^1	74.091	1.62×10^{-1}	2.19×10^0	4.57×10^2	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	7.47×10^{-1}	6.99×10^{-5}	1.22×10^1	81.858	1.62×10^{-1}	1.98×10^0	5.05×10^2	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.73	2.54×10^{-1}	3.99×10^{-5}	1.34×10^0	7.46×10^2	1.62×10^{-1}	2.17×10^{-1}	4.61×10^3	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.73	1.94×10^{-1}	4.85×10^{-5}	7.72×10^{-1}	1.30×10^3	1.62×10^{-1}	1.25×10^{-1}	8.00×10^3	0.0	100.0
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.72	1.67×10^{-1}	5.57×10^{-5}	5.55×10^{-1}	1.80×10^3	1.62×10^{-1}	9.00×10^{-2}	1.11×10^4	0.1	99.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.65	4.55×10^{-2}	3.60×10^{-5}	3.02×10^{-2}	3.31×10^4	1.62×10^{-1}	4.89×10^{-3}	2.04×10^5	0.3	99.7
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.78	2.00×10^{-1}	1.01×10^{-4}	1.01×10^0	9.86×10^2	1.11×10^{-1}	1.12×10^{-1}	8.92×10^3	0.1	99.9
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.78	1.18×10^{-1}	1.38×10^{-4}	3.44×10^{-1}	2.91×10^2	1.11×10^{-1}	3.80×10^{-2}	2.63×10^4	0.7	99.3
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.76	2.63×10^{-1}	7.55×10^{-5}	1.62×10^0	6.16×10^2	1.11×10^{-1}	1.79×10^{-1}	5.57×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.76	5.02×10^{-1}	5.79×10^{-5}	5.74×10^0	1.74×10^2	1.11×10^{-1}	6.35×10^{-1}	1.58×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.74	7.85×10^{-1}	3.17×10^{-5}	1.33×10^1	75.257	1.11×10^{-1}	1.47×10^0	6.81×10^2	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.74	3.88×10^{-1}	6.34×10^{-5}	3.20×10^0	3.12×10^2	1.11×10^{-1}	3.54×10^{-1}	2.82×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.73	4.02×10^{-1}	4.28×10^{-5}	3.33×10^0	3.01×10^2	1.11×10^{-1}	3.68×10^{-1}	2.72×10^3	0.0	100.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.66	3.14×10^{-2}	6.19×10^{-5}	1.52×10^{-2}	6.57×10^4	1.11×10^{-1}	1.68×10^{-3}	5.94×10^5	1.9	98.1
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.78	1.38×10^{-1}	1.44×10^{-4}	4.86×10^{-1}	2.06×10^3	1.05×10^{-1}	5.12×10^{-2}	1.95×10^4	0.5	99.5
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.78	1.87×10^{-1}	6.81×10^{-5}	8.70×10^{-1}	1.15×10^3	1.05×10^{-1}	9.17×10^{-2}	1.09×10^4	0.1	99.9
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.77	2.89×10^{-1}	8.00×10^{-5}	1.97×10^0	5.06×10^2	1.05×10^{-1}	2.08×10^{-1}	4.80×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.76	3.81×10^{-1}	4.89×10^{-5}	3.31×10^0	3.02×10^2	1.05×10^{-1}	3.50×10^{-1}	2.86×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.74	5.06×10^{-1}	5.16×10^{-5}	5.56×10^0	1.80×10^2	1.05×10^{-1}	5.86×10^{-1}	1.71×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.74	7.22×10^{-1}	6.75×10^{-5}	1.11×10^1	89.905	1.05×10^{-1}	1.17×10^0	8.52×10^2	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.73	4.58×10^{-1}	5.84×10^{-5}	4.35×10^0	2.30×10^2	1.05×10^{-1}	4.59×10^{-1}	2.18×10^3	0.0	100.0
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.66	2.58×10^{-2}	5.17×10^{-5}	1.03×10^{-2}	9.67×10^4	1.05×10^{-1}	1.09×10^{-3}	9.17×10^5	1.9	98.1
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.80	1.43×10^{-1}	4.01×10^{-5}	5.42×10^{-1}	1.84×10^3	6.68×10^{-2}	3.62×10^{-2}	2.76×10^4	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.79	1.02×10^{-1}	9.32×10^{-5}	2.73×10^{-1}	3.66×10^3	6.68×10^{-2}	1.83×10^{-2}	5.48×10^4	0.4	99.6
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.78	2.04×10^{-1}	1.02×10^{-4}	1.03×10^0	9.74×10^2	6.68×10^{-2}	6.86×10^{-2}	1.46×10^4	0.1	99.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.77	4.83×10^{-1}	1.62×10^{-4}	5.60×10^0	1.79×10^2	6.68×10^{-2}	3.74×10^{-1}	2.67×10^3	0.1	99.9
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.76	4.31×10^{-1}	6.37×10^{-5}	4.22×10^0	2.37×10^2	6.68×10^{-2}	2.82×10^{-1}	3.54×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.75	6.02×10^{-1}	1.05×10^{-4}	8.12×10^0	1.23×10^2	6.68×10^{-2}	5.42×10^{-1}	1.84×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.74	8.03×10^{-1}	1.59×10^{-4}	1.40×10^1	71.331	6.68×10^{-2}	9.37×10^{-1}	1.07×10^3	0.0	100.0
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.67	4.30×10^{-2}	1.12×10^{-5}	2.99×10^{-2}	3.35×10^4	6.68×10^{-2}	2.00×10^{-3}	5.01×10^5	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.85	5.18×10^{-2}	4.40×10^{-5}	8.83×10^{-2}	1.13×10^4	7.30×10^{-3}	6.45×10^{-4}	1.55×10^6	0.3	99.7
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.85	6.37×10^{-2}	9.99×10^{-6}	1.30×10^{-1}	7.69×10^3	7.30×10^{-3}	9.50×10^{-4}	1.05×10^6	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.83	9.24×10^{-2}	1.65×10^{-5}	2.62×10^{-1}	3.82×10^3	7.30×10^{-3}	1.91×10^{-3}	5.23×10^5	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.83	1.90×10^{-1}	8.40×10^{-5}	1.08×10^0	9.28×10^2	7.30×10^{-3}	7.87×10^{-3}	1.27×10^5	0.1	99.9
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.81	1.41×10^{-1}	5.46×10^{-5}	5.66×10^{-1}	1.77×10^3	7.30×10^{-3}	4.13×10^{-3}	2.42×10^5	0.1	99.9
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.81	2.03×10^{-1}	2.81×10^{-5}	1.15×10^0	8.70×10^2	7.30×10^{-3}	8.39×10^{-3}	1.19×10^5	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.80	2.87×10^{-1}	2.81×10^{-5}	2.23×10^0	4.48×10^2	7.30×10^{-3}	1.63×10^{-2}	6.13×10^4	0.0	100.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.73	9.85×10^{-1}	4.09×10^{-5}	2.00×10^1	50.067	7.30×10^{-3}	1.46×10^{-1}	6.85×10^3	0.0	100.0

Table S9. Detailed Kramers-pair-resolved PL rates for $2V_H Er_{Mg2}^{3+}$. "KP" denotes Kramers pair.

Initial state	Final state	ΔE (eV)	μ_M (μ_B)	μ_E (D)	k_{if} (s^{-1})	τ_{if} (ms)	p_i	$k_{if}^{eff, Kramers}$ (s^{-1})	$\tau_{eff, Kramers}$ (ms)	E (%)	M (%)
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 1	0.75	1.05×10^0	2.44×10^{-3}	2.58×10^1	38.816	2.70×10^{-1}	6.97×10^0	1.44×10^2	2.5	97.5
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 2	0.75	3.38×10^{-1}	2.13×10^{-3}	3.03×10^0	3.30×10^2	2.70×10^{-1}	8.20×10^{-1}	1.22×10^3	16.1	83.9
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 3	0.74	3.53×10^{-1}	1.05×10^{-3}	2.81×10^0	3.56×10^2	2.70×10^{-1}	7.61×10^{-1}	1.31×10^3	4.1	95.9
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 4	0.73	2.38×10^{-1}	1.05×10^{-3}	1.29×10^0	7.74×10^2	2.70×10^{-1}	3.49×10^{-1}	2.86×10^3	8.6	91.4
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 5	0.73	1.50×10^{-1}	1.62×10^{-3}	7.25×10^{-1}	1.38×10^3	2.70×10^{-1}	1.96×10^{-1}	5.10×10^3	36.1	63.9
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 6	0.72	7.13×10^{-2}	1.74×10^{-3}	3.88×10^{-1}	2.58×10^3	2.70×10^{-1}	1.05×10^{-1}	9.54×10^3	74.2	25.8
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 7	0.69	3.09×10^{-2}	1.30×10^{-3}	1.60×10^{-1}	6.25×10^3	2.70×10^{-1}	4.33×10^{-2}	2.31×10^4	89.6	10.4
$^4I_{13/2}$ KP 1	$^4I_{15/2}$ KP 8	0.69	3.21×10^{-2}	1.70×10^{-3}	2.57×10^{-1}	3.89×10^3	2.70×10^{-1}	6.96×10^{-2}	1.44×10^4	93.1	6.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 1	0.76	1.82×10^{-1}	2.84×10^{-3}	1.66×10^0	6.01×10^2	2.16×10^{-1}	3.60×10^{-1}	2.78×10^3	54.2	45.8
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 2	0.76	8.93×10^{-1}	2.05×10^{-3}	1.86×10^1	53.678	2.16×10^{-1}	4.03×10^0	2.48×10^2	2.5	97.5
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 3	0.75	7.14×10^{-1}	2.53×10^{-3}	1.20×10^1	83.353	2.16×10^{-1}	2.59×10^0	3.86×10^2	5.7	94.3
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 4	0.74	2.89×10^{-1}	1.30×10^{-3}	1.97×10^0	5.08×10^2	2.16×10^{-1}	4.25×10^{-1}	2.35×10^3	8.9	91.1
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 5	0.74	1.15×10^{-1}	6.31×10^{-4}	3.18×10^{-1}	3.15×10^3	2.16×10^{-1}	6.87×10^{-2}	1.46×10^4	12.7	87.3
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 6	0.73	9.44×10^{-2}	2.78×10^{-3}	9.32×10^{-1}	1.07×10^3	2.16×10^{-1}	2.02×10^{-1}	4.96×10^3	80.8	19.2
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 7	0.70	4.88×10^{-2}	2.06×10^{-3}	4.12×10^{-1}	6.25×10^3	2.16×10^{-1}	8.90×10^{-2}	1.12×10^4	84.1	15.9
$^4I_{13/2}$ KP 2	$^4I_{15/2}$ KP 8	0.69	5.27×10^{-2}	1.83×10^{-3}	3.36×10^{-1}	2.98×10^3	2.16×10^{-1}	7.26×10^{-2}	1.38×10^4	85.4	14.6
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 1	0.77	8.97×10^{-2}	1.34×10^{-3}	3.98×10^{-1}	2.51×10^3	1.67×10^{-1}	6.64×10^{-2}	1.51×10^4	51.9	48.1
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 2	0.76	5.04×10^{-1}	2.60×10^{-3}	6.70×10^0	1.49×10^2	1.67×10^{-1}	1.12×10^0	8.95×10^2	11.4	88.6
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 3	0.76	6.40×10^{-1}	2.15×10^{-3}	9.84×10^0	1.02×10^2	1.67×10^{-1}	1.64×10^0	6.10×10^2	5.2	94.8
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 4	0.75	8.34×10^{-1}	1.82×10^{-3}	1.57×10^1	63.843	1.67×10^{-1}	2.61×10^0	3.83×10^2	2.3	97.7
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 5	0.74	2.03×10^{-1}	1.84×10^{-3}	1.24×10^0	8.07×10^2	1.67×10^{-1}	2.07×10^{-1}	4.84×10^3	28.5	71.5
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 6	0.73	1.56×10^{-1}	1.78×10^{-3}	8.23×10^{-1}	1.21×10^3	1.67×10^{-1}	1.37×10^{-1}	7.28×10^3	38.4	61.6
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 7	0.70	5.87×10^{-2}	1.94×10^{-3}	4.01×10^{-1}	2.49×10^3	1.67×10^{-1}	6.69×10^{-2}	1.49×10^4	84.1	15.9
$^4I_{13/2}$ KP 3	$^4I_{15/2}$ KP 8	0.70	5.01×10^{-2}	2.82×10^{-3}	7.43×10^{-1}	1.35×10^3	1.67×10^{-1}	1.24×10^{-1}	8.07×10^3	93.9	6.1
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 1	0.77	2.88×10^{-1}	2.47×10^{-3}	2.73×10^0	3.66×10^2	1.32×10^{-1}	3.61×10^{-1}	2.77×10^3	26.2	73.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 2	0.77	2.84×10^{-1}	2.48×10^{-3}	2.65×10^0	3.78×10^2	1.32×10^{-1}	3.50×10^{-1}	2.86×10^3	27.0	73.0
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 3	0.76	2.78×10^{-1}	2.69×10^{-3}	2.62×10^0	3.72×10^2	1.32×10^{-1}	3.46×10^{-1}	2.89×10^3	31.2	68.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 4	0.75	4.74×10^{-1}	1.76×10^{-3}	5.41×10^0	1.85×10^2	1.32×10^{-1}	7.14×10^{-1}	1.40×10^3	6.3	93.7
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 5	0.75	8.46×10^{-1}	2.03×10^{-3}	1.62×10^1	61.567	1.32×10^{-1}	2.14×10^0	4.66×10^2	2.7	97.3
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 6	0.74	4.50×10^{-1}	1.21×10^{-3}	4.44×10^0	2.25×10^2	1.32×10^{-1}	5.86×10^{-1}	1.71×10^3	3.4	96.6
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 7	0.71	7.75×10^{-2}	1.75×10^{-3}	3.94×10^{-1}	2.54×10^3	1.32×10^{-1}	5.21×10^{-2}	1.92×10^4	71.2	28.8
$^4I_{13/2}$ KP 4	$^4I_{15/2}$ KP 8	0.71	6.23×10^{-2}	1.41×10^{-3}	2.53×10^{-1}	3.96×10^3	1.32×10^{-1}	3.33×10^{-2}	3.00×10^4	71.4	28.6
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 1	0.77	2.04×10^{-1}	3.69×10^{-3}	2.63×10^0	3.80×10^2	1.25×10^{-1}	3.29×10^{-1}	3.04×10^3	61.2	38.8
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 2	0.77	1.86×10^{-1}	3.29×10^{-3}	2.09×10^0	4.78×10^2	1.25×10^{-1}	2.61×10^{-1}	3.83×10^3	60.2	39.8
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 3	0.76	2.52×10^{-1}	1.80×10^{-3}	1.86×10^0	5.39×10^2	1.25×10^{-1}	2.32×10^{-1}	4.31×10^3	19.8	80.2
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 4	0.75	2.21×10^{-1}	2.19×10^{-3}	1.64×10^0	6.11×10^2	1.25×10^{-1}	2.04×10^{-1}	4.89×10^3	32.3	67.7
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 5	0.75	5.27×10^{-1}	2.87×10^{-3}	7.05×10^0	1.42×10^2	1.25×10^{-1}	8.81×10^{-1}	1.14×10^3	12.5	87.5
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 6	0.74	8.97×10^{-1}	1.96×10^{-3}	1.76×10^1	56.875	1.25×10^{-1}	2.20×10^0	4.55×10^2	2.3	97.7
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 7	0.71	8.64×10^{-2}	2.39×10^{-3}	6.70×10^{-1}	1.49×10^3	1.25×10^{-1}	8.37×10^{-2}	1.20×10^4	78.8	21.2
$^4I_{13/2}$ KP 5	$^4I_{15/2}$ KP 8	0.71	3.84×10^{-2}	1.16×10^{-3}	1.50×10^{-1}	6.69×10^3	1.25×10^{-1}	1.87×10^{-2}	5.35×10^4	81.5	18.5
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 1	0.80	1.07×10^{-1}	1.05×10^{-3}	4.51×10^{-1}	2.22×10^3	4.64×10^{-2}	2.09×10^{-2}	4.78×10^4	31.7	68.3
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 2	0.80	1.15×10^{-1}	3.55×10^{-3}	1.97×10^0	5.07×10^2	4.64×10^{-2}	9.15×10^{-2}	1.09×10^4	82.2	17.8
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 3	0.79	2.38×10^{-1}	1.16×10^{-3}	1.64×10^0	6.10×10^2	4.64×10^{-2}	7.60×10^{-2}	1.32×10^4	10.3	89.7
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 4	0.78	2.17×10^{-1}	2.91×10^{-3}	2.21×10^0	4.52×10^2	4.64×10^{-2}	1.03×10^{-1}	9.75×10^3	46.5	53.5
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 5	0.78	3.19×10^{-1}	2.75×10^{-3}	3.40×10^0	2.94×10^2	4.64×10^{-2}	1.58×10^{-1}	6.35×10^3	26.4	73.6
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 6	0.77	1.45×10^{-1}	1.38×10^{-3}	7.11×10^{-1}	1.41×10^3	4.64×10^{-2}	3.29×10^{-2}	3.04×10^4	30.5	69.5
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 7	0.74	8.00×10^{-1}	2.75×10^{-3}	1.43×10^1	69.860	4.64×10^{-2}	6.64×10^{-1}	1.51×10^3	5.4	94.6
$^4I_{13/2}$ KP 6	$^4I_{15/2}$ KP 8	0.73	5.72×10^{-1}	2.58×10^{-3}	7.49×10^0	1.33×10^2	4.64×10^{-2}	3.47×10^{-1}	2.88×10^3	9.0	91.0
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 1	0.80	6.76×10^{-2}	1.57×10^{-3}	4.46×10^{-1}	2.24×10^3	4.32×10^{-2}	1.93×10^{-2}	5.19×10^4	72.2	27.8
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 2	0.80	1.75×10^{-1}	2.46×10^{-3}	1.60×10^0	6.26×10^2	4.32×10^{-2}	6.90×10^{-2}	1.45×10^4	48.9	51.1
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 3	0.79	1.40×10^{-1}	3.27×10^{-3}	1.86×10^0	5.37×10^2	4.32×10^{-2}	8.05×10^{-2}	1.24×10^4	72.5	27.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 4	0.78	2.22×10^{-1}	2.61×10^{-3}	2.08×10^0	4.80×10^2	4.32×10^{-2}	9.00×10^{-2}	1.11×10^4	40.1	59.9
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 5	0.78	2.22×10^{-1}	3.50×10^{-3}	2.69×10^0	3.72×10^2	4.32×10^{-2}	1.16×10^{-1}	8.60×10^3	54.5	45.5
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 6	0.77	8.05×10^{-2}	1.14×10^{-3}	3.03×10^{-1}	3.30×10^3	4.32×10^{-2}	1.31×10^{-2}	7.63×10^4	49.2	50.8
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 7	0.74	6.09×10^{-1}	1.75×10^{-3}	8.23×10^0	1.22×10^2	4.32×10^{-2}	3.56×10^{-1}	2.81×10^3	3.8	96.2
$^4I_{13/2}$ KP 7	$^4I_{15/2}$ KP 8	0.74	8.12×10^{-1}	2.72×10^{-3}	1.46×10^1	68.568	4.32×10^{-2}	6.30×10^{-1}	1.59×10^3	5.2	94.8

Table S10. Detailed transition-resolved PL rates for the free Er^{4+} ion.

[illegible]

Table S11. Detailed PL rates for $2V_H Er_{Mg1}^{4+}$ [illegible]Table S12. Detailed PL rates for $2V_H Er_{Mg2}^{4+}$ [illegible]

S2. SAMPLE INPUT FILES

S2.1. VASP

Table S13. VASP input parameters used for the structural relaxation of pristine and Er doped talc.

Category	Parameter	Value
Exchange-correlation	METAGGA	R2SCAN
	LASPH	.TRUE.
Dispersion correction	IVDW	11 (DFT-D3)
Electronic minimization	ALGO	All
Projector operator	LREAL	Auto
Occupations	ISMEAR	1
Smearing width	SIGMA	0.001 eV
Spin treatment	ISPIN	2 (1 if no defect / substitutional / interstitial atom)
Electronic configuration	NELECT	1152 (pristine); 1172 (Er-doped; varies if charged)
Plane-wave basis	ENCUT	440 eV
	ENAUG	900 eV
Electronic convergence	NELM	100
	EDIFF	10^{-6} eV
Geometry optimization	NSW	100 (0 if no relaxation)
	IBRION	2 (conjugate gradient)
	ISIF	2 (Change only parameters)
	EDIFFG	-10^{-3} eV $\text{\AA}^{-1}$
FFT grid	ADDGRID	.TRUE.
Symmetry	ISYM	2

Table S14. Brillouin-zone sampling used in the VASP calculations.

K-point scheme	Mesh
Γ -centered Monkhorst-Pack	$1 \times 1 \times 1$

S2.2. ORCA

The generation of input orbitals by the AVAS method was run as follows.

```
! RI r2scan def2-SVP def2/J noiter
%scf
avas # Selection of seven 4f orbitals by the AVAS method.
system
shell 4,4,4,4,4,4,4
l 3,3,3,3,3,3,3
m_l -3,-2,-1,0,1,2,3
center 0,0,0,0,0,0,0 # Provided that the Er atom comes first in the xyz file.
end
end
end
*xyz (charge) (multiplicity)
(Cluster model geometry in xyz format)
*
```

CASSCF calculations with SOC treatment were run as follows.

```
! RIJCOSX def2-SVP def2/J def2-SVP/C moread
%moinp "AVAS_orbitals.gbw" #AVAS orbitals from the above calculation
%rotate {(Occupied edge orbital),(Empty 4f orbital)} end # Set correct 4f occupancy
%casscf
nel 11 # Or 10 in the case of Er4+.
norb 7
nroots 13
orbstep superci
```

```

switchstep diis
shiftup 4.0 # Large level shift to preserve active space.
shiftdn 4.0
minshift 0.6
maxiter 1000
decomposefosc true # Print electric and magnetic dipoles.
rel
dosoc true
printlevel 4
ninitstates 16 # Initial SOC states of photon absorption. For Er4+, this was set to 17.
end
end
*xyz (charge) (multiplicity)
(Cluster model geometry in xyz format)
*
```

S3. OPTIMIZED GEOMETRIES

S3.1. Supercell models used in VASP

Table S15. Talc cell parameters and atomic composition of the simulated system (3x2x2 system).

Parameter	Value
Formula unit	Mg ₃ Si ₄ O ₁₂ H ₂
Scaling factor	1.0
<i>Lattice vectors ($\text{\AA}$)</i>	
a	(15.84095478, 0.00000000, 0.00000000)
b	(-0.00075482, 18.22700880, 0.00000000)
c	(-0.46513852, -0.12059429, 18.30568513)
<i>Atomic composition</i>	
Mg	35 (36 if talc is pristine)
Si	48
O	144
H	24
Er	1 (if present in the structure)

Table S16: Atomic coordinates of the optimized unit cell

Atom	x	y	z
Mg1	-0.000000	-0.000000	-0.000000
Mg2	0.500000	0.500000	-0.000000
Mg3	0.500007	0.166432	0.000031
Mg4	0.499993	0.833568	-0.000031
Mg5	0.000007	0.666432	0.000031
Mg6	-0.000007	0.333568	-0.000031
Si1	0.844288	0.167655	0.298049
Si2	0.155712	0.832345	0.701951
Si3	0.344288	0.667655	0.298049
Si4	0.655712	0.332345	0.701951

Atom	x	y	z
Si5	0.344299	0.334729	0.297994
Si6	0.655701	0.665271	0.702006
Si7	0.844299	0.834729	0.297994
Si8	0.155701	0.165271	0.702006
O1	0.337558	0.334261	0.119721
O2	0.662442	0.665739	0.880279
O3	0.837558	0.834261	0.119721
O4	0.162442	0.165739	0.880279
O5	0.837497	0.166669	0.119754
O6	0.162503	0.833331	0.880246
O7	0.337497	0.666669	0.119754
O8	0.662503	0.333331	0.880246
O9	0.337463	0.000447	0.116368
O10	0.662537	0.999553	0.883632
O11	0.837463	0.500447	0.116368
O12	0.162537	0.499553	0.883632
O13	0.310460	0.501420	0.359285
O14	0.689540	0.498580	0.640715
O15	0.810460	0.001420	0.359285
O16	0.189540	0.998580	0.640715
O17	0.614919	0.269983	0.356561
O18	0.385081	0.730017	0.643439
O19	0.114919	0.769983	0.356561
O20	0.885081	0.230017	0.643439
O21	0.114857	0.232949	0.356526
O22	0.885143	0.767051	0.643474
O23	0.614857	0.732949	0.356526
O24	0.385143	0.267051	0.643474
H1	0.340237	0.000782	0.222169

Atom	x	y	z
H2	0.659763	0.999218	0.777831
H3	0.840237	0.500782	0.222169
H4	0.159763	0.499218	0.777831

Table S17: Atomic coordinates of the optimized 3×2 pristine talc supercell

Atom	x	y	z
Mg1	0.000000	0.000000	0.500000
Mg2	1.000000	0.500000	0.500000
Mg3	0.333333	0.000000	0.500000
Mg4	0.333333	0.500000	0.500000
Mg5	0.666667	0.000000	0.500000
Mg6	0.666667	0.500000	0.500000
Mg7	0.166667	0.250000	0.500000
Mg8	0.166667	0.750000	0.500000
Mg9	0.500000	0.250000	0.500000
Mg10	0.500000	0.750000	0.500000
Mg11	0.833333	0.250000	0.500000
Mg12	0.833333	0.750000	0.500000
Mg13	0.166670	0.083295	0.499982
Mg14	0.166670	0.583295	0.499982
Mg15	0.500003	0.083295	0.499982
Mg16	0.500003	0.583295	0.499982
Mg17	0.833336	0.083295	0.499982
Mg18	0.833336	0.583295	0.499982
Mg19	0.166664	0.416705	0.500018
Mg20	0.166664	0.916705	0.500018
Mg21	0.499997	0.416705	0.500018
Mg22	0.499997	0.916705	0.500018

Atom	x	y	z
Mg23	0.833330	0.416705	0.500018
Mg24	0.833330	0.916705	0.500018
Mg25	-0.000001	0.333295	0.499982
Mg26	-0.000001	0.833295	0.499982
Mg27	0.333336	0.333295	0.499982
Mg28	0.333336	0.833295	0.499982
Mg29	0.666670	0.333295	0.499982
Mg30	0.666670	0.833295	0.499982
Mg31	0.333330	0.166705	0.500018
Mg32	0.333330	0.666705	0.500018
Mg33	0.666664	0.166705	0.500018
Mg34	0.666664	0.666705	0.500018
Mg35	0.000001	0.166705	0.500018
Mg36	0.000001	0.666705	0.500018
Si1	0.282715	0.084363	0.648389
Si2	0.282715	0.584363	0.648389
Si3	0.616048	0.084363	0.648389
Si4	0.616048	0.584363	0.648389
Si5	0.949381	0.084363	0.648389
Si6	0.949381	0.584363	0.648389
Si7	0.050619	0.415637	0.351611
Si8	0.050619	0.915637	0.351611
Si9	0.383952	0.415637	0.351611
Si10	0.383952	0.915637	0.351611
Si11	0.717285	0.415637	0.351611
Si12	0.717285	0.915637	0.351611
Si13	0.116048	0.334363	0.648389
Si14	0.116048	0.834363	0.648389
Si15	0.449381	0.334363	0.648389

Atom	x	y	z
Si16	0.449381	0.834363	0.648389
Si17	0.782715	0.334363	0.648389
Si18	0.782715	0.834363	0.648389
Si19	0.217285	0.165637	0.351611
Si20	0.217285	0.665637	0.351611
Si21	0.550619	0.165637	0.351611
Si22	0.550619	0.665637	0.351611
Si23	0.883952	0.165637	0.351611
Si24	0.883952	0.665637	0.351611
Si25	0.116050	0.167557	0.648399
Si26	0.116050	0.667557	0.648399
Si27	0.449383	0.167557	0.648399
Si28	0.449383	0.667557	0.648399
Si29	0.782717	0.167557	0.648399
Si30	0.782717	0.667557	0.648399
Si31	0.217283	0.332443	0.351601
Si32	0.217283	0.832443	0.351601
Si33	0.550616	0.332443	0.351601
Si34	0.550617	0.832443	0.351601
Si35	0.883950	0.332443	0.351601
Si36	0.883950	0.832443	0.351601
Si37	0.282717	0.417557	0.648399
Si38	0.282717	0.917557	0.648399
Si39	0.616050	0.417557	0.648399
Si40	0.616050	0.917557	0.648399
Si41	0.949383	0.417557	0.648399
Si42	0.949384	0.917557	0.648399
Si43	0.050617	0.082443	0.351601
Si44	0.050617	0.582443	0.351601

Atom	x	y	z
Si45	0.383950	0.082443	0.351601
Si46	0.383950	0.582443	0.351601
Si47	0.717283	0.082443	0.351601
Si48	0.717283	0.582443	0.351601
O1	0.113091	0.167027	0.559673
O2	0.113091	0.667027	0.559673
O3	0.446424	0.167027	0.559673
O4	0.446424	0.667027	0.559673
O5	0.779757	0.167027	0.559673
O6	0.779757	0.667027	0.559673
O7	0.220243	0.332973	0.440327
O8	0.220243	0.832973	0.440327
O9	0.553576	0.332973	0.440327
O10	0.553576	0.832973	0.440327
O11	0.886909	0.332973	0.440327
O12	0.886909	0.832973	0.440327
O13	0.279757	0.417027	0.559673
O14	0.279757	0.917027	0.559673
O15	0.613091	0.417027	0.559673
O16	0.613091	0.917027	0.559673
O17	0.946424	0.417027	0.559673
O18	0.946424	0.917027	0.559673
O19	0.053576	0.082973	0.440327
O20	0.053576	0.582973	0.440327
O21	0.386909	0.082973	0.440327
O22	0.386909	0.582973	0.440327
O23	0.720243	0.082973	0.440327
O24	0.720243	0.582973	0.440327
O25	0.279737	0.083760	0.559664

Atom	x	y	z
O26	0.279737	0.583760	0.559664
O27	0.613070	0.083760	0.559664
O28	0.613070	0.583760	0.559664
O29	0.946403	0.083760	0.559664
O30	0.946403	0.583760	0.559664
O31	0.053597	0.416240	0.440336
O32	0.053597	0.916240	0.440336
O33	0.386930	0.416240	0.440336
O34	0.386930	0.916240	0.440336
O35	0.720263	0.416240	0.440336
O36	0.720263	0.916240	0.440336
O37	0.113070	0.333760	0.559664
O38	0.113070	0.833760	0.559664
O39	0.446403	0.333760	0.559664
O40	0.446403	0.833760	0.559664
O41	0.779737	0.333760	0.559664
O42	0.779737	0.833760	0.559664
O43	0.220263	0.166240	0.440336
O44	0.220263	0.666240	0.440336
O45	0.553597	0.166240	0.440336
O46	0.553597	0.666240	0.440336
O47	0.886930	0.166240	0.440336
O48	0.886930	0.666240	0.440336
O49	0.112806	0.000410	0.557512
O50	0.112806	0.500410	0.557512
O51	0.446140	0.000410	0.557512
O52	0.446140	0.500410	0.557512
O53	0.779473	0.000410	0.557512
O54	0.779473	0.500410	0.557512

Atom	x	y	z
O55	0.220527	0.499590	0.442488
O56	0.220527	0.999590	0.442488
O57	0.553860	0.499590	0.442488
O58	0.553860	0.999590	0.442488
O59	0.887194	0.499590	0.442488
O60	0.887194	0.999590	0.442488
O61	0.279473	0.250410	0.557512
O62	0.279473	0.750410	0.557512
O63	0.612806	0.250410	0.557512
O64	0.612806	0.750410	0.557512
O65	0.946140	0.250410	0.557512
O66	0.946140	0.750410	0.557512
O67	0.053860	0.249590	0.442488
O68	0.053860	0.749590	0.442488
O69	0.387194	0.249590	0.442488
O70	0.387194	0.749590	0.442488
O71	0.720527	0.249590	0.442488
O72	0.720527	0.749590	0.442488
O73	0.123752	0.251159	0.678533
O74	0.123753	0.751159	0.678533
O75	0.457086	0.251159	0.678533
O76	0.457086	0.751159	0.678533
O77	0.790419	0.251159	0.678533
O78	0.790419	0.751159	0.678533
O79	0.209581	0.248841	0.321467
O80	0.209581	0.748841	0.321467
O81	0.542914	0.248841	0.321467
O82	0.542914	0.748841	0.321467
O83	0.876247	0.248841	0.321467

Atom	x	y	z
O84	0.876247	0.748841	0.321467
O85	0.290419	0.001159	0.678533
O86	0.290419	0.501159	0.678533
O87	0.623753	0.001159	0.678533
O88	0.623753	0.501159	0.678533
O89	0.957086	0.001159	0.678533
O90	0.957086	0.501159	0.678533
O91	0.042914	0.498841	0.321467
O92	0.042914	0.998841	0.321467
O93	0.376248	0.498841	0.321467
O94	0.376247	0.998841	0.321467
O95	0.709581	0.498841	0.321467
O96	0.709581	0.998841	0.321467
O97	0.196950	0.121177	0.678384
O98	0.196950	0.621177	0.678384
O99	0.530284	0.121177	0.678384
O100	0.530284	0.621177	0.678384
O101	0.863617	0.121177	0.678384
O102	0.863617	0.621177	0.678384
O103	0.136383	0.378823	0.321616
O104	0.136383	0.878823	0.321616
O105	0.469716	0.378823	0.321616
O106	0.469716	0.878823	0.321616
O107	0.803050	0.378823	0.321616
O108	0.803050	0.878823	0.321616
O109	0.030284	0.371177	0.678384
O110	0.030284	0.871177	0.678384
O111	0.363617	0.371177	0.678384
O112	0.363617	0.871177	0.678384

Atom	x	y	z
O113	0.696950	0.371177	0.678384
O114	0.696950	0.871177	0.678384
O115	0.303050	0.128823	0.321616
O116	0.303050	0.628823	0.321616
O117	0.636383	0.128823	0.321616
O118	0.636383	0.628823	0.321616
O119	0.969716	0.128823	0.321616
O120	0.969716	0.628823	0.321616
O121	0.030255	0.131200	0.678365
O122	0.030255	0.631200	0.678365
O123	0.363589	0.131200	0.678365
O124	0.363589	0.631200	0.678365
O125	0.696922	0.131200	0.678365
O126	0.696922	0.631200	0.678365
O127	0.303078	0.368800	0.321635
O128	0.303078	0.868800	0.321635
O129	0.636411	0.368800	0.321635
O130	0.636411	0.868800	0.321635
O131	0.969745	0.368800	0.321635
O132	0.969745	0.868800	0.321635
O133	0.196922	0.381200	0.678365
O134	0.196922	0.881200	0.678365
O135	0.530255	0.381200	0.678365
O136	0.530255	0.881200	0.678365
O137	0.863589	0.381200	0.678365
O138	0.863589	0.881200	0.678365
O139	0.136411	0.118800	0.321635
O140	0.136411	0.618800	0.321635
O141	0.469745	0.118800	0.321635

Atom	x	y	z
O142	0.469745	0.618800	0.321635
O143	0.803078	0.118800	0.321635
O144	0.803078	0.618800	0.321635
H1	0.114288	0.000733	0.610111
H2	0.114288	0.500733	0.610111
H3	0.447621	0.000733	0.610111
H4	0.447621	0.500733	0.610111
H5	0.780954	0.000733	0.610111
H6	0.780954	0.500733	0.610111
H7	0.219046	0.499267	0.389889
H8	0.219046	0.999267	0.389889
H9	0.552379	0.499267	0.389889
H10	0.552379	0.999267	0.389889
H11	0.885712	0.499267	0.389889
H12	0.885712	0.999267	0.389889
H13	0.280954	0.250733	0.610111
H14	0.280954	0.750733	0.610111
H15	0.614288	0.250733	0.610111
H16	0.614288	0.750733	0.610111
H17	0.947621	0.250733	0.610111
H18	0.947621	0.750733	0.610111
H19	0.052379	0.249267	0.389889
H20	0.052379	0.749267	0.389889
H21	0.385712	0.249267	0.389889
H22	0.385712	0.749267	0.389889
H23	0.719046	0.249267	0.389889
H24	0.719046	0.749267	0.389889

Table S18: Atomic coordinates of Er_{Mg_2}

Atom	x	y	z
Mg1	0.000306	0.999619	0.499858
Mg2	0.005886	0.503729	0.501490
Mg3	0.333456	0.999755	0.500046
Mg4	0.332917	0.500183	0.500292
Mg5	0.666536	0.999826	0.500074
Mg6	0.661175	0.502006	0.499523
Mg7	0.167851	0.249122	0.500592
Mg8	0.166879	0.750351	0.500398
Mg9	0.498353	0.249346	0.499190
Mg10	0.500000	0.750211	0.500217
Mg11	0.833212	0.245735	0.499315
Mg12	0.833265	0.752369	0.500547
Mg13	0.166899	0.082743	0.500137
Mg14	0.168563	0.584632	0.500561
Mg15	0.499841	0.082921	0.500002
Mg16	0.498194	0.584158	0.500385
Mg17	0.833475	0.082226	0.499596
Mg18	0.833657	0.589843	0.501328
Mg19	0.166871	0.416697	0.500040
Mg20	0.166903	0.916559	0.500041
Mg21	0.498391	0.416603	0.499391
Mg22	0.499973	0.916629	0.500052
Mg23	0.833318	0.917008	0.500034
Mg24	0.003831	0.330658	0.499948
Mg25	0.000175	0.833700	0.500165
Mg26	0.332743	0.333110	0.500113
Mg27	0.333439	0.833375	0.500276
Mg28	0.661963	0.331107	0.499319

Atom	x	y	z
Mg29	0.666407	0.833544	0.500358
Mg30	0.333237	0.166101	0.500019
Mg31	0.333397	0.667397	0.500282
Mg32	0.666028	0.165935	0.499895
Mg33	0.666173	0.667337	0.499889
Mg34	0.000508	0.165684	0.499219
Mg35	0.000538	0.668169	0.500542
Si1	0.282128	0.084396	0.648474
Si2	0.282271	0.585041	0.648802
Si3	0.614993	0.084520	0.648389
Si4	0.614749	0.585298	0.648429
Si5	0.949062	0.084456	0.648192
Si6	0.948861	0.585524	0.650075
Si7	0.047817	0.415845	0.351282
Si8	0.051892	0.914450	0.351775
Si9	0.381333	0.415410	0.351782
Si10	0.384853	0.915045	0.351830
Si11	0.714638	0.413498	0.347517
Si12	0.717601	0.915381	0.351876
Si13	0.116953	0.334405	0.649558
Si14	0.115544	0.834711	0.648656
Si15	0.449482	0.334598	0.648131
Si16	0.448635	0.834790	0.648541
Si17	0.782007	0.332848	0.648451
Si18	0.781896	0.835537	0.648946
Si19	0.218304	0.165121	0.352005
Si20	0.218161	0.665482	0.351851
Si21	0.551067	0.165167	0.351454
Si22	0.551602	0.664679	0.351867

Atom	x	y	z
Si23	0.885818	0.163556	0.350150
Si24	0.884688	0.666610	0.352667
Si25	0.115653	0.167526	0.648501
Si26	0.115517	0.668112	0.649399
Si27	0.448439	0.167778	0.648137
Si28	0.448507	0.668257	0.648912
Si29	0.782024	0.166816	0.648713
Si30	0.781703	0.669171	0.649151
Si31	0.214973	0.332186	0.352119
Si32	0.218442	0.831819	0.351928
Si33	0.547642	0.332255	0.350063
Si34	0.551436	0.831647	0.351883
Si35	0.882475	0.329720	0.347739
Si36	0.884435	0.832776	0.351754
Si37	0.283154	0.417998	0.648521
Si38	0.282097	0.917856	0.648479
Si39	0.615986	0.417924	0.648103
Si40	0.615033	0.918034	0.648549
Si41	0.951843	0.417794	0.649777
Si42	0.948991	0.917940	0.648389
Si43	0.052454	0.080708	0.351527
Si44	0.051659	0.583214	0.352801
Si45	0.384767	0.081801	0.351748
Si46	0.384370	0.582319	0.352114
Si47	0.717767	0.082064	0.351623
Si48	0.718951	0.580921	0.350988
O1	0.113055	0.166793	0.559810
O2	0.112990	0.667700	0.560719
O3	0.445710	0.166734	0.559446

Atom	x	y	z
O4	0.445848	0.667635	0.560199
O5	0.779315	0.165841	0.559935
O6	0.778830	0.669905	0.560432
O7	0.219254	0.332777	0.440914
O8	0.220956	0.832834	0.440662
O9	0.551057	0.332409	0.439066
O10	0.553835	0.832756	0.440618
O11	0.891711	0.323044	0.436912
O12	0.887170	0.833894	0.440532
O13	0.279754	0.417001	0.559866
O14	0.279570	0.917157	0.559790
O15	0.612389	0.416923	0.559348
O16	0.612622	0.917238	0.559857
O17	0.955164	0.417720	0.561105
O18	0.946191	0.917335	0.559715
O19	0.054536	0.081929	0.440311
O20	0.057430	0.585243	0.441547
O21	0.387266	0.082520	0.440480
O22	0.386351	0.583318	0.440856
O23	0.720519	0.082651	0.440425
O24	0.720654	0.581579	0.440122
O25	0.279517	0.083490	0.559789
O26	0.280199	0.584499	0.560117
O27	0.612607	0.083545	0.559692
O28	0.610906	0.585160	0.559707
O29	0.946296	0.083642	0.559474
O30	0.947204	0.585522	0.561500
O31	0.051605	0.415951	0.440373
O32	0.054230	0.915845	0.440507

Atom	x	y	z
O33	0.385361	0.416038	0.440528
O34	0.387359	0.916007	0.440554
O35	0.707237	0.415269	0.436729
O36	0.720356	0.916145	0.440625
O37	0.113961	0.333518	0.560754
O38	0.113049	0.833890	0.559972
O39	0.446133	0.333754	0.559439
O40	0.446157	0.833907	0.559856
O41	0.775818	0.328742	0.559775
O42	0.779216	0.834705	0.560242
O43	0.220960	0.165529	0.440748
O44	0.221141	0.666830	0.440654
O45	0.553327	0.165868	0.440227
O46	0.553774	0.666177	0.440643
O47	0.887690	0.164231	0.439142
O48	0.887222	0.670444	0.441397
O49	0.112813	0.000136	0.557727
O50	0.116221	0.501266	0.558565
O51	0.446031	0.000230	0.557770
O52	0.445639	0.500387	0.557919
O53	0.779274	0.000233	0.557666
O54	0.773937	0.508364	0.560188
O55	0.220335	0.499731	0.442748
O56	0.220909	0.999275	0.442480
O57	0.550157	0.500584	0.442347
O58	0.553932	0.999397	0.442511
O59	0.898050	0.516505	0.442538
O60	0.887621	0.999122	0.442294
O61	0.279974	0.250030	0.558050

Atom	x	y	z
O62	0.279457	0.750722	0.558073
O63	0.610550	0.249114	0.557336
O64	0.612448	0.750808	0.557925
O65	0.946039	0.249840	0.557333
O66	0.946100	0.751527	0.558420
O67	0.056336	0.247885	0.442576
O68	0.054523	0.750419	0.442897
O69	0.385928	0.249325	0.442285
O70	0.387521	0.749811	0.442708
O71	0.719966	0.249030	0.442286
O72	0.720368	0.749940	0.442797
O73	0.124829	0.250967	0.679006
O74	0.124411	0.751735	0.679351
O75	0.457108	0.251371	0.678154
O76	0.457454	0.751753	0.678962
O77	0.790606	0.250262	0.679824
O78	0.790184	0.752506	0.679734
O79	0.209324	0.248353	0.322246
O80	0.210122	0.748497	0.321580
O81	0.541826	0.248067	0.321022
O82	0.543413	0.747988	0.321838
O83	0.881677	0.245586	0.317378
O84	0.875429	0.749446	0.321394
O85	0.291180	0.001342	0.678724
O86	0.290983	0.501692	0.678463
O87	0.623190	0.001524	0.678787
O88	0.623985	0.501760	0.677750
O89	0.958456	0.001451	0.678457
O90	0.956242	0.501702	0.679666

Atom	x	y	z
O91	0.043436	0.499671	0.322680
O92	0.045229	0.997337	0.321236
O93	0.375605	0.498829	0.322121
O94	0.376010	0.998210	0.321732
O95	0.712070	0.497738	0.318650
O96	0.707864	0.998467	0.321836
O97	0.195700	0.120031	0.678443
O98	0.195928	0.620677	0.678853
O99	0.528991	0.120990	0.678158
O100	0.528767	0.620990	0.679040
O101	0.862561	0.119831	0.678342
O102	0.862115	0.621763	0.678964
O103	0.132966	0.377003	0.322265
O104	0.137666	0.878008	0.321838
O105	0.464844	0.376315	0.320865
O106	0.470951	0.878690	0.321969
O107	0.792526	0.363603	0.317991
O108	0.804264	0.880285	0.321930
O109	0.031699	0.371177	0.681343
O110	0.028997	0.870389	0.678338
O111	0.364176	0.371789	0.678438
O112	0.362303	0.870564	0.678438
O113	0.697474	0.371939	0.678115
O114	0.695691	0.871515	0.678784
O115	0.304641	0.129340	0.321964
O116	0.304289	0.629449	0.321907
O117	0.637709	0.129677	0.321924
O118	0.637258	0.627425	0.322171
O119	0.971062	0.125496	0.320937

Atom	x	y	z
O120	0.971644	0.631230	0.323688
O121	0.028892	0.132658	0.678149
O122	0.029604	0.632447	0.680391
O123	0.362232	0.132361	0.678273
O124	0.362323	0.632786	0.679017
O125	0.695578	0.131685	0.678461
O126	0.695476	0.632612	0.678153
O127	0.299270	0.370410	0.321833
O128	0.304490	0.867598	0.321933
O129	0.629705	0.371778	0.317380
O130	0.637710	0.867214	0.322046
O131	0.966423	0.370674	0.318947
O132	0.970938	0.867834	0.321870
O133	0.197670	0.381603	0.679074
O134	0.195668	0.882664	0.678439
O135	0.530587	0.381197	0.678230
O136	0.528897	0.882384	0.678483
O137	0.864139	0.380471	0.674655
O138	0.862454	0.883047	0.678510
O139	0.138255	0.117343	0.321979
O140	0.137797	0.618297	0.321801
O141	0.471186	0.116867	0.321728
O142	0.470759	0.617597	0.322254
O143	0.804117	0.116875	0.321340
O144	0.804240	0.619288	0.322709
H1	0.114287	0.000319	0.610352
H2	0.117714	0.501152	0.611178
H3	0.447344	0.000519	0.610396
H4	0.446636	0.500536	0.610542

Atom	x	y	z
H5	0.780970	0.000619	0.610287
H6	0.774742	0.508505	0.612875
H7	0.218732	0.499732	0.390112
H8	0.219508	0.998945	0.389853
H9	0.550375	0.499581	0.389740
H10	0.552746	0.999178	0.389882
H11	0.886101	0.998943	0.389667
H12	0.281410	0.250309	0.610674
H13	0.280826	0.751104	0.610697
H14	0.611897	0.249791	0.609952
H15	0.613737	0.751029	0.610546
H16	0.948245	0.248826	0.609970
H17	0.948148	0.752371	0.611037
H18	0.053616	0.248519	0.389963
H19	0.052601	0.749045	0.390280
H20	0.384819	0.249091	0.389656
H21	0.386014	0.749216	0.390081
H22	0.718684	0.248819	0.389593
H23	0.719515	0.749512	0.390163
H24	0.883509	0.496416	0.393461
Er1	0.834185	0.419828	0.490894

Table S19: Atomic coordinates of $(Er_{Mg_2})^+$

Atom	x	y	z
Mg1	0.000248	0.999471	0.499838
Mg2	0.005930	0.503154	0.500652
Mg3	0.333278	0.999620	0.500089
Mg4	0.333085	0.500269	0.500162
Mg5	0.666358	0.999526	0.500230

Atom	x	y	z
Mg6	0.660399	0.502975	0.499752
Mg7	0.168278	0.248835	0.500529
Mg8	0.166953	0.750564	0.500063
Mg9	0.497856	0.248858	0.499268
Mg10	0.499678	0.750534	0.500411
Mg11	0.833031	0.244270	0.499740
Mg12	0.833276	0.752179	0.500287
Mg13	0.166871	0.082614	0.499983
Mg14	0.168527	0.584531	0.500045
Mg15	0.499605	0.082646	0.500084
Mg16	0.497919	0.584440	0.500531
Mg17	0.833282	0.081677	0.499964
Mg18	0.833330	0.589636	0.500393
Mg19	0.167906	0.416712	0.500257
Mg20	0.166857	0.916596	0.499939
Mg21	0.498130	0.416676	0.499610
Mg22	0.499751	0.916614	0.500177
Mg23	0.833287	0.916753	0.500154
Mg24	0.005521	0.330496	0.499891
Mg25	0.000293	0.833703	0.499974
Mg26	0.332979	0.332995	0.499998
Mg27	0.333299	0.833461	0.500218
Mg28	0.660547	0.330414	0.499866
Mg29	0.666308	0.833684	0.500484
Mg30	0.333170	0.165828	0.499956
Mg31	0.333296	0.667467	0.500183
Mg32	0.665620	0.165372	0.500533
Mg33	0.665737	0.668106	0.500322
Mg34	0.000733	0.165388	0.499302

Atom	x	y	z
Mg35	0.000849	0.668199	0.500179
Si1	0.281898	0.084258	0.648425
Si2	0.282206	0.584928	0.648541
Si3	0.614459	0.084003	0.648640
Si4	0.614503	0.585438	0.648709
Si5	0.949123	0.084076	0.648221
Si6	0.948532	0.585101	0.648928
Si7	0.050099	0.415662	0.351680
Si8	0.051735	0.914988	0.351505
Si9	0.382542	0.415523	0.351589
Si10	0.384685	0.915091	0.351754
Si11	0.713586	0.415017	0.349069
Si12	0.717557	0.915168	0.351898
Si13	0.117427	0.334045	0.649482
Si14	0.115441	0.834541	0.648460
Si15	0.449261	0.334373	0.647953
Si16	0.448359	0.834722	0.648658
Si17	0.781080	0.331615	0.650483
Si18	0.781902	0.835496	0.648908
Si19	0.218266	0.164948	0.351744
Si20	0.218356	0.665722	0.351507
Si21	0.550916	0.164709	0.351474
Si22	0.551043	0.665427	0.352067
Si23	0.884844	0.163393	0.350347
Si24	0.884882	0.666859	0.351793
Si25	0.115539	0.167289	0.648460
Si26	0.115591	0.667932	0.648470
Si27	0.448165	0.167536	0.648158
Si28	0.448265	0.668286	0.648950

Atom	x	y	z
Si29	0.781715	0.165707	0.649385
Si30	0.781651	0.669258	0.648869
Si31	0.216502	0.331931	0.351970
Si32	0.218257	0.832099	0.351648
Si33	0.548324	0.331521	0.350342
Si34	0.551196	0.832036	0.351929
Si35	0.884665	0.329294	0.348987
Si36	0.884592	0.832998	0.351540
Si37	0.283247	0.417979	0.648427
Si38	0.281891	0.917724	0.648470
Si39	0.615675	0.417963	0.648317
Si40	0.614851	0.917700	0.648652
Si41	0.952168	0.417728	0.650834
Si42	0.949055	0.917624	0.648375
Si43	0.051987	0.081341	0.351325
Si44	0.052035	0.583151	0.351833
Si45	0.384581	0.081622	0.351653
Si46	0.384397	0.582406	0.351884
Si47	0.717487	0.081632	0.351727
Si48	0.718093	0.582536	0.351692
O1	0.112782	0.167024	0.559666
O2	0.112830	0.667250	0.559696
O3	0.445619	0.166638	0.559379
O4	0.445812	0.667528	0.560165
O5	0.779168	0.165770	0.560484
O6	0.778866	0.669259	0.560000
O7	0.219602	0.332800	0.440767
O8	0.220704	0.832824	0.440409
O9	0.551935	0.332605	0.439232

Atom	x	y	z
O10	0.553831	0.832793	0.440689
O11	0.890811	0.326852	0.438452
O12	0.887241	0.833372	0.440321
O13	0.279955	0.417009	0.559669
O14	0.279337	0.917058	0.559706
O15	0.613467	0.416988	0.559302
O16	0.612547	0.917116	0.559893
O17	0.954316	0.418186	0.561323
O18	0.946133	0.917037	0.559602
O19	0.054045	0.082343	0.440117
O20	0.055309	0.584223	0.440674
O21	0.387212	0.082537	0.440409
O22	0.386439	0.583176	0.440657
O23	0.720574	0.082887	0.440556
O24	0.720694	0.582161	0.440741
O25	0.279284	0.083556	0.559663
O26	0.280062	0.584257	0.559757
O27	0.612457	0.083359	0.559857
O28	0.611250	0.585061	0.559843
O29	0.946018	0.083867	0.559391
O30	0.945959	0.583371	0.559908
O31	0.052477	0.416089	0.440693
O32	0.054047	0.916026	0.440274
O33	0.385981	0.416052	0.440342
O34	0.387234	0.915998	0.440509
O35	0.711857	0.416549	0.438635
O36	0.720479	0.916046	0.440664
O37	0.114027	0.333565	0.560603
O38	0.112808	0.833791	0.559691

Atom	x	y	z
O39	0.446327	0.333711	0.559155
O40	0.445924	0.833861	0.559897
O41	0.774854	0.327644	0.561015
O42	0.779323	0.834337	0.560123
O43	0.220719	0.165613	0.440524
O44	0.220791	0.666571	0.440286
O45	0.553569	0.166015	0.440258
O46	0.553763	0.666212	0.440835
O47	0.887286	0.164913	0.439244
O48	0.887657	0.668383	0.440645
O49	0.112605	0.000251	0.557545
O50	0.115584	0.501074	0.558091
O51	0.445870	0.000188	0.557803
O52	0.445983	0.500350	0.557843
O53	0.779160	0.000063	0.557818
O54	0.775250	0.507425	0.561336
O55	0.220215	0.499687	0.442379
O56	0.220734	0.999344	0.442301
O57	0.550797	0.500277	0.442169
O58	0.553988	0.999457	0.442518
O59	0.891538	0.506956	0.439527
O60	0.887439	0.999196	0.442301
O61	0.280071	0.250109	0.557888
O62	0.279242	0.750567	0.557840
O63	0.610291	0.248923	0.557664
O64	0.612366	0.750873	0.558132
O65	0.945624	0.250812	0.556787
O66	0.945990	0.750672	0.557849
O67	0.055841	0.248134	0.442148

Atom	x	y	z
O68	0.054289	0.750095	0.442354
O69	0.386019	0.249330	0.441965
O70	0.387401	0.749715	0.442593
O71	0.720369	0.249808	0.442852
O72	0.720590	0.749762	0.442669
O73	0.125383	0.250809	0.678766
O74	0.124760	0.751313	0.678480
O75	0.458036	0.251262	0.677740
O76	0.457858	0.751632	0.678853
O77	0.791132	0.249324	0.680815
O78	0.791152	0.752292	0.679325
O79	0.208711	0.248323	0.322221
O80	0.208922	0.748627	0.321500
O81	0.541249	0.247824	0.321173
O82	0.542047	0.748380	0.322016
O83	0.875879	0.246492	0.318637
O84	0.875140	0.749405	0.321217
O85	0.291511	0.001245	0.678449
O86	0.291646	0.501614	0.678095
O87	0.623516	0.001141	0.678831
O88	0.625176	0.501736	0.677472
O89	0.959536	0.001170	0.678084
O90	0.956657	0.501590	0.679512
O91	0.041503	0.499179	0.322774
O92	0.043140	0.998028	0.321278
O93	0.375227	0.498831	0.322010
O94	0.375156	0.998190	0.321745
O95	0.709970	0.498727	0.320966
O96	0.707240	0.998257	0.322010

Atom	x	y	z
O97	0.195066	0.119355	0.678211
O98	0.195170	0.619727	0.678084
O99	0.528292	0.120250	0.678112
O100	0.528255	0.620382	0.678936
O101	0.862143	0.118623	0.678448
O102	0.861502	0.620480	0.677662
O103	0.135269	0.378221	0.322207
O104	0.137959	0.879175	0.321784
O105	0.467905	0.378422	0.321130
O106	0.471321	0.879646	0.322068
O107	0.801945	0.377340	0.325791
O108	0.804494	0.880521	0.321996
O109	0.031249	0.370146	0.680772
O110	0.028505	0.869408	0.678139
O111	0.363657	0.370983	0.678078
O112	0.361762	0.870020	0.678333
O113	0.696518	0.370991	0.678643
O114	0.695264	0.870629	0.678557
O115	0.304846	0.129727	0.321943
O116	0.304675	0.629968	0.321744
O117	0.638194	0.130248	0.322129
O118	0.637699	0.629425	0.322440
O119	0.971531	0.128387	0.321204
O120	0.971112	0.630085	0.322738
O121	0.028178	0.133379	0.677810
O122	0.028873	0.632493	0.678162
O123	0.361490	0.132971	0.678055
O124	0.361836	0.633057	0.678690
O125	0.694782	0.131678	0.678682

Atom	x	y	z
O126	0.695463	0.632709	0.677857
O127	0.301606	0.368899	0.321828
O128	0.304786	0.867042	0.321912
O129	0.633980	0.367906	0.318856
O130	0.638073	0.866551	0.322235
O131	0.968778	0.369121	0.321066
O132	0.971278	0.867499	0.321774
O133	0.197202	0.382248	0.678688
O134	0.195206	0.882787	0.678200
O135	0.529852	0.381964	0.677683
O136	0.528518	0.882465	0.678408
O137	0.863211	0.380902	0.673429
O138	0.862076	0.883450	0.678324
O139	0.138079	0.117317	0.321820
O140	0.138327	0.617517	0.321585
O141	0.471344	0.116376	0.321806
O142	0.471430	0.616897	0.322458
O143	0.804260	0.116022	0.321394
O144	0.805165	0.617493	0.323052
H1	0.114332	0.000264	0.610178
H2	0.118165	0.501994	0.610706
H3	0.447062	0.000303	0.610433
H4	0.446338	0.500754	0.610468
H5	0.780727	0.000051	0.610447
H6	0.773389	0.513008	0.613770
H7	0.219881	0.499739	0.389755
H8	0.219713	0.998704	0.389672
H9	0.548141	0.500904	0.389561
H10	0.552347	0.998748	0.389883

Atom	x	y	z
H11	0.885932	0.998283	0.389674
H12	0.281816	0.249914	0.610518
H13	0.280826	0.751327	0.610471
H14	0.610188	0.248816	0.610267
H15	0.613327	0.751856	0.610754
H16	0.948759	0.248469	0.609370
H17	0.948113	0.752274	0.610469
H18	0.056044	0.247137	0.389550
H19	0.053352	0.750340	0.389733
H20	0.384112	0.248288	0.389338
H21	0.385908	0.749731	0.389963
H22	0.717050	0.246533	0.390289
H23	0.718607	0.750692	0.390049
H24	0.892952	0.511126	0.387009
Er1	0.833086	0.417180	0.500005

Table S20: Atomic coordinates of $V_H Er_{Mg1}$

Atom	x	y	z
Mg1	0.000082	0.999997	0.499884
Mg2	0.333320	0.000016	0.500130
Mg3	0.334635	0.500028	0.499798
Mg4	0.666360	0.999986	0.500096
Mg5	0.666262	0.499980	0.500217
Mg6	0.166958	0.250029	0.499903
Mg7	0.166980	0.750061	0.499922
Mg8	0.499858	0.249780	0.500055
Mg9	0.499887	0.750252	0.500097
Mg10	0.832976	0.249009	0.500338
Mg11	0.832973	0.750931	0.500483

Atom	x	y	z
Mg12	0.166937	0.083206	0.499951
Mg13	0.171320	0.582518	0.501291
Mg14	0.499771	0.083213	0.500168
Mg15	0.500246	0.583443	0.500176
Mg16	0.833125	0.082938	0.500093
Mg17	0.830325	0.585207	0.499820
Mg18	0.171201	0.417686	0.501174
Mg19	0.166925	0.916843	0.499879
Mg20	0.500221	0.416605	0.500027
Mg21	0.499775	0.916790	0.500111
Mg22	0.830300	0.414626	0.499698
Mg23	0.833095	0.916994	0.500035
Mg24	0.000166	0.328043	0.499562
Mg25	0.000182	0.835215	0.499833
Mg26	0.334163	0.333004	0.499609
Mg27	0.333304	0.833396	0.500133
Mg28	0.665844	0.332603	0.500645
Mg29	0.666372	0.833615	0.500359
Mg30	0.333318	0.166667	0.499989
Mg31	0.334245	0.667085	0.499537
Mg32	0.666372	0.166361	0.500207
Mg33	0.665883	0.667369	0.500676
Mg34	0.000199	0.164784	0.499742
Mg35	0.000245	0.672007	0.499630
Si1	0.281963	0.084788	0.648283
Si2	0.282037	0.584438	0.647825
Si3	0.614829	0.084521	0.648410
Si4	0.615117	0.584728	0.648608
Si5	0.949002	0.084461	0.648269

Atom	x	y	z
Si6	0.947064	0.587323	0.651487
Si7	0.051835	0.413658	0.349480
Si8	0.051344	0.915483	0.351430
Si9	0.384990	0.415271	0.351439
Si10	0.384622	0.915434	0.351807
Si11	0.717241	0.415011	0.351941
Si12	0.717736	0.915345	0.351779
Si13	0.115502	0.335504	0.648464
Si14	0.115375	0.834370	0.648153
Si15	0.448385	0.334992	0.648268
Si16	0.448509	0.834476	0.648347
Si17	0.780990	0.333491	0.649683
Si18	0.781819	0.835528	0.648577
Si19	0.218088	0.165213	0.351641
Si20	0.218446	0.665475	0.350988
Si21	0.551183	0.165162	0.351816
Si22	0.551154	0.665527	0.351680
Si23	0.884485	0.164974	0.351608
Si24	0.884408	0.665574	0.351230
Si25	0.115412	0.168219	0.648082
Si26	0.115483	0.667073	0.648538
Si27	0.448527	0.168169	0.648267
Si28	0.448426	0.667674	0.648315
Si29	0.781784	0.166859	0.648463
Si30	0.781146	0.668853	0.649829
Si31	0.218235	0.332063	0.351002
Si32	0.218159	0.832286	0.351660
Si33	0.551082	0.331888	0.351673
Si34	0.551173	0.832238	0.351859

Atom	x	y	z
Si35	0.884427	0.331873	0.351091
Si36	0.884441	0.832408	0.351672
Si37	0.281953	0.418268	0.647785
Si38	0.281908	0.917827	0.648315
Si39	0.615107	0.417813	0.648509
Si40	0.614848	0.917992	0.648408
Si41	0.946906	0.414881	0.651358
Si42	0.948951	0.918103	0.648252
Si43	0.051380	0.081885	0.351446
Si44	0.052026	0.584154	0.349583
Si45	0.384608	0.082060	0.351808
Si46	0.385083	0.582110	0.351497
Si47	0.717761	0.082051	0.351780
Si48	0.717299	0.582381	0.352035
O1	0.112921	0.166898	0.559333
O2	0.111772	0.667529	0.559659
O3	0.446025	0.167123	0.559540
O4	0.446783	0.667442	0.559534
O5	0.779128	0.166581	0.559755
O6	0.779173	0.667865	0.560970
O7	0.220596	0.332803	0.439700
O8	0.220733	0.833016	0.440334
O9	0.553862	0.332623	0.440372
O10	0.553871	0.832975	0.440554
O11	0.887405	0.332235	0.439945
O12	0.886911	0.833210	0.440354
O13	0.282621	0.416271	0.559074
O14	0.279472	0.917218	0.559583
O15	0.613213	0.417016	0.559766

Atom	x	y	z
O16	0.612543	0.917296	0.559693
O17	0.941379	0.408357	0.562341
O18	0.945972	0.917858	0.559521
O19	0.054020	0.082066	0.440131
O20	0.055670	0.589924	0.438182
O21	0.387177	0.082799	0.440490
O22	0.388240	0.583150	0.440095
O23	0.720381	0.082758	0.440482
O24	0.719279	0.583628	0.440772
O25	0.279527	0.083829	0.559557
O26	0.282767	0.584854	0.559117
O27	0.612542	0.083675	0.559691
O28	0.613254	0.583990	0.559862
O29	0.946051	0.083125	0.559540
O30	0.941646	0.592519	0.562457
O31	0.055365	0.409244	0.438080
O32	0.053986	0.916915	0.440119
O33	0.388166	0.415854	0.440041
O34	0.387164	0.916239	0.440491
O35	0.719230	0.415313	0.440685
O36	0.720338	0.916196	0.440485
O37	0.111748	0.333657	0.559583
O38	0.112940	0.834130	0.559399
O39	0.446748	0.333636	0.559487
O40	0.446022	0.833934	0.559613
O41	0.779069	0.333000	0.560842
O42	0.779139	0.834311	0.559863
O43	0.220704	0.166037	0.440309
O44	0.220715	0.666285	0.439683

Atom	x	y	z
O45	0.553852	0.165987	0.440510
O46	0.553881	0.666376	0.440386
O47	0.886936	0.165724	0.440288
O48	0.887393	0.666673	0.440093
O49	0.112810	0.000421	0.557476
O50	0.123763	0.500611	0.557023
O51	0.445952	0.000417	0.557738
O52	0.447310	0.500409	0.557462
O53	0.779034	0.000387	0.557683
O54	0.780354	0.500338	0.557489
O55	0.224036	0.499640	0.438982
O56	0.220842	0.999613	0.442270
O57	0.554177	0.499616	0.442442
O58	0.553784	0.999581	0.442462
O59	0.880622	0.499353	0.440376
O60	0.887155	0.999563	0.442264
O61	0.279468	0.250399	0.557213
O62	0.279485	0.750461	0.557245
O63	0.612467	0.249924	0.557883
O64	0.612473	0.750846	0.557949
O65	0.945576	0.247436	0.557408
O66	0.945620	0.753399	0.557476
O67	0.054330	0.246754	0.441755
O68	0.054344	0.752408	0.441741
O69	0.387503	0.249259	0.442096
O70	0.387534	0.750016	0.442132
O71	0.720552	0.249446	0.442878
O72	0.720571	0.749724	0.443007
O73	0.123059	0.251747	0.677992

Atom	x	y	z
O74	0.122794	0.751228	0.678138
O75	0.457207	0.251706	0.678281
O76	0.457242	0.751338	0.678366
O77	0.789504	0.250244	0.679179
O78	0.789673	0.752536	0.679296
O79	0.209918	0.248308	0.321262
O80	0.210324	0.748824	0.321210
O81	0.542645	0.248307	0.321650
O82	0.542674	0.748707	0.321649
O83	0.876126	0.248202	0.321290
O84	0.875917	0.748803	0.321366
O85	0.290177	0.001507	0.678339
O86	0.291956	0.501546	0.677934
O87	0.622327	0.001450	0.678741
O88	0.624732	0.501449	0.678342
O89	0.957881	0.001480	0.678744
O90	0.953392	0.501245	0.673395
O91	0.043548	0.498749	0.324442
O92	0.043028	0.998489	0.320797
O93	0.376650	0.498510	0.321351
O94	0.376272	0.998550	0.321616
O95	0.709208	0.498516	0.322517
O96	0.709115	0.998501	0.321645
O97	0.195924	0.121237	0.678090
O98	0.197477	0.622662	0.678069
O99	0.529215	0.121490	0.678243
O100	0.528854	0.620471	0.678272
O101	0.862643	0.120282	0.678105
O102	0.861129	0.622343	0.682487

Atom	x	y	z
O103	0.137814	0.378316	0.318771
O104	0.137315	0.878870	0.321740
O105	0.470951	0.378934	0.321333
O106	0.470753	0.879230	0.321914
O107	0.803583	0.379017	0.322145
O108	0.803943	0.879346	0.321753
O109	0.029258	0.370703	0.680491
O110	0.029189	0.870798	0.677874
O111	0.362636	0.371142	0.678179
O112	0.362548	0.870999	0.678210
O113	0.694855	0.370070	0.678838
O114	0.695937	0.871953	0.678459
O115	0.304085	0.128833	0.321712
O116	0.304530	0.628946	0.321430
O117	0.637406	0.129175	0.321868
O118	0.637324	0.629435	0.321584
O119	0.970705	0.128863	0.321809
O120	0.969869	0.629028	0.319820
O121	0.029154	0.132335	0.677862
O122	0.029335	0.632079	0.680547
O123	0.362515	0.132153	0.678153
O124	0.362592	0.632117	0.678252
O125	0.695924	0.130920	0.678457
O126	0.694902	0.632830	0.678974
O127	0.304473	0.367931	0.321423
O128	0.304145	0.868223	0.321711
O129	0.637243	0.367537	0.321537
O130	0.637448	0.867724	0.321895
O131	0.969754	0.368267	0.319631

Atom	x	y	z
O132	0.970755	0.867936	0.321849
O133	0.197338	0.380537	0.678025
O134	0.195809	0.881900	0.678136
O135	0.528789	0.382614	0.678214
O136	0.529097	0.881711	0.678272
O137	0.860961	0.380421	0.682368
O138	0.862579	0.882706	0.678124
O139	0.137441	0.117937	0.321753
O140	0.137959	0.618944	0.318706
O141	0.470819	0.117687	0.321888
O142	0.471150	0.617870	0.321379
O143	0.804003	0.117575	0.321736
O144	0.803799	0.617748	0.322284
H1	0.114372	0.000735	0.610104
H2	0.447136	0.000730	0.610364
H3	0.446671	0.500724	0.610059
H4	0.780610	0.000708	0.610309
H5	0.780222	0.500681	0.610116
H6	0.226088	0.499264	0.386463
H7	0.219622	0.999310	0.389648
H8	0.552525	0.499318	0.389820
H9	0.552274	0.999269	0.389836
H10	0.877211	0.498895	0.387709
H11	0.885527	0.999269	0.389639
H12	0.280618	0.251906	0.609836
H13	0.280646	0.749585	0.609866
H14	0.613086	0.250368	0.610503
H15	0.613111	0.751107	0.610569
H16	0.948119	0.248329	0.610011

Atom	x	y	z
H17	0.948174	0.753204	0.610078
H18	0.053340	0.246724	0.389151
H19	0.053300	0.751775	0.389137
H20	0.386098	0.248918	0.389474
H21	0.386125	0.749716	0.389510
H22	0.718940	0.249163	0.390251
H23	0.718973	0.749365	0.390379
Er1	0.007458	0.500090	0.508619

Table S21: Atomic coordinates of $(V_H Er_{Mg_1})^+$

Atom	x	y	z
Mg1	0.000057	0.000007	0.499900
Mg2	0.333535	0.000012	0.499909
Mg3	0.334618	0.499981	0.499693
Mg4	0.666351	0.999982	0.500177
Mg5	0.665717	0.500000	0.500270
Mg6	0.167185	0.248585	0.499518
Mg7	0.167169	0.751453	0.499658
Mg8	0.499973	0.249389	0.500009
Mg9	0.499972	0.750601	0.500069
Mg10	0.832663	0.248286	0.500562
Mg11	0.832648	0.751693	0.500741
Mg12	0.167049	0.082874	0.499665
Mg13	0.172257	0.586440	0.498378
Mg14	0.499902	0.083101	0.500122
Mg15	0.500112	0.583495	0.500104
Mg16	0.833026	0.082738	0.500261
Mg17	0.828775	0.586724	0.501229
Mg18	0.172237	0.413551	0.498143

Atom	x	y	z
Mg19	0.167028	0.917173	0.499661
Mg20	0.500101	0.416479	0.499935
Mg21	0.499912	0.916899	0.500049
Mg22	0.828783	0.413274	0.501055
Mg23	0.832994	0.917198	0.500271
Mg24	0.999867	0.327096	0.500006
Mg25	0.000052	0.835579	0.499997
Mg26	0.334704	0.332359	0.499415
Mg27	0.333568	0.833742	0.499746
Mg28	0.665367	0.332308	0.500685
Mg29	0.666290	0.833834	0.500517
Mg30	0.333591	0.166291	0.499614
Mg31	0.334758	0.667623	0.499436
Mg32	0.666324	0.166123	0.500362
Mg33	0.665367	0.667687	0.500760
Mg34	0.000060	0.164439	0.499864
Mg35	-0.000121	0.672915	0.500111
Si1	0.282075	0.084658	0.648151
Si2	0.281890	0.584568	0.648543
Si3	0.614722	0.084493	0.648561
Si4	0.615038	0.584668	0.648746
Si5	0.948979	0.084327	0.648460
Si6	0.947178	0.586969	0.651544
Si7	0.052646	0.413402	0.348929
Si8	0.051265	0.915643	0.351340
Si9	0.385022	0.415220	0.351277
Si10	0.385098	0.915556	0.351513
Si11	0.717333	0.415154	0.351937
Si12	0.717879	0.915387	0.351837

Atom	x	y	z
Si13	0.115533	0.334839	0.648257
Si14	0.115415	0.834884	0.648074
Si15	0.448486	0.334734	0.648142
Si16	0.448427	0.834562	0.648337
Si17	0.780623	0.333085	0.649910
Si18	0.781665	0.835750	0.648958
Si19	0.218318	0.164498	0.351018
Si20	0.219243	0.666658	0.350080
Si21	0.551442	0.165186	0.351733
Si22	0.551181	0.665612	0.351811
Si23	0.884537	0.164872	0.351743
Si24	0.884143	0.665836	0.351867
Si25	0.115487	0.167672	0.647933
Si26	0.115496	0.667691	0.648341
Si27	0.448444	0.167996	0.648297
Si28	0.448565	0.667822	0.648219
Si29	0.781766	0.166593	0.648822
Si30	0.780757	0.669210	0.650120
Si31	0.219139	0.330961	0.349893
Si32	0.218338	0.833086	0.351120
Si33	0.551247	0.331859	0.351753
Si34	0.551441	0.832264	0.351774
Si35	0.884251	0.331757	0.351703
Si36	0.884531	0.832639	0.351873
Si37	0.281796	0.418031	0.648475
Si38	0.282023	0.917857	0.648169
Si39	0.615009	0.417773	0.648614
Si40	0.614684	0.918048	0.648571
Si41	0.947031	0.415172	0.651474

Atom	x	y	z
Si42	0.948880	0.918123	0.648468
Si43	0.051284	0.081880	0.351304
Si44	0.052659	0.584435	0.349057
Si45	0.385081	0.081995	0.351503
Si46	0.385003	0.582173	0.351385
Si47	0.717872	0.082048	0.351805
Si48	0.717253	0.582382	0.352055
O1	0.112885	0.166881	0.559117
O2	0.112007	0.666551	0.559149
O3	0.445893	0.167198	0.559506
O4	0.446281	0.667111	0.559382
O5	0.779179	0.166562	0.560038
O6	0.778924	0.668274	0.561184
O7	0.221160	0.331732	0.438781
O8	0.220764	0.833171	0.439883
O9	0.553804	0.332780	0.440524
O10	0.554004	0.832901	0.440542
O11	0.887716	0.333038	0.440711
O12	0.887094	0.833102	0.440623
O13	0.279659	0.417422	0.559284
O14	0.279429	0.917058	0.559373
O15	0.613218	0.417086	0.559772
O16	0.612492	0.917263	0.559800
O17	0.942825	0.410549	0.561677
O18	0.945963	0.917784	0.559678
O19	0.054073	0.082281	0.440065
O20	0.056394	0.588443	0.438699
O21	0.387360	0.082792	0.440257
O22	0.386985	0.583008	0.440203

Atom	x	y	z
O23	0.720532	0.082862	0.440572
O24	0.719861	0.583173	0.440963
O25	0.279476	0.083965	0.559352
O26	0.279776	0.583582	0.559362
O27	0.612507	0.083724	0.559789
O28	0.613241	0.583894	0.559898
O29	0.946023	0.083178	0.559666
O30	0.942965	0.590286	0.561739
O31	0.056319	0.410716	0.438586
O32	0.054042	0.916787	0.440103
O33	0.386948	0.415919	0.440099
O34	0.387355	0.916246	0.440268
O35	0.719897	0.415837	0.440856
O36	0.720510	0.916094	0.440607
O37	0.112017	0.334462	0.559062
O38	0.112895	0.834149	0.559256
O39	0.446231	0.333872	0.559308
O40	0.445915	0.833821	0.559548
O41	0.778881	0.332643	0.560994
O42	0.779138	0.834313	0.560174
O43	0.220768	0.165902	0.439777
O44	0.221209	0.667324	0.438948
O45	0.553993	0.166068	0.440491
O46	0.553782	0.666224	0.440582
O47	0.887113	0.165881	0.440502
O48	0.887696	0.665992	0.440876
O49	0.112809	0.000424	0.557388
O50	0.119994	0.500375	0.557755
O51	0.445893	0.000407	0.557683

Atom	x	y	z
O52	0.446424	0.500350	0.557450
O53	0.778992	0.000392	0.557898
O54	0.780980	0.500364	0.557349
O55	0.220922	0.499641	0.440684
O56	0.220991	0.999609	0.442013
O57	0.553752	0.499614	0.442446
O58	0.553959	0.999586	0.442420
O59	0.883677	0.499627	0.442345
O60	0.887245	0.999563	0.442386
O61	0.279259	0.250751	0.556903
O62	0.279284	0.750070	0.556962
O63	0.612324	0.249983	0.558045
O64	0.612308	0.750800	0.558145
O65	0.945541	0.247873	0.557861
O66	0.945571	0.752987	0.557987
O67	0.054363	0.247409	0.441814
O68	0.054355	0.751821	0.441920
O69	0.387638	0.249240	0.441881
O70	0.387647	0.749964	0.441950
O71	0.720669	0.249709	0.443015
O72	0.720679	0.749482	0.443144
O73	0.124229	0.251508	0.677339
O74	0.123959	0.751406	0.677444
O75	0.457486	0.251695	0.678060
O76	0.457599	0.751270	0.678119
O77	0.790385	0.250139	0.679370
O78	0.790342	0.752599	0.679547
O79	0.209176	0.247653	0.320384
O80	0.209463	0.749544	0.320476

Atom	x	y	z
O81	0.542099	0.248454	0.321871
O82	0.541986	0.748610	0.321894
O83	0.875384	0.248431	0.322078
O84	0.875257	0.748720	0.322188
O85	0.291054	0.001457	0.677970
O86	0.291416	0.501482	0.678100
O87	0.622662	0.001462	0.678745
O88	0.625224	0.501385	0.678227
O89	0.958875	0.001424	0.678744
O90	0.955271	0.501211	0.673981
O91	0.042825	0.498767	0.325158
O92	0.041420	0.998559	0.320986
O93	0.375206	0.498523	0.321768
O94	0.376208	0.998579	0.321418
O95	0.708724	0.498589	0.322684
O96	0.708612	0.998513	0.321907
O97	0.195568	0.120436	0.677839
O98	0.196030	0.621202	0.677846
O99	0.528828	0.121112	0.678193
O100	0.528284	0.619821	0.678044
O101	0.862399	0.119698	0.678243
O102	0.860809	0.621490	0.681187
O103	0.138892	0.378857	0.319226
O104	0.137787	0.880098	0.321598
O105	0.471678	0.379958	0.321843
O106	0.471440	0.879659	0.321877
O107	0.804785	0.380468	0.322848
O108	0.804530	0.879929	0.322002
O109	0.028859	0.369923	0.679318

Atom	x	y	z
O110	0.028690	0.869969	0.677765
O111	0.362000	0.370525	0.677564
O112	0.361926	0.870141	0.677982
O113	0.694525	0.369677	0.678816
O114	0.695413	0.871465	0.678561
O115	0.304837	0.129208	0.321444
O116	0.305128	0.629801	0.321053
O117	0.638113	0.129946	0.322024
O118	0.637843	0.630039	0.322038
O119	0.971408	0.130106	0.322011
O120	0.970442	0.629496	0.321307
O121	0.028725	0.133036	0.677642
O122	0.028937	0.632745	0.679373
O123	0.361994	0.132749	0.677977
O124	0.362045	0.632522	0.677638
O125	0.695448	0.131478	0.678494
O126	0.694644	0.633018	0.679023
O127	0.305194	0.367153	0.320884
O128	0.304853	0.867940	0.321499
O129	0.637917	0.367032	0.321987
O130	0.638205	0.866955	0.322090
O131	0.970567	0.367724	0.321201
O132	0.971449	0.866904	0.322138
O133	0.195815	0.382032	0.677803
O134	0.195504	0.882546	0.677921
O135	0.528177	0.383181	0.677911
O136	0.528645	0.882077	0.678210
O137	0.860619	0.381198	0.681109
O138	0.862299	0.883151	0.678266

Atom	x	y	z
O139	0.137868	0.116909	0.321554
O140	0.138880	0.618560	0.319342
O141	0.471427	0.117430	0.321826
O142	0.471683	0.616999	0.321954
O143	0.804496	0.117157	0.321948
O144	0.804742	0.616677	0.323023
H1	0.114518	0.000772	0.610022
H2	0.447200	0.000723	0.610317
H3	0.447508	0.500650	0.610092
H4	0.780347	0.000724	0.610529
H5	0.779883	0.500677	0.609980
H6	0.223810	0.499333	0.388157
H7	0.219906	0.999265	0.389385
H8	0.552079	0.499301	0.389808
H9	0.552517	0.999242	0.389788
H10	0.882363	0.499306	0.389424
H11	0.885415	0.999210	0.389754
H12	0.281018	0.250683	0.609548
H13	0.281082	0.750829	0.609608
H14	0.612971	0.249717	0.610668
H15	0.612933	0.751746	0.610768
H16	0.947511	0.247149	0.610477
H17	0.947562	0.754360	0.610604
H18	0.052926	0.245590	0.389212
H19	0.052900	0.752919	0.389317
H20	0.386891	0.248150	0.389261
H21	0.386910	0.750357	0.389330
H22	0.718479	0.248402	0.390388
H23	0.718490	0.750081	0.390517

Atom	x	y	z
Er1	0.004745	0.500007	0.504576

Table S22: Atomic coordinates of $V_H Er_{Mg_2}$

Atom	x	y	z
Mg1	0.000256	-0.000302	0.499819
Mg2	0.001469	0.503960	0.497822
Mg3	0.333513	-0.000297	0.499985
Mg4	0.332778	0.500200	0.500082
Mg5	0.666652	-0.000359	0.499976
Mg6	0.661459	0.502605	0.499742
Mg7	0.168240	0.249317	0.500811
Mg8	0.166787	0.750237	0.500256
Mg9	0.498872	0.249486	0.499276
Mg10	0.500093	0.750124	0.500100
Mg11	0.833563	0.246705	0.499809
Mg12	0.833670	0.751132	0.499926
Mg13	0.166975	0.082837	0.500107
Mg14	0.167229	0.584189	0.500022
Mg15	0.500001	0.082895	0.499989
Mg16	0.498199	0.584249	0.500294
Mg17	0.833439	0.082400	0.499769
Mg18	0.836085	0.586623	0.498219
Mg19	0.166453	0.417145	0.500068
Mg20	0.166881	0.916608	0.499975
Mg21	0.498760	0.416763	0.499448
Mg22	0.500080	0.916539	0.499960
Mg23	0.833474	0.916672	0.499778
Mg24	0.004840	0.331004	0.500258
Mg25	0.000224	0.833623	0.499898

Atom	x	y	z
Mg26	0.332958	0.333256	0.500135
Mg27	0.333422	0.833287	0.500166
Mg28	0.663152	0.331699	0.499824
Mg29	0.666708	0.833241	0.499977
Mg30	0.333512	0.166173	0.500018
Mg31	0.333026	0.667236	0.500079
Mg32	0.666330	0.166112	0.500069
Mg33	0.666896	0.667089	0.499740
Mg34	0.000660	0.165827	0.499326
Mg35	0.000492	0.667927	0.500236
Si1	0.282402	0.084375	0.648381
Si2	0.282285	0.584956	0.648484
Si3	0.615208	0.084291	0.648306
Si4	0.614978	0.585439	0.648280
Si5	0.949066	0.084504	0.648127
Si6	0.949635	0.585384	0.649946
Si7	0.049606	0.415863	0.351292
Si8	0.051563	0.914993	0.351656
Si9	0.382801	0.415436	0.351798
Si10	0.384695	0.914935	0.351778
Si11	0.713960	0.415176	0.348386
Si12	0.717708	0.914959	0.351736
Si13	0.117176	0.334222	0.649930
Si14	0.115671	0.834815	0.648463
Si15	0.449544	0.334627	0.647935
Si16	0.448812	0.834749	0.648398
Si17	0.782034	0.333059	0.649015
Si18	0.782262	0.834912	0.648310
Si19	0.218358	0.165094	0.352043

Atom	x	y	z
Si20	0.217340	0.665387	0.351670
Si21	0.551036	0.164896	0.351475
Si22	0.551076	0.664840	0.351869
Si23	0.884875	0.163825	0.350342
Si24	0.884704	0.665502	0.351670
Si25	0.115930	0.167359	0.648498
Si26	0.115684	0.668119	0.649244
Si27	0.448745	0.167765	0.648044
Si28	0.448676	0.668263	0.648703
Si29	0.782045	0.167005	0.648820
Si30	0.782680	0.668227	0.648136
Si31	0.216434	0.332108	0.352181
Si32	0.218089	0.831955	0.351870
Si33	0.549112	0.331744	0.350255
Si34	0.551274	0.831629	0.351792
Si35	0.885450	0.329465	0.348413
Si36	0.884684	0.832217	0.351485
Si37	0.283035	0.418033	0.648425
Si38	0.282295	0.917856	0.648359
Si39	0.615900	0.418091	0.648021
Si40	0.615448	0.917702	0.648308
Si41	0.952087	0.417350	0.650870
Si42	0.949033	0.917876	0.648162
Si43	0.051957	0.081476	0.351532
Si44	0.050580	0.582560	0.351710
Si45	0.384678	0.081625	0.351748
Si46	0.383845	0.582352	0.351997
Si47	0.717651	0.081644	0.351631
Si48	0.718555	0.581814	0.351262

Atom	x	y	z
O1	0.113268	0.166834	0.559805
O2	0.112993	0.667657	0.560555
O3	0.446085	0.166791	0.559350
O4	0.445834	0.667623	0.560005
O5	0.779477	0.166266	0.560000
O6	0.780087	0.668173	0.559466
O7	0.219948	0.332761	0.440984
O8	0.220832	0.832967	0.440593
O9	0.552593	0.332524	0.439096
O10	0.553861	0.832767	0.440512
O11	0.892408	0.325417	0.437468
O12	0.887324	0.833559	0.440266
O13	0.279565	0.417084	0.559767
O14	0.279665	0.917192	0.559669
O15	0.612515	0.417035	0.559213
O16	0.612842	0.917069	0.559619
O17	0.954709	0.416083	0.562209
O18	0.946296	0.917401	0.559497
O19	0.054192	0.082363	0.440274
O20	0.056060	0.585213	0.440384
O21	0.387380	0.082540	0.440455
O22	0.386242	0.583200	0.440725
O23	0.720557	0.082785	0.440387
O24	0.719721	0.582152	0.440181
O25	0.279721	0.083548	0.559698
O26	0.279743	0.584248	0.559814
O27	0.612827	0.083541	0.559594
O28	0.610822	0.585135	0.559598
O29	0.946241	0.083842	0.559379

Atom	x	y	z
O30	0.948128	0.586212	0.561721
O31	0.053074	0.415275	0.440162
O32	0.054145	0.916254	0.440386
O33	0.386206	0.415999	0.440503
O34	0.387358	0.916002	0.440492
O35	0.709893	0.416659	0.437437
O36	0.720433	0.916105	0.440454
O37	0.114267	0.333444	0.561123
O38	0.113118	0.834053	0.559796
O39	0.446469	0.333769	0.559217
O40	0.446258	0.833876	0.559718
O41	0.776401	0.329029	0.560320
O42	0.779480	0.834240	0.559635
O43	0.221120	0.165617	0.440779
O44	0.220656	0.666657	0.440483
O45	0.553718	0.165988	0.440201
O46	0.553538	0.666242	0.440620
O47	0.887328	0.165134	0.439178
O48	0.887935	0.669301	0.440371
O49	0.112824	0.000317	0.557651
O50	0.113715	0.501177	0.557056
O51	0.446185	0.000237	0.557674
O52	0.445629	0.500411	0.557793
O53	0.779397	0.000194	0.557529
O54	0.773297	0.506614	0.561894
O55	0.220489	0.499694	0.442436
O56	0.220877	-0.000564	0.442421
O57	0.550587	0.500444	0.442219
O58	0.554016	-0.000523	0.442405

Atom	x	y	z
O59	0.892020	0.507670	0.442932
O60	0.887495	-0.000567	0.442223
O61	0.280362	0.250062	0.558126
O62	0.279440	0.750709	0.557895
O63	0.611115	0.249430	0.557371
O64	0.612827	0.750589	0.557679
O65	0.946443	0.249885	0.557168
O66	0.946283	0.751595	0.558000
O67	0.056431	0.247957	0.442622
O68	0.054625	0.750499	0.442683
O69	0.386483	0.249404	0.442242
O70	0.387397	0.749758	0.442587
O71	0.720637	0.249625	0.442388
O72	0.720596	0.749820	0.442370
O73	0.125171	0.250710	0.679146
O74	0.124283	0.751847	0.679068
O75	0.457444	0.251403	0.677948
O76	0.457160	0.751741	0.678852
O77	0.790156	0.250366	0.680224
O78	0.790627	0.751764	0.678563
O79	0.209671	0.248296	0.322285
O80	0.209706	0.748615	0.321593
O81	0.541559	0.247861	0.320954
O82	0.542754	0.748077	0.321735
O83	0.876693	0.246312	0.317657
O84	0.876502	0.748980	0.321128
O85	0.291461	0.001350	0.678595
O86	0.290907	0.501661	0.678386
O87	0.623486	0.001249	0.678557

Atom	x	y	z
O88	0.623686	0.501866	0.677693
O89	0.957899	0.001457	0.678281
O90	0.957075	0.501467	0.679687
O91	0.045091	0.498960	0.321518
O92	0.044020	0.998106	0.321283
O93	0.375522	0.498697	0.322012
O94	0.376000	0.998124	0.321668
O95	0.709788	0.498512	0.319238
O96	0.708034	0.998170	0.321755
O97	0.195959	0.119889	0.678422
O98	0.196498	0.621232	0.678757
O99	0.529259	0.120896	0.678066
O100	0.529364	0.621614	0.678957
O101	0.862821	0.120305	0.678309
O102	0.862796	0.621258	0.679173
O103	0.135235	0.377583	0.322068
O104	0.137584	0.878736	0.321855
O105	0.468034	0.378185	0.321222
O106	0.470838	0.878757	0.321892
O107	0.801256	0.375532	0.325390
O108	0.804171	0.879594	0.321813
O109	0.031872	0.370516	0.682173
O110	0.029399	0.870914	0.678220
O111	0.364099	0.371629	0.678077
O112	0.362689	0.870850	0.678310
O113	0.697258	0.372085	0.678222
O114	0.696157	0.871100	0.678299
O115	0.304472	0.129017	0.321934
O116	0.303590	0.629211	0.321838

Atom	x	y	z
O117	0.637760	0.129535	0.321860
O118	0.636497	0.627692	0.322041
O119	0.971136	0.127655	0.321114
O120	0.970973	0.630182	0.321511
O121	0.029164	0.132395	0.678052
O122	0.030393	0.632031	0.680859
O123	0.362492	0.132409	0.678149
O124	0.362763	0.632247	0.678598
O125	0.695800	0.131416	0.678424
O126	0.696319	0.632041	0.677561
O127	0.301943	0.368684	0.322011
O128	0.304249	0.867639	0.321885
O129	0.633995	0.367938	0.317641
O130	0.637529	0.867190	0.321901
O131	0.969602	0.368379	0.319303
O132	0.970749	0.868313	0.321704
O133	0.197828	0.381484	0.679322
O134	0.195943	0.882595	0.678323
O135	0.530467	0.381392	0.678042
O136	0.529328	0.882071	0.678294
O137	0.864102	0.380448	0.675887
O138	0.862707	0.882478	0.678113
O139	0.137958	0.117709	0.322004
O140	0.136993	0.618473	0.321483
O141	0.471101	0.116807	0.321725
O142	0.470225	0.617698	0.322227
O143	0.804137	0.116368	0.321236
O144	0.802596	0.620554	0.321717
H1	0.114314	0.000373	0.610276

Atom	x	y	z
H2	0.113770	0.501767	0.609645
H3	0.447439	0.000376	0.610299
H4	0.446431	0.500774	0.610416
H5	0.780973	0.000240	0.610151
H6	0.772527	0.508685	0.614502
H7	0.218383	0.499821	0.389807
H8	0.219319	0.998853	0.389795
H9	0.549858	0.500844	0.389614
H10	0.552577	0.998846	0.389778
H11	0.886015	0.998559	0.389599
H12	0.281847	0.250388	0.610750
H13	0.280705	0.750887	0.610517
H14	0.612159	0.249909	0.609986
H15	0.614476	0.750936	0.610301
H16	0.948646	0.249064	0.609791
H17	0.947923	0.751940	0.610614
H18	0.055618	0.248760	0.390023
H19	0.052577	0.748727	0.390078
H20	0.384664	0.249118	0.389614
H21	0.385741	0.749214	0.389960
H22	0.718501	0.248158	0.389757
H23	0.719993	0.748892	0.389745
Er1	0.836718	0.422547	0.493043

Table S23: Atomic coordinates of $(V_H Er_{Mg_2})^+$

Atom	x	y	z
Mg1	0.000408	0.999485	0.499723
Mg2	0.005816	0.502763	0.501601
Mg3	0.333593	0.999620	0.499939

Atom	x	y	z
Mg4	0.332927	0.500290	0.500101
Mg5	0.666624	0.999631	0.499950
Mg6	0.660025	0.503195	0.499321
Mg7	0.168692	0.248713	0.500509
Mg8	0.166839	0.750559	0.500123
Mg9	0.498652	0.249062	0.499273
Mg10	0.499663	0.750553	0.500287
Mg11	0.834132	0.244930	0.498929
Mg12	0.833292	0.751795	0.500076
Mg13	0.167217	0.082578	0.499906
Mg14	0.168092	0.584347	0.500010
Mg15	0.499988	0.082738	0.499955
Mg16	0.497681	0.584551	0.500414
Mg17	0.833586	0.081821	0.499552
Mg18	0.832906	0.589330	0.501412
Mg19	0.167979	0.416528	0.500086
Mg20	0.166991	0.916641	0.499826
Mg21	0.497974	0.416801	0.499359
Mg22	0.499986	0.916647	0.500017
Mg23	0.833436	0.916692	0.499951
Mg24	0.005885	0.330292	0.499872
Mg25	0.000317	0.833677	0.499895
Mg26	0.333272	0.332913	0.500083
Mg27	0.333350	0.833465	0.500192
Mg28	0.661061	0.331532	0.499163
Mg29	0.666453	0.833646	0.500286
Mg30	0.333640	0.165857	0.499931
Mg31	0.333074	0.667470	0.500196
Mg32	0.666171	0.165702	0.499885

Atom	x	y	z
Mg33	0.665638	0.668039	0.499985
Mg34	0.001157	0.165288	0.499097
Mg35	0.000659	0.667963	0.500149
Si1	0.282545	0.084263	0.648327
Si2	0.282154	0.585047	0.648575
Si3	0.615230	0.084396	0.648348
Si4	0.614430	0.585752	0.648572
Si5	0.949201	0.084516	0.648001
Si6	0.948962	0.585672	0.649468
Si7	0.050032	0.415613	0.351596
Si8	0.051700	0.914862	0.351450
Si9	0.382654	0.415456	0.351574
Si10	0.384770	0.914976	0.351697
Si11	0.714033	0.415284	0.348488
Si12	0.717828	0.914963	0.351745
Si13	0.117912	0.333905	0.649505
Si14	0.115569	0.834981	0.648356
Si15	0.449634	0.334422	0.647951
Si16	0.448669	0.834933	0.648578
Si17	0.782436	0.334026	0.649942
Si18	0.782050	0.835402	0.648750
Si19	0.218559	0.164785	0.351735
Si20	0.217679	0.665563	0.351705
Si21	0.551237	0.164721	0.351320
Si22	0.550730	0.665238	0.352000
Si23	0.885204	0.163396	0.350123
Si24	0.884526	0.665411	0.351155
Si25	0.116078	0.167159	0.648381
Si26	0.115597	0.668291	0.648640

Atom	x	y	z
Si27	0.448805	0.167649	0.648168
Si28	0.448208	0.668493	0.648909
Si29	0.782073	0.166738	0.648255
Si30	0.781704	0.669136	0.649079
Si31	0.216741	0.331732	0.352099
Si32	0.218230	0.832029	0.351674
Si33	0.548589	0.331583	0.350229
Si34	0.551312	0.831919	0.351815
Si35	0.885218	0.329589	0.348524
Si36	0.884770	0.832374	0.351603
Si37	0.283535	0.418032	0.648439
Si38	0.282212	0.917822	0.648386
Si39	0.615516	0.418449	0.647821
Si40	0.615211	0.917940	0.648476
Si41	0.952789	0.417976	0.651216
Si42	0.948960	0.917910	0.648260
Si43	0.052190	0.081227	0.351226
Si44	0.050818	0.582302	0.351272
Si45	0.384850	0.081561	0.351606
Si46	0.383863	0.582388	0.351919
Si47	0.717868	0.081574	0.351396
Si48	0.718078	0.582202	0.351436
O1	0.113185	0.166957	0.559607
O2	0.112590	0.667109	0.559808
O3	0.446391	0.166867	0.559395
O4	0.445668	0.667626	0.560144
O5	0.779570	0.166601	0.559455
O6	0.778870	0.669010	0.560191
O7	0.220059	0.332555	0.440947

Atom	x	y	z
O8	0.220688	0.832812	0.440454
O9	0.552229	0.332730	0.439161
O10	0.553952	0.832754	0.440597
O11	0.891441	0.327427	0.438334
O12	0.887350	0.833057	0.440432
O13	0.280090	0.417000	0.559696
O14	0.279552	0.917137	0.559631
O15	0.613198	0.417332	0.558869
O16	0.612812	0.917261	0.559726
O17	0.953194	0.417143	0.561552
O18	0.946182	0.917164	0.559505
O19	0.054260	0.082253	0.440034
O20	0.053398	0.583310	0.440427
O21	0.387550	0.082561	0.440380
O22	0.386112	0.583168	0.440704
O23	0.720903	0.082985	0.440246
O24	0.720699	0.581995	0.440635
O25	0.279774	0.083546	0.559586
O26	0.279861	0.584235	0.559810
O27	0.612981	0.083756	0.559576
O28	0.611246	0.585206	0.559724
O29	0.946158	0.084017	0.559189
O30	0.946481	0.584228	0.560661
O31	0.052301	0.416017	0.440784
O32	0.054113	0.915994	0.440234
O33	0.386005	0.416022	0.440352
O34	0.387397	0.915966	0.440467
O35	0.712196	0.417178	0.438321
O36	0.720650	0.916009	0.440531

Atom	x	y	z
O37	0.114307	0.333471	0.560639
O38	0.112788	0.833953	0.559607
O39	0.446799	0.333708	0.559176
O40	0.446127	0.833966	0.559822
O41	0.778176	0.332072	0.559534
O42	0.779436	0.834209	0.559975
O43	0.221136	0.165505	0.440538
O44	0.220367	0.666460	0.440536
O45	0.554086	0.166186	0.440157
O46	0.553445	0.666230	0.440819
O47	0.887697	0.164950	0.439024
O48	0.887598	0.666325	0.440315
O49	0.112769	0.000315	0.557504
O50	0.115470	0.500763	0.558355
O51	0.446223	0.000325	0.557713
O52	0.445935	0.500410	0.557824
O53	0.779406	0.000328	0.557601
O54	0.774529	0.506104	0.561059
O55	0.219922	0.499688	0.442430
O56	0.220981	0.999338	0.442243
O57	0.550530	0.500388	0.441967
O58	0.554235	0.999530	0.442387
O59	0.889903	0.504759	0.442636
O60	0.887606	0.999159	0.442118
O61	0.280452	0.250015	0.558041
O62	0.279173	0.750634	0.557897
O63	0.612093	0.249844	0.557554
O64	0.612468	0.750871	0.557943
O65	0.946037	0.250611	0.556635

Atom	x	y	z
O66	0.945853	0.750604	0.557580
O67	0.056176	0.248031	0.442126
O68	0.054110	0.749815	0.442384
O69	0.386601	0.249321	0.442155
O70	0.387256	0.749697	0.442602
O71	0.721075	0.250627	0.442900
O72	0.720822	0.749572	0.442578
O73	0.125417	0.250678	0.678809
O74	0.124857	0.751759	0.678317
O75	0.458216	0.251360	0.677850
O76	0.457953	0.751837	0.678809
O77	0.790980	0.250967	0.678007
O78	0.791207	0.752239	0.679284
O79	0.208831	0.248126	0.322287
O80	0.208780	0.748535	0.321702
O81	0.541334	0.247846	0.321107
O82	0.542212	0.748275	0.321953
O83	0.876028	0.246537	0.318858
O84	0.875583	0.748715	0.321978
O85	0.291933	0.001299	0.678412
O86	0.291391	0.501696	0.678138
O87	0.624425	0.001494	0.678469
O88	0.624798	0.502023	0.677327
O89	0.958263	0.001566	0.677998
O90	0.957927	0.501935	0.679327
O91	0.043214	0.498614	0.321839
O92	0.042971	0.997915	0.321217
O93	0.374989	0.498756	0.322089
O94	0.375321	0.998120	0.321745

Atom	x	y	z
O95	0.709136	0.498663	0.320262
O96	0.707851	0.998124	0.321854
O97	0.195856	0.119587	0.678126
O98	0.195226	0.620066	0.678138
O99	0.529199	0.120651	0.678067
O100	0.528262	0.620688	0.678853
O101	0.862811	0.120529	0.677949
O102	0.861489	0.620368	0.678112
O103	0.135591	0.378000	0.322722
O104	0.138027	0.879202	0.321766
O105	0.468234	0.378647	0.321163
O106	0.471368	0.879502	0.322003
O107	0.801889	0.376721	0.325709
O108	0.804626	0.879921	0.322013
O109	0.031943	0.370401	0.680802
O110	0.028873	0.870266	0.678061
O111	0.364253	0.371388	0.678054
O112	0.362095	0.870198	0.678285
O113	0.697243	0.372232	0.677518
O114	0.695517	0.870745	0.678378
O115	0.305167	0.129660	0.321878
O116	0.303872	0.629622	0.321888
O117	0.638466	0.130168	0.321927
O118	0.636895	0.628606	0.322628
O119	0.971932	0.128453	0.320981
O120	0.970905	0.629820	0.321640
O121	0.028865	0.132971	0.677708
O122	0.028982	0.633279	0.679037
O123	0.362300	0.132774	0.677976

Atom	x	y	z
O124	0.361869	0.633108	0.678696
O125	0.695544	0.132457	0.678045
O126	0.695410	0.632775	0.677971
O127	0.302060	0.368375	0.321928
O128	0.304799	0.866957	0.321964
O129	0.634434	0.367634	0.318981
O130	0.638100	0.866625	0.322135
O131	0.969793	0.368093	0.320468
O132	0.971299	0.867262	0.321842
O133	0.197813	0.381849	0.678804
O134	0.195491	0.883004	0.678094
O135	0.530505	0.381675	0.677711
O136	0.528827	0.882791	0.678259
O137	0.864066	0.382009	0.675512
O138	0.862306	0.883187	0.678219
O139	0.138515	0.116916	0.321885
O140	0.137424	0.617631	0.322301
O141	0.471667	0.116292	0.321829
O142	0.470654	0.617214	0.322459
O143	0.804645	0.116001	0.321120
O144	0.803497	0.618660	0.321932
H1	0.114625	0.000253	0.610137
H2	0.118699	0.502026	0.610956
H3	0.447348	0.000282	0.610343
H4	0.446228	0.500988	0.610447
H5	0.780817	0.000012	0.610229
H6	0.772834	0.509404	0.613689
H7	0.219062	0.499689	0.389788
H8	0.219819	0.998732	0.389613

Atom	x	y	z
H9	0.548183	0.501150	0.389353
H10	0.552485	0.998760	0.389754
H11	0.886234	0.998146	0.389489
H12	0.282208	0.249733	0.610669
H13	0.280779	0.751420	0.610527
H14	0.611499	0.249306	0.610147
H15	0.613565	0.751842	0.610565
H16	0.949129	0.248242	0.609207
H17	0.947762	0.751890	0.610209
H18	0.056340	0.247484	0.389518
H19	0.053043	0.749681	0.389748
H20	0.384593	0.248418	0.389525
H21	0.385739	0.749656	0.389969
H22	0.718227	0.248156	0.390275
H23	0.719198	0.749992	0.389938
Er1	0.834823	0.419867	0.496458

Table S24: Atomic coordinates of $2V_H Er_{Mg1}$

Atom	x	y	z
Mg1	-0.000000	0.000000	0.500000
Mg2	0.333544	0.000004	0.499959
Mg3	0.333701	0.499969	0.499648
Mg4	0.666456	0.999996	0.500041
Mg5	0.666299	0.500031	0.500352
Mg6	0.166913	0.249442	0.499807
Mg7	0.166931	0.750556	0.499864
Mg8	0.500005	0.249973	0.499975
Mg9	0.499995	0.750027	0.500025
Mg10	0.833069	0.249444	0.500136

Atom	x	y	z
Mg11	0.833087	0.750558	0.500193
Mg12	0.166957	0.083063	0.499945
Mg13	0.169098	0.583993	0.499601
Mg14	0.499994	0.083279	0.500051
Mg15	0.499985	0.583305	0.500096
Mg16	0.833042	0.083042	0.500149
Mg17	0.830925	0.584043	0.500560
Mg18	0.169075	0.415957	0.499440
Mg19	0.166958	0.916958	0.499851
Mg20	0.500015	0.416695	0.499904
Mg21	0.500006	0.916721	0.499949
Mg22	0.830902	0.416007	0.500399
Mg23	0.833043	0.916937	0.500055
Mg24	0.999996	0.327752	0.500010
Mg25	0.000003	0.835343	0.500021
Mg26	0.333677	0.333060	0.499587
Mg27	0.333499	0.833373	0.499952
Mg28	0.666306	0.333093	0.500436
Mg29	0.666501	0.833367	0.500188
Mg30	0.333499	0.166633	0.499812
Mg31	0.333694	0.666906	0.499564
Mg32	0.666500	0.166627	0.500048
Mg33	0.666323	0.666940	0.500413
Mg34	0.999997	0.164657	0.499979
Mg35	0.000004	0.672248	0.499990
Si1	0.282191	0.084744	0.648226
Si2	0.281588	0.584516	0.648174
Si3	0.614981	0.084602	0.648345
Si4	0.615199	0.584751	0.648462

Atom	x	y	z
Si5	0.948802	0.084495	0.648443
Si6	0.948067	0.586822	0.651703
Si7	0.051933	0.413178	0.348297
Si8	0.051198	0.915506	0.351557
Si9	0.384801	0.415249	0.351538
Si10	0.385019	0.915398	0.351655
Si11	0.718412	0.415484	0.351826
Si12	0.717808	0.915256	0.351774
Si13	0.115409	0.335031	0.648773
Si14	0.115460	0.834853	0.648196
Si15	0.448518	0.335010	0.648102
Si16	0.448613	0.834432	0.648247
Si17	0.781517	0.334022	0.649477
Si18	0.781840	0.835293	0.648506
Si19	0.218160	0.164707	0.351494
Si20	0.218483	0.665978	0.350523
Si21	0.551387	0.165568	0.351753
Si22	0.551482	0.664990	0.351898
Si23	0.884540	0.165147	0.351804
Si24	0.884591	0.664969	0.351227
Si25	0.115482	0.167819	0.648185
Si26	0.115359	0.667610	0.648785
Si27	0.448630	0.168199	0.648188
Si28	0.448488	0.667638	0.648159
Si29	0.781774	0.167284	0.648420
Si30	0.781581	0.668582	0.649582
Si31	0.218419	0.331418	0.350418
Si32	0.218225	0.832716	0.351580
Si33	0.551512	0.332362	0.351841

Atom	x	y	z
Si34	0.551370	0.831801	0.351812
Si35	0.884641	0.332390	0.351215
Si36	0.884518	0.832181	0.351815
Si37	0.281565	0.418119	0.648119
Si38	0.282172	0.917908	0.648221
Si39	0.615172	0.417899	0.648404
Si40	0.614993	0.917960	0.648333
Si41	0.948020	0.415578	0.651652
Si42	0.948781	0.918188	0.648409
Si43	0.051219	0.081812	0.351591
Si44	0.051980	0.584422	0.348348
Si45	0.385007	0.082040	0.351667
Si46	0.384828	0.582101	0.351596
Si47	0.717828	0.082092	0.351779
Si48	0.718435	0.581881	0.351881
O1	0.113016	0.166722	0.559454
O2	0.111989	0.667447	0.559831
O3	0.446093	0.167223	0.559474
O4	0.446178	0.667154	0.559423
O5	0.779131	0.166843	0.559722
O6	0.779552	0.667670	0.560759
O7	0.220448	0.332330	0.439241
O8	0.220869	0.833157	0.440278
O9	0.553822	0.332846	0.440577
O10	0.553907	0.832777	0.440526
O11	0.888011	0.332553	0.440169
O12	0.886984	0.833278	0.440546
O13	0.279576	0.417160	0.559201
O14	0.279636	0.917178	0.559500

Atom	x	y	z
O15	0.612729	0.417038	0.559697
O16	0.612622	0.917222	0.559628
O17	0.943776	0.409238	0.562707
O18	0.945956	0.917972	0.559702
O19	0.054044	0.082028	0.440298
O20	0.056224	0.590762	0.437293
O21	0.387378	0.082778	0.440372
O22	0.387271	0.582962	0.440303
O23	0.720364	0.082822	0.440500
O24	0.720424	0.582840	0.440799
O25	0.279671	0.083857	0.559500
O26	0.279641	0.583824	0.559256
O27	0.612636	0.083806	0.559636
O28	0.612759	0.584027	0.559757
O29	0.945992	0.083059	0.559733
O30	0.943891	0.591712	0.562729
O31	0.056109	0.408288	0.437271
O32	0.054008	0.916941	0.440267
O33	0.387240	0.415973	0.440243
O34	0.387364	0.916194	0.440364
O35	0.720359	0.416176	0.440744
O36	0.720329	0.916143	0.440500
O37	0.112008	0.333604	0.559812
O38	0.113030	0.834322	0.559465
O39	0.446209	0.333870	0.559363
O40	0.446107	0.833796	0.559528
O41	0.779521	0.333426	0.560666
O42	0.779177	0.834129	0.559803
O43	0.220823	0.165871	0.440197

Atom	x	y	z
O44	0.220479	0.666574	0.439334
O45	0.553893	0.166204	0.440472
O46	0.553791	0.666130	0.440637
O47	0.886970	0.165678	0.440535
O48	0.887992	0.666396	0.440188
O49	0.112867	0.000415	0.557618
O50	0.114041	0.500336	0.554116
O51	0.446111	0.000407	0.557630
O52	0.446122	0.500364	0.557469
O53	0.779039	0.000400	0.557739
O54	0.778190	0.500446	0.559839
O55	0.221810	0.499554	0.440161
O56	0.220961	0.999600	0.442261
O57	0.553878	0.499636	0.442531
O58	0.553889	0.999593	0.442370
O59	0.885959	0.499664	0.445884
O60	0.887133	0.999585	0.442383
O61	0.279375	0.250527	0.557166
O62	0.279391	0.750265	0.557215
O63	0.612587	0.250238	0.557803
O64	0.612571	0.750584	0.557869
O65	0.945594	0.247441	0.557843
O66	0.945649	0.753429	0.557833
O67	0.054351	0.246570	0.442167
O68	0.054406	0.752559	0.442157
O69	0.387429	0.249416	0.442131
O70	0.387413	0.749762	0.442197
O71	0.720609	0.249735	0.442785
O72	0.720625	0.749473	0.442834

Atom	x	y	z
O73	0.123238	0.251364	0.678149
O74	0.123058	0.751674	0.678148
O75	0.456827	0.251800	0.678207
O76	0.456714	0.751233	0.678309
O77	0.789298	0.250695	0.679054
O78	0.789474	0.752291	0.679204
O79	0.210526	0.247709	0.320796
O80	0.210702	0.749305	0.320946
O81	0.543286	0.248767	0.321691
O82	0.543173	0.748200	0.321793
O83	0.876942	0.248326	0.321852
O84	0.876762	0.748636	0.321851
O85	0.290592	0.001522	0.678294
O86	0.290515	0.501506	0.678234
O87	0.622279	0.001472	0.678623
O88	0.623986	0.501513	0.678412
O89	0.957109	0.001533	0.679061
O90	0.953835	0.501359	0.675495
O91	0.046165	0.498641	0.324505
O92	0.042891	0.998467	0.320939
O93	0.376014	0.498487	0.321588
O94	0.377721	0.998528	0.321377
O95	0.709485	0.498494	0.321766
O96	0.709408	0.998478	0.321706
O97	0.196106	0.120997	0.678148
O98	0.197080	0.622660	0.678391
O99	0.529378	0.121671	0.678203
O100	0.529057	0.620839	0.678235
O101	0.862783	0.120946	0.678185

Atom	x	y	z
O102	0.861978	0.622506	0.681901
O103	0.138022	0.377494	0.318099
O104	0.137217	0.879054	0.321816
O105	0.470943	0.379161	0.321765
O106	0.470622	0.878329	0.321798
O107	0.802920	0.377340	0.321609
O108	0.803893	0.879003	0.321852
O109	0.029850	0.370733	0.681121
O110	0.029422	0.871332	0.678017
O111	0.362694	0.371566	0.677709
O112	0.362718	0.871016	0.678146
O113	0.695403	0.370772	0.678640
O114	0.696126	0.872030	0.678432
O115	0.303874	0.127970	0.321568
O116	0.304597	0.629228	0.321360
O117	0.637282	0.128984	0.321854
O118	0.637306	0.628434	0.322291
O119	0.970578	0.128668	0.321983
O120	0.970150	0.629267	0.318879
O121	0.029315	0.131963	0.678017
O122	0.029839	0.632223	0.681127
O123	0.362639	0.132196	0.678114
O124	0.362611	0.631592	0.677790
O125	0.696050	0.131020	0.678426
O126	0.695375	0.632362	0.678716
O127	0.304625	0.367638	0.321284
O128	0.303950	0.868980	0.321574
O129	0.637389	0.368408	0.322210
O130	0.637361	0.867804	0.321887

Atom	x	y	z
O131	0.970161	0.367777	0.318873
O132	0.970685	0.868038	0.321983
O133	0.197001	0.380539	0.678403
O134	0.196036	0.882152	0.678155
O135	0.528968	0.382352	0.678185
O136	0.529324	0.881440	0.678213
O137	0.861888	0.380464	0.681915
O138	0.862721	0.882243	0.678202
O139	0.137279	0.117757	0.321798
O140	0.138112	0.619536	0.318085
O141	0.470676	0.118560	0.321788
O142	0.471032	0.617648	0.321815
O143	0.803964	0.117848	0.321845
O144	0.802999	0.619461	0.321597
H1	0.114480	0.000727	0.610244
H2	0.447359	0.000718	0.610256
H3	0.446768	0.500663	0.610096
H4	0.780504	0.000713	0.610364
H5	0.777083	0.500764	0.612422
H6	0.222917	0.499236	0.387578
H7	0.219496	0.999287	0.389636
H8	0.553232	0.499337	0.389904
H9	0.552641	0.999282	0.389744
H10	0.885520	0.999273	0.389756
H11	0.280520	0.251434	0.609798
H12	0.280536	0.750011	0.609846
H13	0.613716	0.250548	0.610428
H14	0.613715	0.750917	0.610494
H15	0.947431	0.248338	0.610452

Atom	x	y	z
H16	0.947481	0.753191	0.610440
H17	0.052519	0.246809	0.389560
H18	0.052569	0.751662	0.389548
H19	0.386285	0.249083	0.389506
H20	0.386284	0.749452	0.389572
H21	0.719464	0.249989	0.390154
H22	0.719480	0.748566	0.390202
Er1	0.000000	0.500000	0.500000

Table S25: Atomic coordinates of $(2V_HEr_{Mg_1})^-$

Atom	x	y	z
Mg1	-0.000000	0.000000	0.500000
Mg2	0.333473	0.000010	0.499959
Mg3	0.333482	0.499982	0.499550
Mg4	0.666528	0.999990	0.500041
Mg5	0.666518	0.500018	0.500451
Mg6	0.166747	0.250430	0.499843
Mg7	0.166716	0.749571	0.499940
Mg8	0.500019	0.250277	0.499984
Mg9	0.499981	0.749723	0.500016
Mg10	0.833284	0.250429	0.500060
Mg11	0.833253	0.749570	0.500157
Mg12	0.166884	0.083293	0.500015
Mg13	0.168271	0.581197	0.502136
Mg14	0.500007	0.083380	0.500029
Mg15	0.499979	0.583237	0.500085
Mg16	0.833121	0.083277	0.500063
Mg17	0.831773	0.581168	0.498017
Mg18	0.168227	0.418832	0.501983

Atom	x	y	z
Mg19	0.166879	0.916724	0.499938
Mg20	0.500021	0.416763	0.499915
Mg21	0.499993	0.916620	0.499971
Mg22	0.831729	0.418803	0.497864
Mg23	0.833116	0.916707	0.499985
Mg24	-0.000000	0.328515	0.499979
Mg25	-0.000008	0.835009	0.500076
Mg26	0.333391	0.333352	0.499466
Mg27	0.333339	0.833151	0.500039
Mg28	0.666613	0.333351	0.500569
Mg29	0.666614	0.833134	0.500116
Mg30	0.333386	0.166866	0.499884
Mg31	0.333387	0.666649	0.499431
Mg32	0.666661	0.166849	0.499961
Mg33	0.666609	0.666648	0.500534
Mg34	0.000008	0.164991	0.499924
Mg35	0.000000	0.671485	0.500021
Si1	0.282106	0.084795	0.648195
Si2	0.281568	0.584296	0.647760
Si3	0.615066	0.084664	0.648274
Si4	0.615170	0.584692	0.648499
Si5	0.948776	0.084519	0.648333
Si6	0.948311	0.586734	0.651437
Si7	0.051689	0.413266	0.348563
Si8	0.051224	0.915481	0.351668
Si9	0.384830	0.415308	0.351501
Si10	0.384934	0.915336	0.351726
Si11	0.718432	0.415704	0.352240
Si12	0.717895	0.915205	0.351805

Atom	x	y	z
Si13	0.115335	0.335385	0.648879
Si14	0.115434	0.834411	0.648300
Si15	0.448364	0.335191	0.648227
Si16	0.448619	0.834323	0.648211
Si17	0.781921	0.334589	0.649047
Si18	0.781905	0.834916	0.648257
Si19	0.218095	0.165084	0.351743
Si20	0.218079	0.665411	0.350953
Si21	0.551381	0.165676	0.351788
Si22	0.551636	0.664809	0.351773
Si23	0.884566	0.165589	0.351700
Si24	0.884665	0.664615	0.351121
Si25	0.115424	0.168124	0.648197
Si26	0.115314	0.667072	0.648985
Si27	0.448617	0.168311	0.648142
Si28	0.448353	0.667452	0.648250
Si29	0.781850	0.167637	0.648205
Si30	0.782036	0.667899	0.649086
Si31	0.217964	0.332101	0.350915
Si32	0.218150	0.832363	0.351796
Si33	0.551647	0.332548	0.351750
Si34	0.551383	0.831689	0.351858
Si35	0.884686	0.332928	0.351015
Si36	0.884576	0.831876	0.351803
Si37	0.281471	0.418224	0.647687
Si38	0.282093	0.917851	0.648210
Si39	0.615135	0.417865	0.648441
Si40	0.615098	0.917898	0.648277
Si41	0.948233	0.415533	0.651310

Atom	x	y	z
Si42	0.948798	0.918071	0.648329
Si43	0.051202	0.081929	0.351671
Si44	0.051768	0.584467	0.348690
Si45	0.384902	0.082102	0.351723
Si46	0.384864	0.582135	0.351559
Si47	0.717907	0.082149	0.351790
Si48	0.718529	0.581776	0.352313
O1	0.113115	0.166617	0.559525
O2	0.112025	0.668380	0.560292
O3	0.446149	0.167110	0.559480
O4	0.446385	0.667395	0.559560
O5	0.779112	0.166811	0.559582
O6	0.779603	0.667202	0.560444
O7	0.220397	0.332798	0.439556
O8	0.220886	0.833189	0.440420
O9	0.553615	0.332605	0.440440
O10	0.553851	0.832890	0.440520
O11	0.887975	0.331620	0.439708
O12	0.886884	0.833383	0.440475
O13	0.281818	0.416211	0.559091
O14	0.279722	0.917290	0.559542
O15	0.612106	0.416854	0.559889
O16	0.612633	0.917255	0.559626
O17	0.943363	0.407604	0.563144
O18	0.945999	0.918063	0.559687
O19	0.054001	0.081938	0.440313
O20	0.056637	0.592396	0.436856
O21	0.387367	0.082745	0.440374
O22	0.387894	0.583147	0.440111

Atom	x	y	z
O23	0.720278	0.082710	0.440458
O24	0.718183	0.583788	0.440909
O25	0.279780	0.083741	0.559530
O26	0.281884	0.584752	0.559163
O27	0.612647	0.083746	0.559620
O28	0.612117	0.584151	0.559947
O29	0.946010	0.082931	0.559686
O30	0.943456	0.593273	0.563240
O31	0.056544	0.406727	0.436760
O32	0.053990	0.917069	0.440314
O33	0.387883	0.415849	0.440052
O34	0.387353	0.916254	0.440380
O35	0.718116	0.415248	0.440837
O36	0.720220	0.916259	0.440469
O37	0.112058	0.332575	0.560187
O38	0.113139	0.834388	0.559619
O39	0.446454	0.333635	0.559531
O40	0.446147	0.833907	0.559548
O41	0.779573	0.333776	0.560401
O42	0.779132	0.834183	0.559638
O43	0.220868	0.165817	0.440362
O44	0.220427	0.666224	0.439599
O45	0.553853	0.166093	0.440452
O46	0.553546	0.666365	0.440469
O47	0.886861	0.165612	0.440381
O48	0.887942	0.667425	0.439813
O49	0.112972	0.000406	0.557573
O50	0.119245	0.500356	0.556106
O51	0.446161	0.000413	0.557566

Atom	x	y	z
O52	0.446358	0.500363	0.557373
O53	0.779057	0.000400	0.557673
O54	0.776206	0.500401	0.561017
O55	0.223794	0.499599	0.438983
O56	0.220943	0.999600	0.442327
O57	0.553642	0.499637	0.442627
O58	0.553839	0.999587	0.442434
O59	0.880755	0.499644	0.443894
O60	0.887028	0.999594	0.442427
O61	0.279588	0.250150	0.557144
O62	0.279560	0.750640	0.557238
O63	0.612554	0.250057	0.557795
O64	0.612527	0.750720	0.557850
O65	0.945600	0.246871	0.557728
O66	0.945594	0.753864	0.557810
O67	0.054406	0.246136	0.442190
O68	0.054400	0.753129	0.442271
O69	0.387473	0.249280	0.442150
O70	0.387446	0.749943	0.442205
O71	0.720440	0.249360	0.442762
O72	0.720412	0.749850	0.442856
O73	0.122857	0.251346	0.678706
O74	0.122650	0.751536	0.678789
O75	0.456713	0.251759	0.678404
O76	0.456570	0.751262	0.678505
O77	0.789030	0.250926	0.678864
O78	0.789088	0.751985	0.678847
O79	0.210912	0.248015	0.321153
O80	0.210970	0.749074	0.321136

Atom	x	y	z
O81	0.543430	0.248737	0.321495
O82	0.543287	0.748241	0.321596
O83	0.877350	0.248465	0.321211
O84	0.877143	0.748654	0.321294
O85	0.290475	0.001523	0.678410
O86	0.291176	0.501452	0.678219
O87	0.622210	0.001479	0.678693
O88	0.623387	0.501462	0.678812
O89	0.956694	0.001494	0.679139
O90	0.952948	0.501290	0.675640
O91	0.047052	0.498711	0.324360
O92	0.043306	0.998505	0.320861
O93	0.376613	0.498538	0.321188
O94	0.377790	0.998521	0.321307
O95	0.708824	0.498549	0.321780
O96	0.709525	0.998477	0.321590
O97	0.196103	0.121037	0.678247
O98	0.198041	0.623528	0.678716
O99	0.529408	0.121669	0.678270
O100	0.529327	0.621277	0.678664
O101	0.862765	0.121056	0.678169
O102	0.862349	0.622794	0.682639
O103	0.137651	0.377206	0.317361
O104	0.137235	0.878944	0.321832
O105	0.470673	0.378723	0.321335
O106	0.470592	0.878331	0.321730
O107	0.801959	0.376472	0.321284
O108	0.803897	0.878963	0.321753
O109	0.030011	0.370768	0.681953

Atom	x	y	z
O110	0.029635	0.871644	0.678191
O111	0.362882	0.371742	0.678201
O112	0.362916	0.871300	0.678279
O113	0.695479	0.370818	0.678667
O114	0.696336	0.872139	0.678451
O115	0.303664	0.127861	0.321549
O116	0.304521	0.629182	0.321333
O117	0.637084	0.128700	0.321721
O118	0.637118	0.628258	0.321799
O119	0.970364	0.128356	0.321809
O120	0.969989	0.629233	0.318047
O121	0.029500	0.131554	0.678123
O122	0.030054	0.632009	0.682079
O123	0.362766	0.131990	0.678222
O124	0.362849	0.631360	0.678247
O125	0.696208	0.130965	0.678416
O126	0.695536	0.632151	0.678697
O127	0.304464	0.367848	0.321303
O128	0.303791	0.869035	0.321584
O129	0.637151	0.368640	0.321753
O130	0.637234	0.868010	0.321778
O131	0.969947	0.367991	0.317921
O132	0.970500	0.868446	0.321877
O133	0.197951	0.379444	0.678681
O134	0.196082	0.882012	0.678293
O135	0.529175	0.381968	0.678639
O136	0.529394	0.881422	0.678294
O137	0.862164	0.380212	0.682570
O138	0.862731	0.882044	0.678186

Atom	x	y	z
O139	0.137269	0.117955	0.321814
O140	0.137837	0.619788	0.317430
O141	0.470606	0.118578	0.321706
O142	0.470825	0.618032	0.321360
O143	0.803918	0.117988	0.321707
O144	0.802049	0.620556	0.321319
H1	0.114467	0.000720	0.610193
H2	0.447257	0.000733	0.610185
H3	0.445925	0.500656	0.609965
H4	0.780708	0.000714	0.610291
H5	0.776166	0.500750	0.613598
H6	0.223834	0.499250	0.386402
H7	0.219292	0.999286	0.389709
H8	0.554075	0.499344	0.390035
H9	0.552743	0.999267	0.389815
H10	0.885533	0.999281	0.389807
H11	0.280127	0.252316	0.609732
H12	0.280134	0.749131	0.609825
H13	0.613879	0.251136	0.610408
H14	0.613882	0.750298	0.610462
H15	0.947797	0.249447	0.610276
H16	0.947801	0.751975	0.610357
H17	0.052199	0.248025	0.389643
H18	0.052203	0.750553	0.389723
H19	0.386118	0.249702	0.389538
H20	0.386121	0.748864	0.389592
H21	0.719866	0.250869	0.390175
H22	0.719873	0.747684	0.390267
Er1	0.000000	0.500000	0.500000

Table S26: Atomic coordinates of $2V_HEr_{Mg_2}$

Atom	x	y	z
Mg1	0.000052	-0.000322	0.499980
Mg2	0.002673	0.502892	0.499725
Mg3	0.333326	-0.000245	0.499962
Mg4	0.333318	0.500304	0.500032
Mg5	0.666564	-0.000331	0.499978
Mg6	0.664129	0.502893	0.500444
Mg7	0.167849	0.249528	0.500735
Mg8	0.166547	0.750145	0.500196
Mg9	0.498850	0.249554	0.499210
Mg10	0.500065	0.750122	0.499861
Mg11	0.833393	0.247070	0.499925
Mg12	0.833332	0.750433	0.500026
Mg13	0.166789	0.082921	0.500111
Mg14	0.167376	0.584106	0.499942
Mg15	0.499855	0.082931	0.499932
Mg16	0.499261	0.584062	0.500161
Mg17	0.833333	0.082453	0.500012
Mg18	0.833314	0.585534	0.500157
Mg19	0.167173	0.417049	0.500320
Mg20	0.166671	0.916604	0.499948
Mg21	0.499528	0.417046	0.499567
Mg22	0.499970	0.916597	0.499942
Mg23	0.833293	0.916515	0.499962
Mg24	0.004192	0.331804	0.500473
Mg25	-0.000050	0.833331	0.500130
Mg26	0.333319	0.333314	0.500042
Mg27	0.333304	0.833277	0.500047
Mg28	0.662529	0.331814	0.499578

Atom	x	y	z
Mg29	0.666646	0.833304	0.500016
Mg30	0.333331	0.166315	0.499908
Mg31	0.333310	0.667178	0.499951
Mg32	0.666181	0.166081	0.500155
Mg33	0.666725	0.667266	0.499607
Mg34	0.000521	0.166084	0.499704
Mg35	-0.000078	0.667264	0.500406
Si1	0.282255	0.084380	0.648241
Si2	0.282649	0.584958	0.648244
Si3	0.615089	0.084254	0.648268
Si4	0.616105	0.584977	0.648391
Si5	0.948896	0.084490	0.648266
Si6	0.948981	0.584982	0.649833
Si7	0.050034	0.416032	0.351885
Si8	0.051243	0.915042	0.351753
Si9	0.383109	0.415513	0.351680
Si10	0.384472	0.915213	0.351724
Si11	0.714695	0.415202	0.347871
Si12	0.717814	0.915146	0.351740
Si13	0.117471	0.334309	0.649893
Si14	0.115501	0.834698	0.648343
Si15	0.450060	0.334632	0.647757
Si16	0.448762	0.834666	0.648204
Si17	0.782181	0.333915	0.650505
Si18	0.782084	0.834550	0.648304
Si19	0.218032	0.165202	0.351961
Si20	0.217297	0.665513	0.351678
Si21	0.551000	0.164940	0.351432
Si22	0.550900	0.665273	0.351321

Atom	x	y	z
Si23	0.884840	0.164473	0.351122
Si24	0.884080	0.664972	0.351527
Si25	0.115741	0.167441	0.648526
Si26	0.115700	0.667859	0.648760
Si27	0.448644	0.167737	0.647923
Si28	0.449258	0.668073	0.648293
Si29	0.781843	0.167066	0.648772
Si30	0.782559	0.667489	0.648554
Si31	0.216612	0.332158	0.352211
Si32	0.217889	0.832094	0.351799
Si33	0.549288	0.331828	0.350082
Si34	0.551150	0.832087	0.351685
Si35	0.884624	0.331256	0.349423
Si36	0.884542	0.832013	0.351768
Si37	0.283575	0.417998	0.648325
Si38	0.282189	0.917766	0.648229
Si39	0.616621	0.418508	0.648072
Si40	0.615368	0.917654	0.648252
Si41	0.952144	0.417793	0.652186
Si42	0.948793	0.917752	0.648268
Si43	0.051619	0.081673	0.351695
Si44	0.050430	0.582485	0.351645
Si45	0.384462	0.081855	0.351705
Si46	0.383906	0.582424	0.351805
Si47	0.717779	0.081906	0.351719
Si48	0.717724	0.582440	0.350350
O1	0.112998	0.167078	0.559791
O2	0.112944	0.667342	0.560004
O3	0.445996	0.166831	0.559205

Atom	x	y	z
O4	0.446050	0.667554	0.559542
O5	0.779383	0.166611	0.559962
O6	0.779583	0.667867	0.559736
O7	0.220011	0.332759	0.440987
O8	0.220514	0.832925	0.440502
O9	0.552700	0.332617	0.438915
O10	0.553786	0.832961	0.440388
O11	0.889681	0.329427	0.438962
O12	0.887220	0.833159	0.440506
O13	0.279985	0.417070	0.559631
O14	0.279477	0.917176	0.559526
O15	0.613210	0.416836	0.559170
O16	0.612755	0.917186	0.559542
O17	0.954109	0.416408	0.563010
O18	0.946152	0.917309	0.559566
O19	0.053969	0.082601	0.440421
O20	0.054585	0.584049	0.440444
O21	0.387179	0.082660	0.440398
O22	0.386670	0.583155	0.440507
O23	0.720551	0.082926	0.440467
O24	0.719116	0.583812	0.438906
O25	0.279517	0.083661	0.559547
O26	0.279944	0.584176	0.559538
O27	0.612735	0.083593	0.559541
O28	0.612043	0.585022	0.559596
O29	0.946128	0.083939	0.559512
O30	0.947619	0.584794	0.561274
O31	0.053447	0.415873	0.440791
O32	0.053856	0.916163	0.440461

Atom	x	y	z
O33	0.386667	0.416129	0.440369
O34	0.387154	0.916184	0.440426
O35	0.712758	0.415230	0.437033
O36	0.720411	0.916264	0.440438
O37	0.114043	0.333621	0.561067
O38	0.112843	0.834005	0.559642
O39	0.446664	0.333722	0.558987
O40	0.446129	0.833949	0.559501
O41	0.777197	0.330547	0.560966
O42	0.779412	0.834136	0.559560
O43	0.220647	0.165820	0.440685
O44	0.220514	0.666603	0.440436
O45	0.553692	0.166099	0.440165
O46	0.553653	0.666335	0.440072
O47	0.887310	0.165594	0.439928
O48	0.887101	0.666835	0.440344
O49	0.112695	0.000402	0.557631
O50	0.114430	0.501004	0.557626
O51	0.446021	0.000316	0.557603
O52	0.446065	0.500477	0.557623
O53	0.779309	0.000292	0.557617
O54	0.776224	0.503495	0.556822
O55	0.220566	0.499725	0.442408
O56	0.220624	0.999514	0.442351
O57	0.552316	0.500201	0.442411
O58	0.553942	0.999585	0.442328
O59	0.890570	0.502837	0.443131
O60	0.887316	0.999470	0.442337
O61	0.280170	0.250181	0.557913

Atom	x	y	z
O62	0.279341	0.750632	0.557700
O63	0.611420	0.249580	0.557383
O64	0.612623	0.750712	0.557413
O65	0.946030	0.250527	0.557117
O66	0.946001	0.750909	0.557812
O67	0.055308	0.248762	0.442618
O68	0.053969	0.749917	0.442652
O69	0.386484	0.249415	0.442049
O70	0.387288	0.749828	0.442325
O71	0.720660	0.249754	0.442881
O72	0.720673	0.750088	0.442239
O73	0.124968	0.250782	0.679135
O74	0.124090	0.751624	0.678591
O75	0.457313	0.251323	0.677774
O76	0.457177	0.751654	0.678445
O77	0.789844	0.250524	0.679694
O78	0.790332	0.751540	0.678305
O79	0.209290	0.248428	0.322192
O80	0.209542	0.748699	0.321491
O81	0.541916	0.247904	0.320838
O82	0.542571	0.748623	0.321429
O83	0.876828	0.247515	0.320158
O84	0.876252	0.748620	0.321774
O85	0.291216	0.001319	0.678382
O86	0.290866	0.501661	0.678198
O87	0.623483	0.001241	0.678495
O88	0.621741	0.501766	0.678420
O89	0.957565	0.001414	0.678329
O90	0.957858	0.501635	0.680721

Atom	x	y	z
O91	0.044682	0.498893	0.321560
O92	0.043144	0.998246	0.321544
O93	0.375807	0.498745	0.321771
O94	0.375585	0.998386	0.321560
O95	0.708986	0.498707	0.319449
O96	0.709039	0.998422	0.321687
O97	0.195827	0.119949	0.678270
O98	0.196793	0.621329	0.678273
O99	0.529081	0.120773	0.677954
O100	0.529998	0.621746	0.678178
O101	0.862677	0.120483	0.678333
O102	0.864103	0.622892	0.679614
O103	0.135433	0.377910	0.322358
O104	0.137396	0.879025	0.321855
O105	0.468122	0.378058	0.320933
O106	0.470747	0.879317	0.321835
O107	0.801369	0.376215	0.322715
O108	0.804094	0.879282	0.321925
O109	0.032592	0.371079	0.682200
O110	0.029350	0.870936	0.678194
O111	0.364701	0.371813	0.677966
O112	0.362583	0.870759	0.678125
O113	0.697023	0.371707	0.679080
O114	0.696050	0.871081	0.678185
O115	0.304255	0.129307	0.321923
O116	0.303211	0.628928	0.321787
O117	0.637597	0.129328	0.321849
O118	0.636015	0.628332	0.320466
O119	0.970949	0.128325	0.321582

Atom	x	y	z
O120	0.970495	0.629646	0.321522
O121	0.029053	0.132370	0.678111
O122	0.030525	0.631508	0.679721
O123	0.362390	0.132327	0.677989
O124	0.363213	0.632119	0.678207
O125	0.695658	0.131462	0.678355
O126	0.696082	0.632579	0.678465
O127	0.302070	0.368780	0.322060
O128	0.304081	0.867768	0.321870
O129	0.634226	0.368126	0.317817
O130	0.637367	0.867788	0.321813
O131	0.969841	0.368559	0.320817
O132	0.970658	0.867947	0.321845
O133	0.198525	0.381071	0.679081
O134	0.195843	0.882432	0.678142
O135	0.531207	0.380839	0.677593
O136	0.529131	0.882176	0.678139
O137	0.865457	0.379148	0.677274
O138	0.862493	0.882327	0.678095
O139	0.137678	0.117683	0.321964
O140	0.136632	0.618662	0.321848
O141	0.470905	0.117030	0.321718
O142	0.469813	0.618337	0.321808
O143	0.804057	0.117369	0.321627
O144	0.802600	0.619874	0.320473
H1	0.114249	0.000338	0.610257
H2	0.115138	0.502147	0.610231
H3	0.447389	0.000360	0.610230
H4	0.447886	0.501073	0.610257

Atom	x	y	z
H5	0.780740	0.000019	0.610240
H6	0.218756	0.499669	0.389774
H7	0.219229	0.998918	0.389725
H8	0.551614	0.500674	0.389806
H9	0.552386	0.998888	0.389702
H10	0.885891	0.998566	0.389713
H11	0.281905	0.250521	0.610540
H12	0.280853	0.750751	0.610326
H13	0.612086	0.250579	0.609999
H14	0.614587	0.750192	0.610034
H15	0.947928	0.250192	0.609759
H16	0.946819	0.750598	0.610432
H17	0.054613	0.249157	0.390002
H18	0.052021	0.748748	0.390030
H19	0.384700	0.249135	0.389422
H20	0.385800	0.749311	0.389698
H21	0.718722	0.248793	0.390238
H22	0.719790	0.749118	0.389617
Er1	0.833422	0.424265	0.499978

Table S27: Atomic coordinates of $(2V_H Er_{Mg_2})^+$

Atom	x	y	z
Mg1	0.000255	0.999551	0.499920
Mg2	0.005912	0.503023	0.502131
Mg3	0.333324	0.999676	0.499992
Mg4	0.333320	0.500332	0.500026
Mg5	0.666427	0.999549	0.500053
Mg6	0.660733	0.502885	0.497992
Mg7	0.168322	0.248949	0.500652

Atom	x	y	z
Mg8	0.166908	0.750585	0.500027
Mg9	0.498384	0.248978	0.499199
Mg10	0.499720	0.750587	0.500019
Mg11	0.833351	0.244784	0.499989
Mg12	0.833293	0.751870	0.500054
Mg13	0.166940	0.082688	0.500043
Mg14	0.168317	0.584407	0.499916
Mg15	0.499714	0.082705	0.499990
Mg16	0.498287	0.584388	0.500216
Mg17	0.833351	0.081763	0.499998
Mg18	0.833404	0.589962	0.500241
Mg19	0.168270	0.416708	0.500370
Mg20	0.166856	0.916673	0.499887
Mg21	0.498433	0.416719	0.499499
Mg22	0.499821	0.916682	0.500017
Mg23	0.833351	0.916685	0.499952
Mg24	0.005780	0.331118	0.500707
Mg25	0.000260	0.833686	0.499923
Mg26	0.333339	0.332963	0.500025
Mg27	0.333324	0.833496	0.500061
Mg28	0.660899	0.331057	0.499400
Mg29	0.666367	0.833687	0.500265
Mg30	0.333336	0.165935	0.499920
Mg31	0.333292	0.667461	0.499958
Mg32	0.665830	0.165489	0.500283
Mg33	0.665852	0.668013	0.499768
Mg34	0.000865	0.165505	0.499584
Mg35	0.000768	0.668031	0.500241
Si1	0.281996	0.084277	0.648361

Atom	x	y	z
Si2	0.282566	0.584990	0.648321
Si3	0.614657	0.084124	0.648497
Si4	0.615685	0.585119	0.648780
Si5	0.948867	0.084334	0.648344
Si6	0.948682	0.585441	0.649561
Si7	0.050190	0.415943	0.352112
Si8	0.051610	0.915139	0.351527
Si9	0.382670	0.415510	0.351551
Si10	0.384629	0.915189	0.351655
Si11	0.714057	0.415415	0.347765
Si12	0.717788	0.915109	0.351726
Si13	0.118163	0.334112	0.649760
Si14	0.115500	0.834775	0.648317
Si15	0.450118	0.334375	0.647769
Si16	0.448586	0.834786	0.648403
Si17	0.782532	0.333491	0.651238
Si18	0.781947	0.835227	0.648601
Si19	0.218279	0.164991	0.351789
Si20	0.217710	0.665728	0.351551
Si21	0.551124	0.164755	0.351364
Si22	0.550689	0.665436	0.351667
Si23	0.885076	0.163764	0.350962
Si24	0.884618	0.665830	0.350704
Si25	0.115545	0.167283	0.648567
Si26	0.115842	0.668030	0.648399
Si27	0.448320	0.167526	0.648099
Si28	0.448786	0.668289	0.648408
Si29	0.781575	0.166248	0.648953
Si30	0.781926	0.668455	0.649414

Atom	x	y	z
Si31	0.216658	0.331875	0.352180
Si32	0.218129	0.832216	0.351601
Si33	0.548595	0.331636	0.350118
Si34	0.551195	0.832167	0.351724
Si35	0.884383	0.330843	0.348592
Si36	0.884751	0.832609	0.351470
Si37	0.284028	0.418007	0.648418
Si38	0.282080	0.917760	0.648352
Si39	0.616605	0.418442	0.647926
Si40	0.615073	0.917749	0.648471
Si41	0.952585	0.418159	0.652185
Si42	0.948904	0.917738	0.648302
Si43	0.051969	0.081536	0.351473
Si44	0.050865	0.582551	0.351275
Si45	0.384630	0.081747	0.351641
Si46	0.383913	0.582445	0.351724
Si47	0.717791	0.081735	0.351657
Si48	0.717943	0.582795	0.350633
O1	0.112761	0.167184	0.559743
O2	0.112878	0.667113	0.559544
O3	0.445989	0.166754	0.559306
O4	0.446069	0.667514	0.559606
O5	0.779197	0.166263	0.560091
O6	0.778852	0.667956	0.560256
O7	0.219896	0.332651	0.441012
O8	0.220621	0.832915	0.440371
O9	0.552412	0.332739	0.439041
O10	0.553924	0.832880	0.440501
O11	0.889210	0.329732	0.439094

Atom	x	y	z
O12	0.887321	0.833142	0.440292
O13	0.280417	0.417050	0.559648
O14	0.279415	0.917130	0.559586
O15	0.614390	0.417370	0.558769
O16	0.612658	0.917189	0.559702
O17	0.952810	0.417650	0.562295
O18	0.946100	0.917150	0.559520
O19	0.054031	0.082561	0.440269
O20	0.053348	0.583377	0.440401
O21	0.387293	0.082636	0.440396
O22	0.386426	0.583137	0.440505
O23	0.720752	0.083011	0.440487
O24	0.720354	0.582942	0.439640
O25	0.279352	0.083630	0.559599
O26	0.280155	0.584176	0.559540
O27	0.612640	0.083570	0.559705
O28	0.613371	0.584332	0.559650
O29	0.945925	0.084054	0.559504
O30	0.946467	0.584207	0.560582
O31	0.052315	0.416378	0.441254
O32	0.053992	0.916126	0.440295
O33	0.386230	0.416083	0.440315
O34	0.387254	0.916099	0.440411
O35	0.713290	0.416065	0.437621
O36	0.720555	0.916101	0.440501
O37	0.114345	0.333707	0.560844
O38	0.112744	0.833925	0.559542
O39	0.446871	0.333635	0.558938
O40	0.446068	0.833959	0.559640

Atom	x	y	z
O41	0.777632	0.330896	0.560724
O42	0.779361	0.834159	0.559779
O43	0.220644	0.165739	0.440590
O44	0.220463	0.666541	0.440361
O45	0.553919	0.166163	0.440193
O46	0.553705	0.666114	0.440520
O47	0.887469	0.165352	0.439820
O48	0.887700	0.666927	0.439853
O49	0.112594	0.000379	0.557583
O50	0.115728	0.500891	0.558471
O51	0.445961	0.000285	0.557688
O52	0.446561	0.500458	0.557639
O53	0.779205	0.000155	0.557696
O54	0.777763	0.504804	0.557602
O55	0.220086	0.499697	0.442376
O56	0.220700	0.999453	0.442277
O57	0.550946	0.500115	0.441573
O58	0.554083	0.999567	0.442383
O59	0.889545	0.504434	0.442750
O60	0.887489	0.999356	0.442249
O61	0.280273	0.250126	0.557950
O62	0.279324	0.750587	0.557694
O63	0.611598	0.249582	0.557640
O64	0.612500	0.750693	0.557754
O65	0.945708	0.251165	0.556721
O66	0.945711	0.750569	0.557499
O67	0.055069	0.248781	0.442337
O68	0.054116	0.749887	0.442341
O69	0.386408	0.249343	0.441964

Atom	x	y	z
O70	0.387317	0.749777	0.442337
O71	0.720977	0.250281	0.443269
O72	0.720896	0.749748	0.442585
O73	0.125254	0.250772	0.678912
O74	0.124989	0.751539	0.678121
O75	0.458128	0.251223	0.677635
O76	0.458105	0.751654	0.678366
O77	0.790779	0.250216	0.679063
O78	0.791061	0.752073	0.678632
O79	0.208416	0.248319	0.322305
O80	0.208536	0.748712	0.321567
O81	0.541377	0.247873	0.321081
O82	0.541747	0.748542	0.321891
O83	0.875837	0.247281	0.320680
O84	0.875553	0.749071	0.321444
O85	0.291764	0.001279	0.678336
O86	0.291592	0.501695	0.678007
O87	0.624096	0.001251	0.678581
O88	0.623834	0.501710	0.677969
O89	0.958663	0.001349	0.678120
O90	0.957994	0.502016	0.680069
O91	0.042805	0.498776	0.322043
O92	0.042477	0.998257	0.321450
O93	0.374924	0.498778	0.321944
O94	0.374949	0.998332	0.321716
O95	0.708691	0.498974	0.320117
O96	0.708060	0.998336	0.321912
O97	0.195128	0.119320	0.678155
O98	0.195765	0.620138	0.677862

Atom	x	y	z
O99	0.528373	0.120102	0.678029
O100	0.528996	0.620601	0.677752
O101	0.862103	0.119539	0.678373
O102	0.862757	0.621813	0.678792
O103	0.135543	0.378358	0.322926
O104	0.138063	0.879696	0.321804
O105	0.468192	0.378655	0.321084
O106	0.471364	0.879939	0.321968
O107	0.801662	0.377248	0.323754
O108	0.804595	0.880144	0.321954
O109	0.032649	0.371105	0.681055
O110	0.028699	0.869897	0.678004
O111	0.364938	0.371630	0.677962
O112	0.361962	0.870029	0.678119
O113	0.697293	0.371548	0.678419
O114	0.695416	0.870594	0.678235
O115	0.304991	0.130004	0.321997
O116	0.303944	0.629791	0.321769
O117	0.638369	0.130187	0.322025
O118	0.636920	0.629338	0.321702
O119	0.971792	0.129156	0.321534
O120	0.971058	0.630090	0.321450
O121	0.028235	0.133265	0.677899
O122	0.029512	0.632651	0.678523
O123	0.361585	0.133024	0.677914
O124	0.362480	0.632888	0.678229
O125	0.694794	0.132191	0.678437
O126	0.695391	0.633208	0.678619
O127	0.302013	0.368407	0.321997

Atom	x	y	z
O128	0.304783	0.867013	0.321883
O129	0.634263	0.367819	0.318612
O130	0.638059	0.866778	0.322044
O131	0.969768	0.368324	0.321497
O132	0.971339	0.867454	0.321791
O133	0.198595	0.381441	0.678873
O134	0.195319	0.882976	0.678044
O135	0.531306	0.381157	0.677073
O136	0.528642	0.882668	0.678205
O137	0.865320	0.379936	0.676410
O138	0.862078	0.883220	0.678094
O139	0.138281	0.117051	0.321925
O140	0.137528	0.617621	0.322203
O141	0.471493	0.116400	0.321847
O142	0.470730	0.617211	0.322206
O143	0.804550	0.116576	0.321646
O144	0.803814	0.618764	0.321310
H1	0.114412	0.000249	0.610216
H2	0.118777	0.502415	0.611079
H3	0.447112	0.000294	0.610319
H4	0.447310	0.501098	0.610278
H5	0.780606	0.999757	0.610323
H6	0.219323	0.499673	0.389737
H7	0.219576	0.998762	0.389647
H8	0.547926	0.500967	0.388966
H9	0.552280	0.998757	0.389749
H10	0.886119	0.998250	0.389622
H11	0.282247	0.249812	0.610579
H12	0.280879	0.751297	0.610327

Atom	x	y	z
H13	0.611136	0.249502	0.610247
H14	0.613681	0.751292	0.610389
H15	0.948459	0.249295	0.609338
H16	0.947286	0.751432	0.610142
H17	0.055594	0.248029	0.389732
H18	0.052904	0.749815	0.389706
H19	0.384436	0.248404	0.389335
H20	0.385729	0.749837	0.389705
H21	0.718237	0.247800	0.390649
H22	0.719325	0.750041	0.389944
Er1	0.833322	0.419823	0.499539

Table S28: Atomic coordinates of $(2V_HEr_{Mg_2})^-$

Atom	x	y	z
Mg1	0.999919	0.999767	0.500035
Mg2	0.000799	0.503616	0.497640
Mg3	0.333313	0.999802	0.499977
Mg4	0.333334	0.500209	0.500039
Mg5	0.666665	0.999731	0.499953
Mg6	0.666074	0.503454	0.502469
Mg7	0.167525	0.249935	0.500871
Mg8	0.166344	0.749824	0.500351
Mg9	0.499107	0.249909	0.499052
Mg10	0.500324	0.749761	0.499686
Mg11	0.833249	0.248360	0.499877
Mg12	0.833350	0.750115	0.500016
Mg13	0.166618	0.083065	0.500179
Mg14	0.167151	0.584027	0.500231
Mg15	0.499981	0.083050	0.499873

Atom	x	y	z
Mg16	0.499560	0.583949	0.499889
Mg17	0.833289	0.082873	0.500041
Mg18	0.833412	0.583442	0.500153
Mg19	0.166302	0.417200	0.500379
Mg20	0.166561	0.916537	0.500043
Mg21	0.500373	0.417173	0.499549
Mg22	0.500074	0.916519	0.499850
Mg23	0.833292	0.916490	0.499963
Mg24	0.002651	0.332316	0.500264
Mg25	0.999812	0.833188	0.500227
Mg26	0.333326	0.333485	0.500018
Mg27	0.333323	0.833141	0.500056
Mg28	0.663984	0.332251	0.499616
Mg29	0.666794	0.833124	0.499920
Mg30	0.333313	0.166483	0.499934
Mg31	0.333345	0.667071	0.499993
Mg32	0.666431	0.166450	0.500111
Mg33	0.667377	0.666804	0.499498
Mg34	0.000146	0.166500	0.499724
Mg35	0.999342	0.666908	0.500502
Si1	0.282201	0.084392	0.648254
Si2	0.282737	0.584951	0.648301
Si3	0.615168	0.084210	0.648154
Si4	0.616512	0.584751	0.647958
Si5	0.948752	0.084437	0.648301
Si6	0.949100	0.584856	0.650397
Si7	0.049270	0.415887	0.351796
Si8	0.051204	0.914958	0.351870
Si9	0.383141	0.415462	0.351708

Atom	x	y	z
Si10	0.384515	0.915191	0.351758
Si11	0.714581	0.415039	0.348302
Si12	0.717936	0.915030	0.351752
Si13	0.117168	0.334422	0.650057
Si14	0.115424	0.834558	0.648466
Si15	0.450437	0.334755	0.647788
Si16	0.448808	0.834505	0.648065
Si17	0.782143	0.333353	0.649759
Si18	0.782085	0.834065	0.648229
Si19	0.217944	0.165335	0.352157
Si20	0.216976	0.665303	0.351698
Si21	0.551027	0.164972	0.351381
Si22	0.551210	0.665049	0.350767
Si23	0.884706	0.164725	0.350865
Si24	0.883933	0.664442	0.352064
Si25	0.115616	0.167490	0.648540
Si26	0.115520	0.667700	0.649326
Si27	0.448653	0.167776	0.647792
Si28	0.449742	0.667783	0.648302
Si29	0.781884	0.167359	0.649025
Si30	0.782854	0.666838	0.647999
Si31	0.216220	0.332382	0.352208
Si32	0.217905	0.831983	0.351934
Si33	0.549563	0.331940	0.349870
Si34	0.551225	0.831933	0.351597
Si35	0.884434	0.330653	0.349937
Si36	0.884598	0.831596	0.351816
Si37	0.283576	0.417906	0.648284
Si38	0.282173	0.917733	0.648208

Atom	x	y	z
Si39	0.617297	0.418334	0.648153
Si40	0.615480	0.917510	0.648107
Si41	0.952284	0.417743	0.651713
Si42	0.948651	0.917666	0.648278
Si43	0.051470	0.081676	0.351824
Si44	0.050209	0.582335	0.352041
Si45	0.384419	0.081888	0.351733
Si46	0.383921	0.582441	0.351792
Si47	0.717821	0.081788	0.351733
Si48	0.717784	0.582241	0.349808
O1	0.113130	0.166815	0.559893
O2	0.113121	0.667719	0.560666
O3	0.445844	0.166692	0.559145
O4	0.445927	0.667686	0.559573
O5	0.779407	0.166222	0.560245
O6	0.779908	0.669209	0.559498
O7	0.220140	0.332754	0.440933
O8	0.220588	0.833008	0.440582
O9	0.552481	0.332308	0.438608
O10	0.553644	0.833049	0.440234
O11	0.890658	0.326358	0.438324
O12	0.887280	0.833501	0.440495
O13	0.279905	0.416995	0.559665
O14	0.279503	0.917224	0.559562
O15	0.612278	0.416141	0.559521
O16	0.612726	0.917200	0.559455
O17	0.956675	0.416397	0.563403
O18	0.946220	0.917433	0.559645
O19	0.053953	0.082482	0.440494

Atom	x	y	z
O20	0.056763	0.585337	0.440515
O21	0.387127	0.082581	0.440370
O22	0.386650	0.583298	0.440431
O23	0.720389	0.082659	0.440412
O24	0.717750	0.584996	0.437885
O25	0.279533	0.083568	0.559619
O26	0.280025	0.584312	0.559660
O27	0.612679	0.083446	0.559482
O28	0.610037	0.586210	0.559481
O29	0.946228	0.083742	0.559611
O30	0.949154	0.586158	0.562319
O31	0.054314	0.415208	0.440436
O32	0.053891	0.916212	0.440529
O33	0.386771	0.416048	0.440331
O34	0.387118	0.916216	0.440404
O35	0.710257	0.414872	0.436587
O36	0.720320	0.916373	0.440380
O37	0.114136	0.333392	0.561323
O38	0.113012	0.834095	0.559828
O39	0.446509	0.333667	0.559063
O40	0.446103	0.833997	0.559421
O41	0.775679	0.327496	0.561363
O42	0.779381	0.834443	0.559546
O43	0.220756	0.165734	0.440807
O44	0.220716	0.666764	0.440428
O45	0.553457	0.165809	0.440024
O46	0.553557	0.666628	0.439425
O47	0.887208	0.165227	0.439651
O48	0.886888	0.668300	0.440560

Atom	x	y	z
O49	0.112750	0.000341	0.557681
O50	0.114376	0.501284	0.557152
O51	0.446023	0.000277	0.557499
O52	0.445650	0.500456	0.557532
O53	0.779325	0.000258	0.557551
O54	0.772899	0.507746	0.558828
O55	0.221016	0.499694	0.442527
O56	0.220600	0.999506	0.442464
O57	0.552417	0.500434	0.442926
O58	0.553853	0.999512	0.442289
O59	0.893987	0.506994	0.441566
O60	0.887279	0.999487	0.442450
O61	0.280176	0.250085	0.557885
O62	0.279379	0.750773	0.557719
O63	0.610745	0.249165	0.556956
O64	0.612495	0.751013	0.557144
O65	0.946399	0.249848	0.557610
O66	0.946234	0.751614	0.558057
O67	0.055876	0.248395	0.442944
O68	0.054142	0.750262	0.442933
O69	0.386435	0.249291	0.442065
O70	0.387288	0.749947	0.442354
O71	0.720145	0.248808	0.442219
O72	0.720447	0.750730	0.442047
O73	0.124841	0.250665	0.679393
O74	0.123983	0.751715	0.679195
O75	0.456862	0.251232	0.677904
O76	0.456892	0.751603	0.678526
O77	0.789648	0.250151	0.681311

Atom	x	y	z
O78	0.790006	0.751283	0.678438
O79	0.209716	0.248431	0.322115
O80	0.209881	0.748702	0.321425
O81	0.541903	0.247773	0.320517
O82	0.542642	0.748673	0.320899
O83	0.876976	0.247022	0.318382
O84	0.876584	0.748447	0.321611
O85	0.291111	0.001287	0.678550
O86	0.290564	0.501606	0.678361
O87	0.623215	0.001112	0.678512
O88	0.620302	0.501711	0.678627
O89	0.957424	0.001302	0.678570
O90	0.957723	0.501497	0.681469
O91	0.046025	0.498878	0.321365
O92	0.043523	0.998169	0.321485
O93	0.376039	0.498742	0.321649
O94	0.375611	0.998365	0.321448
O95	0.709208	0.498491	0.318740
O96	0.709050	0.998261	0.321481
O97	0.195829	0.119922	0.678462
O98	0.197410	0.621919	0.678771
O99	0.528998	0.120619	0.677933
O100	0.530511	0.622081	0.678656
O101	0.862571	0.120153	0.678586
O102	0.864755	0.623706	0.680522
O103	0.134883	0.377390	0.321891
O104	0.137448	0.878983	0.321860
O105	0.467698	0.377554	0.320585
O106	0.470755	0.879323	0.321688

Atom	x	y	z
O107	0.800667	0.375035	0.322794
O108	0.804165	0.879140	0.321834
O109	0.032974	0.371276	0.683206
O110	0.029454	0.871166	0.678415
O111	0.365057	0.372086	0.678078
O112	0.362711	0.870879	0.678170
O113	0.697433	0.371631	0.679763
O114	0.696154	0.871117	0.678242
O115	0.304028	0.129080	0.321870
O116	0.303024	0.628792	0.321699
O117	0.637330	0.128799	0.321623
O118	0.635660	0.627990	0.318915
O119	0.970722	0.127801	0.321354
O120	0.970685	0.629919	0.321639
O121	0.029178	0.131989	0.678335
O122	0.031075	0.631168	0.681313
O123	0.362481	0.132123	0.678113
O124	0.363637	0.631786	0.678357
O125	0.695769	0.130994	0.678575
O126	0.696063	0.632725	0.678359
O127	0.301732	0.369090	0.321958
O128	0.304036	0.867864	0.321791
O129	0.633778	0.368316	0.316746
O130	0.637322	0.867889	0.321625
O131	0.969358	0.368455	0.320153
O132	0.970616	0.868035	0.321762
O133	0.199050	0.380377	0.679369
O134	0.195894	0.882385	0.678319
O135	0.531796	0.380141	0.678104

Atom	x	y	z
O136	0.529150	0.882091	0.678132
O137	0.865992	0.378104	0.676752
O138	0.862467	0.882102	0.678207
O139	0.137633	0.117698	0.322034
O140	0.136342	0.619001	0.321307
O141	0.470789	0.116997	0.321514
O142	0.469398	0.618753	0.321341
O143	0.804041	0.117001	0.321442
O144	0.802103	0.620694	0.319642
H1	0.113963	0.000377	0.610297
H2	0.112469	0.501882	0.609656
H3	0.447609	0.000429	0.610121
H4	0.448562	0.501027	0.610148
H5	0.780811	0.000280	0.610167
H6	0.218139	0.499599	0.389912
H7	0.219006	0.999000	0.389842
H8	0.554318	0.500374	0.390422
H9	0.552657	0.998928	0.389671
H10	0.885771	0.998851	0.389830
H11	0.281740	0.251008	0.610501
H12	0.280765	0.750326	0.610327
H13	0.612862	0.251503	0.609530
H14	0.615167	0.749210	0.609719
H15	0.947629	0.250643	0.610226
H16	0.946465	0.750026	0.610620
H17	0.053794	0.250057	0.390369
H18	0.051416	0.747774	0.390359
H19	0.384896	0.249575	0.389450
H20	0.385898	0.748834	0.389742

Atom	x	y	z
H21	0.718936	0.249053	0.389607
H22	0.720154	0.748501	0.389483
Er1	0.833492	0.427709	0.500145

Table S29: Atomic coordinates of the optimized 3x2x3 pristine talc supercell

Atom	x	y	z
Mg1	0.000426	0.000106	0.330506
Mg2	0.999574	0.999894	0.669494
Mg3	0.000426	0.500106	0.330506
Mg4	0.999574	0.499894	0.669494
Mg5	0.333760	0.000106	0.330506
Mg6	0.332907	0.999893	0.669494
Mg7	0.333760	0.500106	0.330506
Mg8	0.332907	0.499893	0.669494
Mg9	0.667093	0.000107	0.330506
Mg10	0.666240	0.999894	0.669494
Mg11	0.667093	0.500107	0.330506
Mg12	0.666240	0.499894	0.669494
Mg13	0.167093	0.250107	0.330506
Mg14	0.166240	0.249894	0.669494
Mg15	0.167093	0.750107	0.330506
Mg16	0.166240	0.749894	0.669494
Mg17	0.500426	0.250106	0.330506
Mg18	0.499574	0.249894	0.669494
Mg19	0.500426	0.750106	0.330506
Mg20	0.499574	0.749894	0.669494
Mg21	0.833760	0.250106	0.330506
Mg22	0.832907	0.249893	0.669494

Atom	x	y	z
Mg23	0.833760	0.750106	0.330506
Mg24	0.832907	0.749893	0.669494
Mg25	0.166944	0.083303	0.330664
Mg26	0.166393	0.083093	0.669364
Mg27	0.166944	0.583303	0.330664
Mg28	0.166393	0.583093	0.669364
Mg29	0.500278	0.083303	0.330664
Mg30	0.499728	0.083093	0.669365
Mg31	0.500278	0.583303	0.330664
Mg32	0.499728	0.583093	0.669365
Mg33	0.833610	0.083303	0.330664
Mg34	0.833060	0.083092	0.669364
Mg35	0.833610	0.583303	0.330664
Mg36	0.833060	0.583092	0.669364
Mg37	0.166940	0.416908	0.330636
Mg38	0.166390	0.416697	0.669337
Mg39	0.166940	0.916908	0.330636
Mg40	0.166390	0.916697	0.669337
Mg41	0.500272	0.416907	0.330635
Mg42	0.499722	0.416697	0.669336
Mg43	0.500272	0.916907	0.330635
Mg44	0.499722	0.916697	0.669336
Mg45	0.833607	0.416907	0.330636
Mg46	0.833056	0.416697	0.669336
Mg47	0.833607	0.916907	0.330636
Mg48	0.833056	0.916697	0.669336
Mg49	0.000275	0.333303	0.330664
Mg50	0.999726	0.333093	0.669365
Mg51	0.000275	0.833303	0.330664

Atom	x	y	z
Mg52	0.999726	0.833093	0.669365
Mg53	0.333610	0.333303	0.330664
Mg54	0.333060	0.333092	0.669364
Mg55	0.333610	0.833303	0.330664
Mg56	0.333060	0.833092	0.669364
Mg57	0.666944	0.333303	0.330664
Mg58	0.666393	0.333093	0.669364
Mg59	0.666944	0.833303	0.330664
Mg60	0.666393	0.833093	0.669364
Mg61	0.000274	0.166907	0.330635
Mg62	0.999725	0.166697	0.669336
Mg63	0.000274	0.666907	0.330635
Mg64	0.999725	0.666697	0.669336
Mg65	0.333607	0.166907	0.330636
Mg66	0.333056	0.166697	0.669336
Mg67	0.333607	0.666907	0.330636
Mg68	0.333056	0.666697	0.669336
Mg69	0.666940	0.166908	0.330636
Mg70	0.666390	0.166697	0.669337
Mg71	0.666940	0.666908	0.330636
Mg72	0.666390	0.666697	0.669337
Si1	0.281947	0.084247	0.430511
Si2	0.280894	0.084237	0.769344
Si3	0.281947	0.584247	0.430511
Si4	0.280894	0.584237	0.769344
Si5	0.615280	0.084248	0.430512
Si6	0.614226	0.084235	0.769344
Si7	0.615280	0.584248	0.430512
Si8	0.614226	0.584235	0.769344

Atom	x	y	z
Si9	0.948610	0.084245	0.430510
Si10	0.947560	0.084235	0.769344
Si11	0.948610	0.584245	0.430510
Si12	0.947560	0.584235	0.769344
Si13	0.052440	0.415765	0.230656
Si14	0.051390	0.415755	0.569490
Si15	0.052440	0.915765	0.230656
Si16	0.051390	0.915755	0.569490
Si17	0.385774	0.415765	0.230656
Si18	0.384720	0.415752	0.569488
Si19	0.385774	0.915765	0.230656
Si20	0.384720	0.915752	0.569488
Si21	0.719106	0.415763	0.230656
Si22	0.718053	0.415753	0.569489
Si23	0.719106	0.915763	0.230656
Si24	0.718053	0.915753	0.569489
Si25	0.115280	0.334248	0.430512
Si26	0.114226	0.334235	0.769344
Si27	0.115280	0.834248	0.430512
Si28	0.114226	0.834235	0.769344
Si29	0.448610	0.334245	0.430510
Si30	0.447560	0.334235	0.769344
Si31	0.448610	0.834245	0.430510
Si32	0.447560	0.834235	0.769344
Si33	0.781947	0.334247	0.430511
Si34	0.780894	0.334237	0.769344
Si35	0.781947	0.834247	0.430511
Si36	0.780894	0.834237	0.769344
Si37	0.219106	0.165763	0.230656

Atom	x	y	z
Si38	0.218053	0.165753	0.569489
Si39	0.219106	0.665763	0.230656
Si40	0.218053	0.665753	0.569489
Si41	0.552440	0.165765	0.230656
Si42	0.551390	0.165755	0.569490
Si43	0.552440	0.665765	0.230656
Si44	0.551390	0.665755	0.569490
Si45	0.885774	0.165765	0.230656
Si46	0.884720	0.165752	0.569488
Si47	0.885774	0.665765	0.230656
Si48	0.884720	0.665752	0.569488
Si49	0.115287	0.167507	0.430502
Si50	0.114226	0.167109	0.769344
Si51	0.115287	0.667507	0.430502
Si52	0.114226	0.667109	0.769344
Si53	0.448624	0.167509	0.430502
Si54	0.447560	0.167110	0.769345
Si55	0.448624	0.667509	0.430502
Si56	0.447560	0.667110	0.769345
Si57	0.781956	0.167508	0.430502
Si58	0.780893	0.167110	0.769345
Si59	0.781956	0.667508	0.430502
Si60	0.780893	0.667110	0.769345
Si61	0.219107	0.332890	0.230655
Si62	0.218044	0.332492	0.569498
Si63	0.219107	0.832890	0.230655
Si64	0.218044	0.832492	0.569498
Si65	0.552440	0.332890	0.230655
Si66	0.551376	0.332491	0.569498

Atom	x	y	z
Si67	0.552440	0.832890	0.230655
Si68	0.551376	0.832491	0.569498
Si69	0.885774	0.332891	0.230656
Si70	0.884713	0.332493	0.569498
Si71	0.885774	0.832891	0.230656
Si72	0.884713	0.832493	0.569498
Si73	0.281956	0.417508	0.430502
Si74	0.280893	0.417110	0.769345
Si75	0.281956	0.917508	0.430502
Si76	0.280893	0.917110	0.769345
Si77	0.615287	0.417507	0.430502
Si78	0.614226	0.417109	0.769344
Si79	0.615287	0.917507	0.430502
Si80	0.614226	0.917109	0.769344
Si81	0.948624	0.417509	0.430502
Si82	0.947560	0.417110	0.769345
Si83	0.948624	0.917509	0.430502
Si84	0.947560	0.917110	0.769345
Si85	0.052440	0.082890	0.230655
Si86	0.051376	0.082491	0.569498
Si87	0.052440	0.582890	0.230655
Si88	0.051376	0.582491	0.569498
Si89	0.385774	0.082891	0.230656
Si90	0.384713	0.082493	0.569498
Si91	0.385774	0.582891	0.230656
Si92	0.384713	0.582493	0.569498
Si93	0.719107	0.082890	0.230655
Si94	0.718044	0.082492	0.569498
Si95	0.719107	0.582890	0.230655

Atom	x	y	z
Si96	0.718044	0.582492	0.569498
O1	0.113098	0.166941	0.370925
O2	0.112248	0.166528	0.709628
O3	0.113098	0.666941	0.370925
O4	0.112248	0.666528	0.709628
O5	0.446431	0.166941	0.370925
O6	0.445581	0.166528	0.709628
O7	0.446431	0.666941	0.370925
O8	0.445581	0.666528	0.709628
O9	0.779764	0.166941	0.370925
O10	0.778914	0.166528	0.709628
O11	0.779764	0.666941	0.370925
O12	0.778914	0.666528	0.709628
O13	0.221086	0.333472	0.290372
O14	0.220236	0.333059	0.629075
O15	0.221086	0.833472	0.290372
O16	0.220236	0.833059	0.629075
O17	0.554419	0.333472	0.290372
O18	0.553569	0.333059	0.629075
O19	0.554420	0.833472	0.290372
O20	0.553569	0.833059	0.629075
O21	0.887752	0.333472	0.290372
O22	0.886902	0.333059	0.629075
O23	0.887752	0.833472	0.290372
O24	0.886902	0.833059	0.629075
O25	0.279764	0.416941	0.370925
O26	0.278914	0.416528	0.709628
O27	0.279764	0.916941	0.370925
O28	0.278914	0.916528	0.709628

Atom	x	y	z
O29	0.613098	0.416941	0.370925
O30	0.612248	0.416528	0.709628
O31	0.613098	0.916941	0.370925
O32	0.612248	0.916528	0.709628
O33	0.946431	0.416941	0.370925
O34	0.945581	0.416528	0.709628
O35	0.946431	0.916941	0.370925
O36	0.945580	0.916528	0.709628
O37	0.054419	0.083472	0.290372
O38	0.053569	0.083059	0.629075
O39	0.054420	0.583472	0.290372
O40	0.053569	0.583059	0.629075
O41	0.387752	0.083472	0.290372
O42	0.386902	0.083059	0.629075
O43	0.387753	0.583472	0.290372
O44	0.386902	0.583059	0.629075
O45	0.721086	0.083472	0.290372
O46	0.720236	0.083059	0.629075
O47	0.721086	0.583472	0.290372
O48	0.720236	0.583059	0.629075
O49	0.279729	0.083897	0.370928
O50	0.278926	0.083878	0.709634
O51	0.279729	0.583897	0.370928
O52	0.278926	0.583878	0.709634
O53	0.613060	0.083903	0.370930
O54	0.612259	0.083878	0.709633
O55	0.613060	0.583903	0.370930
O56	0.612259	0.583878	0.709633
O57	0.946395	0.083897	0.370928

Atom	x	y	z
O58	0.945592	0.083878	0.709633
O59	0.946395	0.583897	0.370928
O60	0.945592	0.583878	0.709633
O61	0.054408	0.416122	0.290367
O62	0.053605	0.416103	0.629072
O63	0.054407	0.916122	0.290367
O64	0.053605	0.916103	0.629072
O65	0.387741	0.416122	0.290367
O66	0.386940	0.416097	0.629070
O67	0.387741	0.916122	0.290367
O68	0.386940	0.916097	0.629070
O69	0.721074	0.416122	0.290366
O70	0.720271	0.416103	0.629072
O71	0.721074	0.916122	0.290366
O72	0.720271	0.916103	0.629072
O73	0.113060	0.333903	0.370930
O74	0.112259	0.333878	0.709633
O75	0.113060	0.833903	0.370930
O76	0.112259	0.833878	0.709633
O77	0.446395	0.333897	0.370928
O78	0.445592	0.333878	0.709633
O79	0.446395	0.833897	0.370928
O80	0.445592	0.833878	0.709633
O81	0.779729	0.333897	0.370928
O82	0.778926	0.333878	0.709634
O83	0.779729	0.833897	0.370928
O84	0.778926	0.833878	0.709634
O85	0.221074	0.166122	0.290366
O86	0.220271	0.166103	0.629072

Atom	x	y	z
O87	0.221074	0.666122	0.290366
O88	0.220271	0.666103	0.629072
O89	0.554408	0.166122	0.290367
O90	0.553605	0.166103	0.629072
O91	0.554408	0.666122	0.290367
O92	0.553605	0.666103	0.629072
O93	0.887741	0.166122	0.290367
O94	0.886940	0.166097	0.629070
O95	0.887741	0.666122	0.290367
O96	0.886940	0.666097	0.629070
O97	0.112417	0.000360	0.369033
O98	0.111922	0.000146	0.707248
O99	0.112417	0.500360	0.369033
O100	0.111922	0.500146	0.707248
O101	0.445751	0.000360	0.369033
O102	0.445255	0.000145	0.707248
O103	0.445751	0.500360	0.369033
O104	0.445255	0.500145	0.707248
O105	0.779084	0.000360	0.369032
O106	0.778589	0.000146	0.707247
O107	0.779084	0.500360	0.369032
O108	0.778589	0.500146	0.707247
O109	0.221411	0.499854	0.292753
O110	0.220916	0.499640	0.630968
O111	0.221411	0.999854	0.292753
O112	0.220916	0.999640	0.630968
O113	0.554745	0.499855	0.292752
O114	0.554249	0.499640	0.630968
O115	0.554745	0.999855	0.292752

Atom	x	y	z
O116	0.554249	0.999640	0.630968
O117	0.888078	0.499855	0.292752
O118	0.887583	0.499640	0.630967
O119	0.888078	0.999855	0.292752
O120	0.887583	0.999640	0.630967
O121	0.279084	0.250360	0.369032
O122	0.278589	0.250146	0.707247
O123	0.279084	0.750360	0.369032
O124	0.278589	0.750146	0.707247
O125	0.612417	0.250360	0.369033
O126	0.611922	0.250146	0.707248
O127	0.612417	0.750360	0.369033
O128	0.611922	0.750146	0.707248
O129	0.945751	0.250360	0.369033
O130	0.945255	0.250145	0.707248
O131	0.945751	0.750360	0.369033
O132	0.945255	0.750145	0.707248
O133	0.054745	0.249855	0.292752
O134	0.054249	0.249640	0.630968
O135	0.054745	0.749855	0.292752
O136	0.054249	0.749640	0.630968
O137	0.388078	0.249854	0.292752
O138	0.387583	0.249640	0.630967
O139	0.388078	0.749854	0.292752
O140	0.387583	0.749640	0.630967
O141	0.721411	0.249854	0.292753
O142	0.720916	0.249640	0.630968
O143	0.721411	0.749854	0.292753
O144	0.720916	0.749640	0.630968

Atom	x	y	z
O145	0.107366	0.250995	0.451021
O146	0.115631	0.250791	0.789730
O147	0.107366	0.750995	0.451021
O148	0.115631	0.750791	0.789730
O149	0.440700	0.250994	0.451021
O150	0.448964	0.250792	0.789730
O151	0.440700	0.750994	0.451021
O152	0.448964	0.750792	0.789730
O153	0.774032	0.250995	0.451021
O154	0.782297	0.250793	0.789729
O155	0.774032	0.750995	0.451021
O156	0.782297	0.750793	0.789729
O157	0.217703	0.249207	0.210271
O158	0.225968	0.249005	0.548979
O159	0.217703	0.749207	0.210271
O160	0.225968	0.749005	0.548979
O161	0.551036	0.249208	0.210270
O162	0.559300	0.249006	0.548979
O163	0.551036	0.749208	0.210270
O164	0.559300	0.749006	0.548979
O165	0.884369	0.249209	0.210270
O166	0.892634	0.249005	0.548979
O167	0.884369	0.749209	0.210270
O168	0.892634	0.749005	0.548979
O169	0.274032	0.000995	0.451021
O170	0.282297	0.000793	0.789729
O171	0.274033	0.500995	0.451021
O172	0.282297	0.500793	0.789729
O173	0.607366	0.000995	0.451021

Atom	x	y	z
O174	0.615631	0.000791	0.789730
O175	0.607366	0.500995	0.451021
O176	0.615631	0.500791	0.789730
O177	0.940700	0.000994	0.451021
O178	0.948964	0.000792	0.789730
O179	0.940700	0.500994	0.451021
O180	0.948964	0.500792	0.789730
O181	0.051036	0.499208	0.210270
O182	0.059300	0.499006	0.548979
O183	0.051036	0.999208	0.210270
O184	0.059300	0.999006	0.548979
O185	0.384369	0.499209	0.210270
O186	0.392634	0.499005	0.548979
O187	0.384369	0.999209	0.210270
O188	0.392634	0.999005	0.548979
O189	0.717703	0.499206	0.210271
O190	0.725968	0.499005	0.548979
O191	0.717703	0.999206	0.210271
O192	0.725968	0.999005	0.548979
O193	0.203810	0.132724	0.450655
O194	0.197980	0.125303	0.790001
O195	0.203810	0.632724	0.450655
O196	0.197980	0.625303	0.790001
O197	0.537143	0.132724	0.450655
O198	0.531314	0.125302	0.790000
O199	0.537143	0.632724	0.450655
O200	0.531314	0.625303	0.790000
O201	0.870476	0.132724	0.450655
O202	0.864648	0.125302	0.790000

Atom	x	y	z
O203	0.870476	0.632724	0.450655
O204	0.864648	0.625302	0.790000
O205	0.135352	0.374698	0.210000
O206	0.129524	0.367276	0.549345
O207	0.135352	0.874698	0.210000
O208	0.129524	0.867276	0.549345
O209	0.468686	0.374698	0.210000
O210	0.462857	0.367276	0.549345
O211	0.468686	0.874698	0.210000
O212	0.462857	0.867276	0.549345
O213	0.802020	0.374697	0.209999
O214	0.796190	0.367276	0.549345
O215	0.802020	0.874697	0.209999
O216	0.796190	0.867276	0.549345
O217	0.037143	0.382724	0.450655
O218	0.031314	0.375302	0.790000
O219	0.037143	0.882724	0.450655
O220	0.031314	0.875302	0.790000
O221	0.370476	0.382724	0.450655
O222	0.364648	0.375302	0.790000
O223	0.370476	0.882724	0.450655
O224	0.364648	0.875302	0.790000
O225	0.703810	0.382724	0.450655
O226	0.697980	0.375303	0.790001
O227	0.703810	0.882724	0.450655
O228	0.697980	0.875303	0.790001
O229	0.302020	0.124697	0.209999
O230	0.296190	0.117276	0.549345
O231	0.302020	0.624698	0.209999

Atom	x	y	z
O232	0.296190	0.617276	0.549345
O233	0.635352	0.124698	0.210000
O234	0.629524	0.117276	0.549345
O235	0.635352	0.624698	0.210000
O236	0.629524	0.617276	0.549345
O237	0.968686	0.124698	0.210000
O238	0.962857	0.117276	0.549345
O239	0.968686	0.624698	0.210000
O240	0.962857	0.617276	0.549345
O241	0.037108	0.119310	0.450630
O242	0.031273	0.126371	0.790008
O243	0.037108	0.619310	0.450630
O244	0.031273	0.626371	0.790008
O245	0.370451	0.119314	0.450631
O246	0.364608	0.126372	0.790009
O247	0.370451	0.619314	0.450631
O248	0.364608	0.626372	0.790009
O249	0.703783	0.119314	0.450630
O250	0.697939	0.126370	0.790008
O251	0.703784	0.619314	0.450630
O252	0.697939	0.626370	0.790008
O253	0.302061	0.373629	0.209992
O254	0.296216	0.380686	0.549370
O255	0.302061	0.873629	0.209992
O256	0.296217	0.880686	0.549370
O257	0.635392	0.373628	0.209991
O258	0.629549	0.380686	0.549369
O259	0.635392	0.873628	0.209991
O260	0.629549	0.880686	0.549369

Atom	x	y	z
O261	0.968727	0.373629	0.209992
O262	0.962892	0.380690	0.549370
O263	0.968727	0.873629	0.209992
O264	0.962892	0.880690	0.549370
O265	0.203784	0.369314	0.450630
O266	0.197939	0.376370	0.790008
O267	0.203783	0.869314	0.450630
O268	0.197939	0.876370	0.790008
O269	0.537108	0.369310	0.450630
O270	0.531273	0.376371	0.790008
O271	0.537108	0.869310	0.450630
O272	0.531273	0.876371	0.790008
O273	0.870451	0.369314	0.450631
O274	0.864608	0.376372	0.790009
O275	0.870451	0.869314	0.450631
O276	0.864608	0.876372	0.790009
O277	0.135392	0.123628	0.209991
O278	0.129549	0.130686	0.549369
O279	0.135392	0.623628	0.209991
O280	0.129549	0.630686	0.549369
O281	0.468727	0.123629	0.209992
O282	0.462892	0.130690	0.549370
O283	0.468727	0.623629	0.209992
O284	0.462892	0.630690	0.549370
O285	0.802061	0.123630	0.209992
O286	0.796216	0.130686	0.549370
O287	0.802061	0.623630	0.209992
O288	0.796217	0.630686	0.549370
H1	0.112890	0.000591	0.404675

Atom	x	y	z
H2	0.112843	0.000392	0.742940
H3	0.112890	0.500591	0.404675
H4	0.112843	0.500392	0.742940
H5	0.446223	0.000591	0.404675
H6	0.446176	0.000392	0.742940
H7	0.446223	0.500591	0.404675
H8	0.446176	0.500392	0.742940
H9	0.779557	0.000591	0.404675
H10	0.779510	0.000393	0.742940
H11	0.779557	0.500591	0.404675
H12	0.779510	0.500393	0.742940
H13	0.220490	0.499607	0.257060
H14	0.220443	0.499409	0.595325
H15	0.220490	0.999607	0.257060
H16	0.220443	0.999409	0.595325
H17	0.553824	0.499608	0.257060
H18	0.553777	0.499409	0.595325
H19	0.553824	0.999608	0.257060
H20	0.553777	0.999409	0.595325
H21	0.887157	0.499608	0.257060
H22	0.887110	0.499409	0.595325
H23	0.887157	0.999608	0.257060
H24	0.887110	0.999410	0.595325
H25	0.279557	0.250591	0.404675
H26	0.279510	0.250392	0.742940
H27	0.279557	0.750591	0.404675
H28	0.279510	0.750392	0.742940
H29	0.612890	0.250591	0.404675
H30	0.612843	0.250392	0.742940

Atom	x	y	z
H31	0.612890	0.750590	0.404675
H32	0.612843	0.750392	0.742940
H33	0.946223	0.250591	0.404675
H34	0.946176	0.250392	0.742940
H35	0.946223	0.750591	0.404675
H36	0.946176	0.750392	0.742940
H37	0.053824	0.249608	0.257060
H38	0.053777	0.249409	0.595325
H39	0.053824	0.749608	0.257060
H40	0.053777	0.749409	0.595325
H41	0.387157	0.249608	0.257060
H42	0.387110	0.249409	0.595325
H43	0.387157	0.749608	0.257060
H44	0.387110	0.749409	0.595325
H45	0.720490	0.249607	0.257060
H46	0.720443	0.249409	0.595325
H47	0.720490	0.749607	0.257060
H48	0.720443	0.749409	0.595325

Table S30: Atomic coordinates of Er^{3+} in the 3x2x3 talc

in the 3x2x3 talctom	x	y	z
Mg1	0.001234	0.001785	0.331839
Mg2	0.998766	0.998215	0.668161
Mg3	0.001506	0.499728	0.332181
Mg4	0.998494	0.500272	0.667819
Mg5	0.333977	0.000589	0.332444
Mg6	0.332613	0.997121	0.667922
Mg7	0.330631	0.499920	0.329520
Mg8	0.332990	0.500206	0.668648

Atom	x	y	z
Mg9	0.667387	0.002879	0.332078
Mg10	0.666023	0.999411	0.667556
Mg11	0.667010	0.499794	0.331352
Mg12	0.669369	0.500080	0.670480
Mg13	0.167020	0.250115	0.331580
Mg14	0.165084	0.248846	0.669115
Mg15	0.165181	0.751006	0.331199
Mg16	0.166968	0.749857	0.667716
Mg17	0.500248	0.250879	0.331996
Mg18	0.506860	0.251443	0.670388
Mg19	0.493140	0.748557	0.329612
Mg20	0.499752	0.749121	0.668004
Mg21	0.833032	0.250143	0.332284
Mg22	0.834819	0.248994	0.668801
Mg23	0.834916	0.751154	0.330885
Mg24	0.832980	0.749885	0.668420
Mg25	0.167430	0.083988	0.332167
Mg26	0.164157	0.080505	0.668233
Mg27	0.163528	0.583690	0.330289
Mg28	0.168767	0.585501	0.666515
Mg29	0.499981	0.083905	0.332513
Mg30	0.500234	0.083299	0.667135
Mg31	0.497251	0.582605	0.329127
Mg32	0.499866	0.582326	0.668608
Mg33	0.833566	0.084702	0.331867
Mg34	0.833130	0.082079	0.667808
Mg35	0.834232	0.583355	0.332323
Mg36	0.834290	0.583558	0.668931
Mg37	0.165710	0.416442	0.331069

Atom	x	y	z
Mg38	0.165768	0.416645	0.667677
Mg39	0.166870	0.917921	0.332192
Mg40	0.166434	0.915298	0.668133
Mg41	0.500134	0.417674	0.331392
Mg42	0.502749	0.417395	0.670873
Mg43	0.499766	0.916701	0.332865
Mg44	0.500019	0.916095	0.667487
Mg45	0.831233	0.414499	0.333485
Mg46	0.836472	0.416310	0.669711
Mg47	0.835843	0.919495	0.331767
Mg48	0.832570	0.916012	0.667833
Mg49	0.999787	0.333706	0.331675
Mg50	0.001223	0.332946	0.669603
Mg51	0.000465	0.834708	0.331518
Mg52	0.999771	0.832341	0.668023
Mg53	0.332992	0.333675	0.331389
Mg54	0.328481	0.336962	0.675183
Mg55	0.331487	0.833665	0.332312
Mg56	0.333625	0.831850	0.667791
Mg57	0.665560	0.334362	0.332838
Mg58	0.671224	0.333761	0.669195
Mg59	0.672005	0.841758	0.328222
Mg60	0.666366	0.832661	0.667801
Mg61	0.000229	0.167659	0.331977
Mg62	0.999535	0.165292	0.668482
Mg63	0.998777	0.667054	0.330397
Mg64	0.000213	0.666294	0.668325
Mg65	0.333634	0.167339	0.332199
Mg66	0.327995	0.158242	0.671778

Atom	x	y	z
Mg67	0.328776	0.666239	0.330806
Mg68	0.334440	0.665638	0.667162
Mg69	0.666375	0.168150	0.332209
Mg70	0.668513	0.166335	0.667688
Mg71	0.671519	0.663038	0.324817
Mg72	0.667008	0.666325	0.668611
Si1	0.282811	0.084949	0.432050
Si2	0.279155	0.080757	0.768267
Si3	0.275575	0.582743	0.430642
Si4	0.282107	0.584027	0.767716
Si5	0.613739	0.084438	0.431966
Si6	0.613269	0.084333	0.766113
Si7	0.614652	0.630112	0.418863
Si8	0.615055	0.583355	0.768052
Si9	0.947486	0.085561	0.431623
Si10	0.946786	0.082042	0.767298
Si11	0.948926	0.583404	0.431478
Si12	0.947072	0.583371	0.768259
Si13	0.052928	0.416629	0.231741
Si14	0.051074	0.416596	0.568522
Si15	0.053214	0.917958	0.232702
Si16	0.052514	0.914439	0.568377
Si17	0.384945	0.416645	0.231948
Si18	0.385348	0.369888	0.581137
Si19	0.386731	0.915667	0.233887
Si20	0.386261	0.915562	0.568034
Si21	0.717893	0.415973	0.232284
Si22	0.724425	0.417257	0.569358
Si23	0.720845	0.919243	0.231733

Atom	x	y	z
Si24	0.717189	0.915051	0.567950
Si25	0.113988	0.332927	0.431322
Si26	0.116659	0.333247	0.769625
Si27	0.114901	0.835866	0.431451
Si28	0.114178	0.833420	0.767329
Si29	0.447624	0.338678	0.431464
Si30	0.449724	0.333837	0.767707
Si31	0.448377	0.830584	0.431981
Si32	0.447989	0.833205	0.766974
Si33	0.778893	0.334652	0.432219
Si34	0.784513	0.332432	0.768240
Si35	0.782906	0.836409	0.431292
Si36	0.779916	0.834654	0.767267
Si37	0.220084	0.165346	0.232733
Si38	0.217094	0.163591	0.568708
Si39	0.215487	0.667568	0.231760
Si40	0.221107	0.665348	0.567781
Si41	0.552011	0.166795	0.233026
Si42	0.551623	0.169416	0.568019
Si43	0.550276	0.666163	0.232293
Si44	0.552376	0.661322	0.568536
Si45	0.885822	0.166580	0.232671
Si46	0.885099	0.164134	0.568549
Si47	0.883341	0.666753	0.230375
Si48	0.886012	0.667073	0.568678
Si49	0.114828	0.166868	0.431570
Si50	0.113269	0.165060	0.767766
Si51	0.113170	0.669438	0.430861
Si52	0.114022	0.667648	0.767041

Atom	x	y	z
Si53	0.448637	0.170877	0.432089
Si54	0.445640	0.167362	0.765900
Si55	0.441550	0.664026	0.430757
Si56	0.448608	0.666595	0.767296
Si57	0.780392	0.168026	0.432038
Si58	0.780930	0.165486	0.767244
Si59	0.784531	0.670055	0.431009
Si60	0.780758	0.668008	0.767734
Si61	0.219242	0.331992	0.232266
Si62	0.215469	0.329945	0.568991
Si63	0.219070	0.834514	0.232756
Si64	0.219608	0.831974	0.567962
Si65	0.551392	0.333405	0.232704
Si66	0.558450	0.335974	0.569243
Si67	0.554360	0.832638	0.234100
Si68	0.551363	0.829123	0.567911
Si69	0.885978	0.332352	0.232959
Si70	0.886830	0.330562	0.569139
Si71	0.886730	0.834940	0.232234
Si72	0.885172	0.833132	0.568430
Si73	0.277929	0.417843	0.431058
Si74	0.280310	0.417605	0.770171
Si75	0.283025	0.917602	0.431897
Si76	0.281205	0.915117	0.767628
Si77	0.616747	0.431567	0.432808
Si78	0.618187	0.416108	0.768401
Si79	0.614525	0.917024	0.431878
Si80	0.613354	0.917572	0.766699
Si81	0.947441	0.416821	0.431820

Atom	x	y	z
Si82	0.951024	0.417067	0.769394
Si83	0.949168	0.919791	0.431337
Si84	0.947327	0.915767	0.767245
Si85	0.052673	0.084233	0.232755
Si86	0.050832	0.080209	0.568663
Si87	0.048976	0.582933	0.230606
Si88	0.052559	0.583179	0.568180
Si89	0.386646	0.082428	0.233301
Si90	0.385475	0.082976	0.568122
Si91	0.381813	0.583892	0.231599
Si92	0.383253	0.568433	0.567192
Si93	0.718795	0.084883	0.232372
Si94	0.716975	0.082398	0.568103
Si95	0.719690	0.582395	0.229829
Si96	0.722071	0.582157	0.568942
O1	0.113210	0.167500	0.372233
O2	0.113021	0.164966	0.707981
O3	0.111208	0.667808	0.371497
O4	0.112949	0.666899	0.707578
O5	0.446217	0.169335	0.372856
O6	0.443140	0.169841	0.705502
O7	0.443149	0.665442	0.371752
O8	0.446115	0.665644	0.707607
O9	0.778201	0.167675	0.372606
O10	0.779448	0.165871	0.707608
O11	0.778361	0.668442	0.371385
O12	0.778687	0.666729	0.708045
O13	0.221313	0.333270	0.291955
O14	0.221639	0.331558	0.628615

Atom	x	y	z
O15	0.220552	0.834129	0.292392
O16	0.221799	0.832325	0.627394
O17	0.553885	0.334356	0.292393
O18	0.556851	0.334558	0.628248
O19	0.556860	0.830159	0.294498
O20	0.553783	0.830665	0.627144
O21	0.887051	0.333101	0.292422
O22	0.888792	0.332192	0.628503
O23	0.886979	0.835034	0.292019
O24	0.886790	0.832500	0.627767
O25	0.278715	0.417681	0.371939
O26	0.275356	0.418811	0.710258
O27	0.280383	0.917341	0.372564
O28	0.279287	0.915352	0.707976
O29	0.611334	0.420484	0.372769
O30	0.615295	0.415757	0.708717
O31	0.613172	0.914525	0.372292
O32	0.611390	0.916693	0.707053
O33	0.945370	0.417073	0.372408
O34	0.949147	0.417126	0.709427
O35	0.946736	0.918590	0.371944
O36	0.944962	0.915539	0.707651
O37	0.055038	0.084461	0.292349
O38	0.053264	0.081410	0.628056
O39	0.050853	0.582874	0.290573
O40	0.054630	0.582927	0.627592
O41	0.388610	0.083307	0.292947
O42	0.386828	0.085475	0.627708
O43	0.384705	0.584243	0.291283

Atom	x	y	z
O44	0.388666	0.579516	0.627231
O45	0.720713	0.084648	0.292024
O46	0.719617	0.082659	0.627436
O47	0.724644	0.581189	0.289742
O48	0.721285	0.582319	0.628061
O49	0.280616	0.084026	0.372722
O50	0.275970	0.078769	0.708530
O51	0.276937	0.582869	0.371557
O52	0.279764	0.582968	0.708129
O53	0.611948	0.084076	0.372597
O54	0.611497	0.084442	0.706467
O55	0.612390	0.587052	0.368043
O56	0.612943	0.583075	0.708386
O57	0.945615	0.084697	0.372240
O58	0.944984	0.082207	0.707704
O59	0.946285	0.584191	0.372158
O60	0.946232	0.582748	0.708513
O61	0.053768	0.417252	0.291487
O62	0.053715	0.415809	0.627842
O63	0.055016	0.917793	0.292296
O64	0.054385	0.915303	0.627760
O65	0.387058	0.416925	0.291614
O66	0.387610	0.412948	0.631957
O67	0.388503	0.915558	0.293533
O68	0.388052	0.915924	0.627403
O69	0.720236	0.417032	0.291871
O70	0.723063	0.417131	0.628443
O71	0.724030	0.921231	0.291470
O72	0.719384	0.915973	0.627278

Atom	x	y	z
O73	0.112557	0.333729	0.372002
O74	0.114926	0.334413	0.709539
O75	0.112767	0.834473	0.372061
O76	0.112588	0.832620	0.707764
O77	0.445953	0.336145	0.372601
O78	0.446219	0.331353	0.707403
O79	0.447830	0.829353	0.372521
O80	0.445771	0.833113	0.707338
O81	0.777686	0.333421	0.372725
O82	0.781599	0.333027	0.708475
O83	0.777030	0.834074	0.371748
O84	0.778145	0.833557	0.707644
O85	0.221855	0.166443	0.292356
O86	0.222970	0.165926	0.628252
O87	0.218401	0.666973	0.291525
O88	0.222314	0.666579	0.627275
O89	0.554229	0.166887	0.292662
O90	0.552171	0.170647	0.627478
O91	0.553781	0.668647	0.292597
O92	0.554047	0.663855	0.627399
O93	0.887412	0.167380	0.292236
O94	0.887233	0.165527	0.627939
O95	0.885075	0.665587	0.290461
O96	0.887443	0.666271	0.627998
O97	0.113307	0.001248	0.371238
O98	0.111176	0.998155	0.706613
O99	0.112795	0.500532	0.370527
O100	0.112331	0.484456	0.753684
O101	0.446699	0.999873	0.371805

Atom	x	y	z
O102	0.445246	0.001111	0.705592
O103	0.443596	0.501615	0.368314
O104	0.445735	0.499079	0.707573
O105	0.779089	0.001012	0.370987
O106	0.777964	0.999666	0.706051
O107	0.778040	0.501446	0.371159
O108	0.781143	0.499906	0.707570
O109	0.218857	0.500094	0.292430
O110	0.221960	0.498554	0.628841
O111	0.222036	0.000334	0.293949
O112	0.220911	0.998988	0.629013
O113	0.554265	0.500921	0.292427
O114	0.556404	0.498385	0.631686
O115	0.554754	0.998889	0.294408
O116	0.553301	0.000127	0.628195
O117	0.887669	0.515544	0.246316
O118	0.887205	0.499468	0.629473
O119	0.888824	0.001845	0.293387
O120	0.886693	0.998752	0.628763
O121	0.279658	0.251263	0.371025
O122	0.281293	0.247736	0.705264
O123	0.278594	0.749847	0.370871
O124	0.279653	0.748864	0.706024
O125	0.611435	0.251569	0.371431
O126	0.615886	0.250428	0.707250
O127	0.606958	0.718484	0.395891
O128	0.611911	0.749586	0.706120
O129	0.945714	0.250958	0.370940
O130	0.947012	0.249265	0.707079

Atom	x	y	z
O131	0.945201	0.750887	0.370103
O132	0.945526	0.749503	0.706589
O133	0.054474	0.250497	0.293411
O134	0.054799	0.249113	0.629898
O135	0.052988	0.750735	0.292921
O136	0.054286	0.749042	0.629060
O137	0.388089	0.250414	0.293880
O138	0.393042	0.281516	0.604109
O139	0.384114	0.749572	0.292750
O140	0.388565	0.748431	0.628569
O141	0.720347	0.251136	0.293976
O142	0.721406	0.250153	0.629129
O143	0.718707	0.752264	0.294736
O144	0.720342	0.748737	0.628975
O145	0.104430	0.250183	0.452168
O146	0.124783	0.248253	0.787224
O147	0.102770	0.752552	0.451467
O148	0.126689	0.750283	0.787504
O149	0.441034	0.255654	0.452860
O150	0.456676	0.250063	0.786871
O151	0.437620	0.746393	0.452728
O152	0.461759	0.750061	0.786676
O153	0.768065	0.251234	0.452622
O154	0.793423	0.248626	0.787341
O155	0.774835	0.753031	0.451652
O156	0.790108	0.751581	0.787391
O157	0.209892	0.248419	0.212609
O158	0.225165	0.246969	0.548348
O159	0.206577	0.751375	0.212659

Atom	x	y	z
O160	0.231935	0.748766	0.547378
O161	0.538241	0.249939	0.213324
O162	0.562380	0.253607	0.547272
O163	0.543324	0.749937	0.213129
O164	0.558966	0.744346	0.547140
O165	0.873311	0.249717	0.212496
O166	0.897230	0.247448	0.548533
O167	0.875217	0.751747	0.212776
O168	0.895570	0.749817	0.547832
O169	0.277286	0.001212	0.452651
O170	0.294304	0.998364	0.788338
O171	0.262879	0.500559	0.451943
O172	0.291648	0.501439	0.789527
O173	0.600601	0.000317	0.451403
O174	0.624127	0.001389	0.786118
O175	0.887277	0.496780	0.297792
O176	0.626831	0.499909	0.787892
O177	0.936475	0.002485	0.452036
O178	0.959993	0.999086	0.787122
O179	0.939108	0.500584	0.452195
O180	0.951199	0.500785	0.789884
O181	0.048801	0.499214	0.210117
O182	0.060892	0.499416	0.547805
O183	0.040007	0.000914	0.212878
O184	0.063525	0.997515	0.547964
O185	0.373169	0.500090	0.212108
O186	0.112723	0.503220	0.702208
O187	0.375873	0.998611	0.213882
O188	0.399399	0.999683	0.548597

Atom	x	y	z
O189	0.708352	0.498561	0.210474
O190	0.737121	0.499441	0.548057
O191	0.705696	0.001636	0.211662
O192	0.722714	0.998788	0.547349
O193	0.203903	0.132912	0.451763
O194	0.191397	0.114470	0.787741
O195	0.204335	0.637887	0.450606
O196	0.192128	0.616080	0.786636
O197	0.537627	0.135970	0.452054
O198	0.524150	0.117599	0.784654
O199	0.528751	0.619142	0.450805
O200	0.526158	0.615908	0.787260
O201	0.870870	0.136248	0.451532
O202	0.857997	0.114261	0.787019
O203	0.870408	0.632668	0.451162
O204	0.860750	0.620614	0.787451
O205	0.139250	0.379386	0.212549
O206	0.129592	0.367332	0.548838
O207	0.142003	0.885739	0.212981
O208	0.129130	0.863752	0.548468
O209	0.473842	0.384092	0.212740
O210	0.471249	0.380858	0.549195
O211	0.475850	0.882401	0.215346
O212	0.462373	0.864030	0.547946
O213	0.807872	0.383920	0.213364
O214	0.795665	0.362113	0.549394
O215	0.808603	0.885530	0.212259
O216	0.796097	0.867088	0.548237
O217	0.037409	0.383438	0.451360

Atom	x	y	z
O218	0.028759	0.366570	0.789825
O219	0.038885	0.887177	0.451205
O220	0.025642	0.865727	0.786936
O221	0.372067	0.392654	0.451875
O222	0.364412	0.371707	0.786466
O223	0.372076	0.881298	0.451163
O224	0.359175	0.864579	0.787016
O225	0.700991	0.384377	0.451428
O226	0.696981	0.367176	0.788061
O227	0.704628	0.884814	0.451544
O228	0.692192	0.868911	0.786787
O229	0.307807	0.131089	0.213213
O230	0.295372	0.115186	0.548456
O231	0.303019	0.632824	0.211939
O232	0.299009	0.615623	0.548572
O233	0.640825	0.135421	0.212984
O234	0.627924	0.118702	0.548837
O235	0.635588	0.628293	0.213534
O236	0.627933	0.607346	0.548125
O237	0.974358	0.134273	0.213064
O238	0.961115	0.112823	0.548795
O239	0.971241	0.633430	0.210175
O240	0.962591	0.616562	0.548640
O241	0.037582	0.117527	0.451471
O242	0.024856	0.132439	0.787013
O243	0.037795	0.618234	0.451273
O244	0.027638	0.632072	0.787226
O245	0.370388	0.122677	0.452152
O246	0.357498	0.133674	0.784846

Atom	x	y	z
O247	0.370227	0.608341	0.451056
O248	0.359893	0.634602	0.787279
O249	0.704290	0.116045	0.451680
O250	0.691190	0.134401	0.786288
O251	0.700993	0.625277	0.450607
O252	0.693341	0.633465	0.787628
O253	0.306659	0.366535	0.212372
O254	0.299007	0.374723	0.549393
O255	0.308810	0.865599	0.213712
O256	0.295710	0.883955	0.548320
O257	0.640107	0.365398	0.212721
O258	0.629773	0.391659	0.548944
O259	0.642502	0.866326	0.215154
O260	0.629612	0.877323	0.547848
O261	0.972362	0.367928	0.212774
O262	0.962205	0.381766	0.548727
O263	0.975143	0.867561	0.212987
O264	0.962418	0.882473	0.548529
O265	0.205186	0.364467	0.451318
O266	0.201066	0.373293	0.791804
O267	0.205126	0.868304	0.451318
O268	0.192460	0.883503	0.787255
O269	0.530255	0.383505	0.453905
O270	0.530544	0.380489	0.786916
O271	0.540158	0.861976	0.450668
O272	0.525325	0.884570	0.786571
O273	0.869235	0.367995	0.451541
O274	0.863953	0.379983	0.788076
O275	0.872064	0.869420	0.450557

Atom	x	y	z
O276	0.858943	0.883742	0.787127
O277	0.141057	0.116258	0.212874
O278	0.127936	0.130580	0.549443
O279	0.136047	0.620017	0.211924
O280	0.130765	0.632005	0.548459
O281	0.474675	0.115430	0.213429
O282	0.459842	0.138024	0.549332
O283	0.469456	0.619511	0.213085
O284	0.469745	0.616495	0.546095
O285	0.807540	0.116497	0.212745
O286	0.794874	0.131696	0.548682
O287	0.798935	0.626707	0.208196
O288	0.794814	0.635533	0.548682
H1	0.113078	0.001813	0.406508
H2	0.111755	0.998239	0.741904
H3	0.112281	0.500670	0.405790
H4	0.131260	0.529207	0.770751
H5	0.447237	0.001285	0.407075
H6	0.446767	0.000199	0.740898
H7	0.432927	0.503258	0.402654
H8	0.447108	0.500942	0.742865
H9	0.781517	0.003150	0.406248
H10	0.779781	0.999733	0.741350
H11	0.775981	0.501940	0.406415
H12	0.784395	0.500683	0.742864
H13	0.215605	0.499317	0.257136
H14	0.224019	0.498060	0.593585
H15	0.220219	0.000267	0.258650
H16	0.218483	0.996850	0.593752

Atom	x	y	z
H17	0.552892	0.499058	0.257135
H18	0.567073	0.496741	0.597346
H19	0.553233	0.999801	0.259102
H20	0.552763	0.998715	0.592925
H21	0.868741	0.470793	0.229249
H22	0.887719	0.499330	0.594210
H23	0.888245	0.001761	0.258096
H24	0.886922	0.998187	0.593492
H25	0.278006	0.250388	0.406248
H26	0.283559	0.246677	0.740676
H27	0.274989	0.751087	0.406035
H28	0.281228	0.749684	0.741314
H29	0.615287	0.252072	0.406671
H30	0.619997	0.249845	0.742520
H31	0.616716	0.757056	0.420160
H32	0.612917	0.749899	0.741422
H33	0.946385	0.250678	0.406222
H34	0.948292	0.249444	0.742391
H35	0.948153	0.751422	0.405375
H36	0.946197	0.750215	0.741883
H37	0.053803	0.249785	0.258117
H38	0.051847	0.248577	0.594625
H39	0.051708	0.750556	0.257609
H40	0.053615	0.749322	0.593778
H41	0.387083	0.250101	0.258578
H42	0.383284	0.242944	0.579840
H43	0.380003	0.750155	0.257480
H44	0.384713	0.747928	0.593329
H45	0.718772	0.250316	0.258685

Atom	x	y	z
H46	0.725011	0.248913	0.593965
H47	0.716441	0.753323	0.259324
H48	0.721994	0.749612	0.593752
Er1	0.500000	0.500000	0.500000

S3.2. Cluster models used in ORCA

Table S31: Cartesian coordinates of cluster models in Angstroms.

Atom	x	y	z
Er³⁺_{Mg1}			
Si	11.847178347	26.782531241	-1.988320840
Er	13.479899797	27.544797365	0.784745787
Si	11.843197990	29.763938126	-1.050558005
Si	10.242598353	24.732436245	-0.387937868
Si	13.470225815	25.979987075	-4.414434045
Si	10.241724956	21.832983743	-1.305040212
Si	8.619548708	25.544404597	2.066032892
Si	8.618339898	28.455492174	2.982325287
Si	7.004501664	23.477058592	3.585372461
Si	10.239918587	30.531047097	1.436485043
Si	7.002354551	29.281550233	5.411326410
Si	10.240113741	33.433645479	2.347663783
Si	13.466487118	31.816121112	-2.574938285
Si	15.092332653	30.971838473	-5.004634182
Si	13.469157991	34.704984657	-1.641438465
Si	15.094405445	28.070192632	-5.917487149
H	16.259872327	32.654633190	-6.393864754
H	16.262637226	27.486467212	-8.019828189
Si	13.470991168	23.078592695	-5.304014712
H	14.639418626	22.507204656	-7.409499643
Si	11.850758633	21.016120798	-3.757368012
H	11.652885612	18.695032637	-4.579432931
Si	8.623372740	19.764271800	0.227028352
H	8.430317330	17.438918675	-0.600844539

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Atom	x	y	z
Si	7.006135211	20.580925994	2.669017533
H	5.543037556	18.903998539	3.756712360
Si	5.386159619	24.306098752	6.020578672
Si	5.384086826	27.207744594	6.933431638
H	3.921055260	22.613535397	7.092133003
H	3.917791797	27.976168840	8.781447552
Si	7.004448284	32.180130551	6.320373830
Si	8.623351236	34.250477495	4.790385926
H	5.543090337	32.928143349	8.175189814
Si	11.851611674	35.508798619	0.809662318
H	14.639158930	36.379158878	-3.038866036
Si	18.315373603	26.638069480	-1.430486424
Si	18.313489861	29.550396768	-0.512153293
H	19.769797664	31.224651458	-1.588382445
Si	16.691011239	30.360791708	1.944852265
Si	16.694764694	24.563444295	0.118341079
H	19.771306446	25.881557961	-3.271558175
Si	16.686303404	21.660789385	-0.794823268
Si	15.095825595	25.324830799	2.609549655
H	18.143843028	20.913620568	-2.650249678
Si	15.073017205	19.587109892	0.743619019
H	15.272248944	17.216811858	0.081544530
Si	13.456462042	20.388145872	3.196786277
Si	11.830731214	18.327647496	4.730034021
Si	13.467506021	23.276536687	4.132483742
Si	11.839785567	24.124582050	6.559454173
Si	11.837227856	27.027326888	7.472190311
Si	10.219410906	22.049012497	8.077466640
Si	13.462190732	29.116480113	5.970974955

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Atom	x	y	z
Si	10.217928576	27.854537398	9.906139382
Si	15.089427021	28.312561825	3.551258385
Si	13.455946207	32.018609617	6.856757593
Si	15.074016117	34.081898488	5.309651441
Si	11.830358678	32.821350051	9.296065694
Si	10.211280033	30.749714141	10.821877812
H	9.045005317	31.325987771	12.929351836
Si	8.605244034	25.786302889	11.425912528
Si	16.685198966	33.262878329	2.859010887
H	18.145056709	34.936248391	1.766980458
Si	8.607128389	22.873975838	10.507578643
H	7.427507788	26.352596399	13.542870635
H	7.430951509	21.194505029	11.917304891
Si	10.212059278	19.149863170	7.168564458
H	9.044345145	17.469934432	8.564392316
H	12.022982843	15.953565498	4.073461212
O	13.161991305	26.419433149	-1.076908063
O	11.422767806	28.316649453	-1.659029342
O	10.651849382	25.786847761	-1.559934486
O	12.251669125	26.619753783	-3.538611652
O	9.732610427	23.357215246	-1.063624158
O	11.539119909	24.438523920	0.554951971
O	9.062295500	25.382336509	0.511892712
O	9.897561443	25.233082990	3.023626390
O	8.123394312	27.069002272	2.304086142
O	7.420352694	24.518678027	2.411590106
O	9.061163135	29.479709412	1.801325827
O	9.895761505	28.156823628	3.944183951
O	7.419326531	29.099411964	3.852883909

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Atom	x	y	z
O	10.649095329	30.338387528	-0.128580711
O	11.535762938	30.227660693	2.376836149
O	9.730116006	32.045509432	1.672743319
O	13.155170107	29.535420981	-0.093529677
O	12.249605325	30.786258978	-2.227179091
O	14.747485461	31.508869607	-1.619136298
O	13.891116812	31.614230647	-4.123028607
O	12.949676941	33.326066246	-2.324536314
O	14.575207885	29.585366507	-5.667001162
O	16.371966966	30.667028933	-4.049290917
O	15.515185220	32.008609955	-6.174330948
O	16.374078006	27.765246548	-4.962449084
O	15.518848203	27.891839906	-7.469781947
O	13.893571771	27.038229601	-5.562778838
O	12.954303827	24.601184620	-5.078754865
O	14.750630998	25.677387229	-3.456900689
O	13.888794118	22.895429781	-6.856377504
O	12.269494436	22.058708123	-4.926189059
O	14.754345294	22.786353630	-4.351187721
O	13.138131935	20.707521245	-2.814553176
O	11.324715773	19.638187580	-4.428226747
O	10.662877828	21.662267093	-2.860655997
O	9.040591885	20.811281527	-0.940368442
O	11.526487290	21.533084000	-0.356303189
O	9.908152695	19.462193174	1.175206815
O	8.111530713	18.385841491	-0.453154749
O	7.426199743	20.402492714	1.114055120
O	5.803815526	19.558959186	3.033441040
O	8.291189197	20.280385232	3.617240270

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Atom	x	y	z
O	6.490299780	22.099322914	2.911409734
O	8.288726957	23.176212174	4.535339444
O	5.810602377	24.127746026	4.468283874
O	6.665832179	24.001152668	6.975616737
O	4.866962059	25.821272628	6.271064659
O	4.185325944	23.274135722	6.375286983
O	6.663721139	26.902935054	7.888774904
O	5.806939394	28.244516075	5.763734873
O	4.182870985	27.850136767	7.815037214
O	8.285763502	28.976727513	6.361131320
O	6.489379092	30.797728832	5.646158627
O	8.288593413	31.875765210	7.268761386
O	7.424721519	33.220016172	5.150258036
O	5.803712319	32.808925430	7.206704775
O	9.040737537	34.064642543	3.233056083
O	9.907745670	33.946941518	5.738667143
O	8.111993421	35.769413227	5.027291507
O	10.662875417	34.465040764	1.171154324
O	11.524218975	33.129940813	3.296200669
O	12.270861647	35.329353034	-0.746316191
O	13.138616315	35.214228854	1.757277704
O	11.325178480	37.021759316	1.052219509
O	14.752895945	34.392320020	-0.695231849
O	13.888546491	35.743392921	-2.809775196
O	18.807666998	28.024513669	-0.749418636
O	17.036726823	29.862095844	-1.470518294
O	19.512363727	30.576065374	-0.858201741
O	17.871228043	29.713017570	1.042465316
O	17.038985466	26.937195930	-2.393182147

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Atom	x	y	z
O	17.874156251	25.612066673	-0.250794127
O	19.513811805	25.994291466	-2.301461444
O	17.199450884	23.047302477	-0.119035391
O	15.398278162	24.867668461	-0.820403779
O	16.292596246	24.758421770	1.685799099
O	17.884145881	21.027209584	-1.680840101
O	16.261748875	20.631074377	0.382372876
O	15.402958427	21.965546997	-1.743816449
O	15.601289373	18.075423242	0.499418779
O	13.786343137	19.880628682	-0.204790052
O	14.654543327	19.765846280	2.299698531
O	13.037121491	19.346913790	4.362200311
O	12.174069537	20.701791220	2.249444610
O	13.977254100	21.763574029	3.885473299
O	12.187528070	23.585495752	3.175828675
O	14.691366459	24.299286876	3.783938993
O	13.044074341	23.484205051	5.680213331
O	10.561304618	24.428744530	5.602388680
O	11.415285496	23.086166899	7.726861656
O	10.558676374	27.331754005	6.515462728
O	13.038898543	28.059586538	7.120551783
O	11.412688846	27.204975223	9.024032143
O	12.182646362	29.416915664	5.011805870
O	14.685057771	28.474905334	5.101119758
O	13.977272319	30.497631949	6.631140114
O	15.506354013	26.776380000	3.217125326
O	16.286456398	29.304304134	3.117583715
O	13.775088931	28.680225554	2.641038388
O	13.783274713	25.548283307	1.652136321

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Atom	x	y	z
O	12.172277138	32.309746289	5.903991689
O	14.654926369	33.041660717	6.480581479
O	13.035096928	32.196852743	8.408744872
O	11.412683148	31.772158013	10.457504241
O	10.549139323	33.125162125	8.344145344
O	8.926855926	31.050122460	9.872991021
O	10.729477470	29.232146868	10.581556563
O	9.790365046	30.927258844	12.376582338
O	8.934828257	28.155173056	8.954742459
O	9.804118513	26.811971733	11.079863326
O	16.261871714	33.433872989	4.413994357
O	15.601751467	35.458994740	5.979865788
O	13.786668433	34.389682492	4.366786063
O	17.885794198	34.285190812	2.494309117
O	15.401477327	33.562772133	1.909315008
O	17.195655554	31.738475759	2.619740266
O	15.394805167	30.653058312	1.001648334
O	9.099421784	24.260420027	11.188646431
O	7.328480996	26.098001965	10.467547526
O	8.162982216	25.948923691	12.980531137
O	9.805566591	22.230197824	9.636603624
O	7.330739639	23.173102050	9.544883674
O	8.165910425	21.847972794	11.687271694
O	8.936218327	22.354961946	7.128085465
O	11.412170235	18.517465667	6.283699649
O	9.790048741	18.113417714	8.340885241
O	8.928251756	19.454865930	6.220263637
O	10.549761070	18.632728186	3.778074098
O	12.343676138	16.810223903	4.501704352

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Atom	x	y	z
O	11.430400009	27.305125853	1.560881614
H	12.881951183	26.331293926	4.633962112
O	12.151403809	26.520814989	4.033987931
H	10.617935762	27.469045657	1.064457353
Mg	11.799570693	28.401759817	3.311858502
Mg	11.802238287	25.394452743	2.366278887
Mg	13.469152062	24.541853749	-0.167915441
Mg	13.464246179	21.714343691	-1.061688437
O	13.171424627	23.567294218	-1.894843632
H	12.409619058	23.725426887	-2.462804688
H	14.524947338	22.547437450	1.237249619
O	13.762668216	22.748462279	0.683661481
O	14.784834611	28.573953694	-2.481534399
H	14.054141654	28.762888024	-3.081553218
H	16.339624138	27.630137761	0.474506688
O	15.519496706	27.788944517	-0.010769242
Mg	15.135284874	26.693251776	-1.758921665
Mg	15.132853777	29.699285918	-0.812839851
Mg	13.462353628	33.381302595	2.613546760
Mg	13.465013744	30.551673327	1.724642683
O	13.169760589	32.341699504	0.869266517
H	12.409176915	32.538628017	0.311843172
H	14.521532372	31.377374044	4.019160723
O	13.759852319	31.531113931	3.449821148
Mg	11.848966816	31.288668786	4.158942754
Mg	15.079511689	32.551212962	0.149012802
Mg	10.228849392	32.095060072	6.591271082
H	9.179356106	31.227128667	4.298130083
O	9.945265132	31.038864695	4.851667561

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Atom	x	y	z
H	11.276122240	30.073182030	7.995786699
O	10.523027469	30.242153346	7.419126213
Mg	10.224082088	29.201044933	5.702210185
Mg	8.608843166	30.024527840	8.117227542
Mg	8.610130016	27.118634267	7.200949765
O	8.315403482	26.066732739	5.471325633
H	7.555436562	26.243468336	4.906065164
H	9.672627064	25.089713033	8.580677933
O	8.910502257	25.265197678	8.017928377
Mg	8.613464406	24.213000213	6.288341628
Mg	10.220696136	26.286456805	4.775071842
O	12.355108929	25.511400012	7.222991781
Mg	10.226578562	23.367032470	3.865293732
O	9.948855364	22.349607466	2.116146318
H	9.182693567	22.513298762	1.555194206
H	11.278208353	21.336196301	5.246988275
O	10.526123229	21.529206354	4.676615840
Mg	10.231938191	20.485764847	2.936584759
Mg	8.611433635	21.306318922	5.372307469
O	10.730145502	20.532701296	7.839659664
Mg	7.006264759	25.044747983	8.715871663
Mg	16.714510586	28.808841862	-3.222194158
Mg	15.082032966	23.806699333	-2.604798850
Mg	11.852715710	22.542438465	1.406129532
H	17.750281958	32.586157480	-0.002114155
O	16.982785757	32.745616309	-0.562492383
Mg	16.706740334	31.727696738	-2.311624246
H	19.380872278	28.853806675	-3.357387134
O	18.618748084	29.029291558	-3.920137444

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Atom	x	y	z
Mg	16.707879493	25.894110977	-4.150199954
H	17.752486647	23.864756237	-2.749420021
O	16.985092164	24.055144036	-3.300195781
Mg	15.078991139	20.925004666	-3.506773363
H	16.135257949	18.903042426	-2.115369112
O	15.371892734	19.079461833	-2.676135012
Mg	13.461851577	18.856377827	-1.964529376
O	11.551595721	18.633046554	-1.252595106
H	10.788333563	18.810341319	-1.813217486
H	12.897359164	17.642429362	1.880122492
O	12.138788893	17.821714712	1.313871888
Mg	11.846007500	19.666203479	0.487830284
Mg	10.226391498	17.599641399	2.019748010
O	8.315500028	17.378570213	2.722598789
H	7.555758266	17.556814222	2.157559142
Mg	8.607893857	18.416752704	4.459971512
O	6.697764182	21.090962356	6.070399072
H	5.945199081	21.262923017	5.493954788
Mg	6.999633666	22.130017098	7.787865867
O	5.076588784	24.809859815	9.456531421
H	4.345896440	24.998794382	8.856511849
Mg	6.998494507	27.963602859	9.626441575
O	6.695329340	29.800459803	8.814076313
H	5.942205942	29.990770373	8.244184546
Mg	8.608100563	32.913385607	9.029030300
O	8.315962123	34.762141711	8.203045798
H	7.556220974	34.940385957	7.638005398
O	12.344138845	34.193795639	9.982150608
Mg	10.226854206	34.983212180	7.500193965

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Atom	x	y	z
H	12.897821871	35.026001097	7.360568748
O	12.139251600	35.205286448	6.794318144
Mg	11.845976765	34.170909111	5.058747710
O	11.552058428	36.016617336	4.227850849
H	10.788796270	36.193913054	3.667228769
Mg	13.462314284	36.239949563	3.515916880
H	16.135720043	36.286613924	3.365077898
O	15.372355442	36.463033568	2.804311244
Mg	15.079609122	35.429086134	1.064450926
H	8.226123812	36.523782925	5.689107654
H	11.431616149	37.774661662	1.716981933
H	12.233501065	35.192379872	9.878763903
H	15.495824999	36.457228201	5.868467668
Er³⁺_{Mg2}			
Si	10.687766827	26.309472280	-0.112531725
Er	10.685373603	25.352355326	3.049481725
Si	13.258810011	23.866763256	4.499115056
Si	8.107068072	26.817355704	1.580923096
Si	10.677512615	22.180836170	3.959131737
H	10.378606836	24.934706929	5.876724450
H	10.999066195	28.183931713	2.682513470
Si	8.186047385	28.942242926	3.772665924
Si	5.622269939	25.161491206	1.073137689
Si	10.696378255	24.170377688	-2.251550939
Si	13.196822121	27.950630499	0.477684970
Si	13.224692231	30.097937367	2.647376314
Si	15.708106129	27.449972710	-1.171257570
Si	10.703409978	30.593451224	4.301301185
Si	15.731654544	31.731842368	3.151186094

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Atom	x	y	z
Si	10.697731003	32.720413128	6.456885651
Si	8.180303315	33.190266804	8.095777026
Si	13.218424170	34.345965231	6.954413489
Si	5.670577301	31.553264452	7.582826191
H	3.593832600	32.127298488	8.802896293
Si	5.668760708	29.420359612	5.421230487
Si	3.154822342	27.785810284	4.906283211
Si	3.127120710	25.648588190	2.741683117
H	1.080818896	28.365011301	6.124791398
H	1.049189333	24.432503266	2.157402414
Si	5.665464842	23.022261153	-1.088114726
H	3.592934082	21.806836990	-1.678574370
Si	8.179131124	22.530625891	-2.729653689
H	8.064528936	20.929041236	-4.608169383
Si	13.221966100	23.685954787	-3.873767879
H	13.110814095	22.087606850	-5.753513970
Si	15.732364759	25.323295213	-3.348236764
H	17.729009961	25.102381054	-4.795140387
Si	18.210672987	29.096581943	-0.654438947
Si	18.238374619	31.233804038	1.510161147
H	20.194670498	28.869010697	-2.125945696
H	20.242704212	32.671602866	1.752680426
Si	15.730997716	33.858018275	5.313752928
H	17.730140359	35.298024557	5.557016592
O	10.984094452	20.780154432	3.228017319
O	9.546108656	22.038923703	5.101764933
O	10.125227141	23.237123945	2.833284030
O	12.034330812	22.803780710	4.603092178
O	11.241370186	25.171139166	0.930847171

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Atom	x	y	z
O	12.828204905	25.007486459	3.400987844
O	8.541496484	25.702849681	2.704564800
O	10.125005283	25.538446609	5.166019267
O	11.253695616	27.465625857	3.276294946
Si	10.680361506	20.075044425	1.788892560
Si	8.170893654	22.743812456	5.615436806
Si	5.658894410	21.104977158	5.090314132
Si	8.154601349	24.876949138	7.798728640
Si	5.647929237	25.359730659	9.441870412
Si	10.676340988	26.523085493	8.320273002
Si	13.193536148	26.021315346	6.661303830
Si	10.680553679	28.649392495	10.479062715
Si	15.711082360	27.662350469	7.164711612
Si	15.745345635	23.384517542	2.835090297
Si	15.711199052	21.257807302	0.663746589
Si	18.240411650	25.043825108	3.349137102
Si	13.199625851	19.622739756	0.145880702
H	17.783524508	20.684854113	-0.559206555
H	13.317009414	17.767419762	-1.481470483
Si	8.153715377	18.462625382	1.286174391
Si	5.643255323	18.964343131	2.930099280
H	8.267694588	16.606779937	-0.338924040
H	3.647031055	17.520512194	2.689834751
Si	3.156859372	21.595831355	6.745259166
Si	3.140943298	23.726014565	8.918048488
H	1.169634059	20.133263801	6.498895212
H	1.137247317	23.944449368	10.359721320
Si	5.647906822	27.492450093	11.599242781
H	3.647878871	27.714382836	13.042012778

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Atom	x	y	z
Si	8.159472793	29.127401162	12.111067133
Si	13.198867031	30.282687297	10.971782796
Si	15.708949832	29.792922132	9.328713471
H	17.784178847	31.007871418	9.921051581
Si	18.224494623	27.174008101	5.521926638
H	20.297817289	28.384607416	6.121174381
H	20.314813060	24.475140800	2.120994158
O	7.903958129	28.229438840	2.335645392
O	6.753248059	26.317923603	0.866697533
O	9.323007637	26.934676875	0.509842584
O	10.396340195	25.600594046	-1.527953241
O	11.814125384	27.458706281	-0.226781933
O	13.690239829	26.842122558	1.565165285
O	12.917012651	29.353392149	1.237009924
O	14.330450509	28.138319654	-0.657769793
O	13.731090562	29.003019290	3.738228984
O	11.854315921	30.786442212	3.174869648
O	14.370762093	31.216204786	2.430287503
O	11.202725851	29.502410685	5.399580422
O	9.352779729	30.049598079	3.579110755
O	10.399451596	32.001162905	5.031973318
O	11.194731226	31.615490867	7.540161898
O	9.337001851	33.424181816	6.983759910
O	11.852248898	33.835549432	6.246241108
O	6.828527526	32.668026465	7.371350216
O	8.681605172	32.092862891	9.184363388
O	7.871139416	34.594196635	8.844090969
O	4.313071383	32.265007369	8.107316077
O	6.167680426	30.453117592	8.670255694

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Atom	x	y	z
O	5.376974241	30.828516660	6.161730001
O	4.315972475	28.898073158	4.698053400
O	6.167280708	28.320634148	6.508757254
O	6.823393346	29.634363122	4.297215888
O	8.683791175	27.824227310	4.849197748
O	2.862675284	27.061314807	3.486443179
O	1.797042153	28.499350034	5.425450744
O	3.642821663	26.683944558	5.996442995
O	1.754059485	25.147148528	2.045419294
O	3.635625628	24.548396800	3.823575702
O	4.259451355	25.853431556	1.598476769
O	6.134932470	24.067803002	2.163684320
O	4.312246036	22.503807678	-1.808659620
O	6.830583398	23.252143629	-2.191620676
O	6.163106743	21.929201182	0.007083703
O	8.683035275	21.437638777	-1.636089246
O	7.871858317	21.803968405	-4.141821358
O	9.332192045	23.651772108	-2.948508434
O	11.854410139	24.391102934	-3.356572964
O	11.191306822	23.077766043	-1.151828098
O	13.710677876	22.586363352	-2.781012715
O	12.931400330	22.968485159	-5.293118374
O	14.369124042	24.814172840	-4.061345146
O	16.885244219	25.547937071	-4.464022270
O	16.226863409	24.221095022	-2.261030606
O	15.435591667	26.728656417	-2.594498453
O	16.211726445	26.352011712	-0.083322596
O	16.837611762	28.595142281	-1.350702770
O	17.946227562	30.509308560	0.090321115

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Atom	x	y	z
O	18.719176953	27.996390336	0.427453853
O	19.343003633	29.301425310	-1.797645295
O	16.880594431	31.947343787	2.029328679
O	18.726373940	30.131938311	2.600320930
O	19.399524753	32.346066911	1.301931336
O	16.225658785	30.631914212	4.240793349
O	14.366793112	34.561034250	5.833331470
O	16.224974658	32.756595297	6.401455417
O	16.883788741	34.977342738	5.108739769
O	13.710703593	33.247990315	8.046603899
O	12.930681429	35.758713389	7.692793953
O	7.027332965	21.617329830	5.798946678
O	7.679389766	23.845937873	4.520531070
O	8.464601613	23.480595931	7.027892658
O	7.008763606	24.644761260	8.915071733
O	7.647510009	25.981044062	6.717006991
O	9.524814000	25.394303726	8.495452932
O	10.177000527	27.633784502	7.241502782
O	12.028215941	25.810177742	7.767552740
O	10.977674301	27.234252646	9.739030637
O	13.474495470	24.596125440	5.922754534
O	12.695672057	27.112149378	5.557751082
O	14.555417638	26.536334121	7.362644762
O	14.605888147	23.153672808	3.979072667
O	16.016381504	21.978256403	2.085799357
O	15.235929186	24.487232720	1.752574490
O	17.098406058	23.908700127	3.548289683
O	14.544264289	20.153403341	0.880053069
O	17.063503938	20.543568402	0.134845839

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Atom	x	y	z
O	15.212726335	22.364401208	-0.417427094
O	12.695891398	20.729050558	-0.934340401
O	13.511166968	18.222061021	-0.600729789
O	12.042896080	19.383677543	1.259459947
O	9.519983603	18.970748375	2.000258697
O	10.184649961	21.188038605	0.710056953
O	7.005663717	18.257483288	2.410366829
O	7.666179964	19.566731977	0.197733365
O	8.445845343	17.053565043	0.549189341
O	4.489227776	17.847166722	3.141610694
O	5.148042406	20.063438173	1.840323057
O	5.945057007	19.696888136	4.345769766
O	5.157584629	22.205848063	4.004410243
O	4.522246920	20.898105212	6.224751402
O	2.650224147	22.690857261	5.657158052
O	3.436361005	22.320671191	8.165920811
O	2.014853781	20.460706374	6.944411748
O	2.651299570	24.829235366	7.829773911
O	1.980064255	23.498156646	10.027181975
O	4.496887670	24.236683790	9.642067925
O	5.153551673	26.460912008	8.353514621
O	5.946935286	26.082027005	10.857612152
O	5.153938541	28.592028625	10.509692149
O	4.494306910	27.271067584	12.714703808
O	7.010232138	28.004316939	12.311281788
O	9.526146053	28.425612543	11.592331786
O	7.667562846	30.231047299	11.024862230
O	8.445126441	29.843793273	13.535101668
O	10.184279028	29.744918520	9.385994277

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Atom	x	y	z
O	12.040975582	29.168511885	11.190337720
O	14.550387911	29.564590886	10.439928726
O	12.697530905	31.384129794	9.887191145
O	13.510448067	31.012289251	12.385182538
O	15.211948698	30.893132294	8.241008268
O	16.004434650	28.382256196	8.583728779
O	17.065216560	30.310067900	10.048579933
O	15.212294057	28.763183813	6.078405387
O	17.063615580	26.946150182	6.631060125
O	18.519913283	25.768664944	4.769798746
O	17.734851848	28.277229120	4.433651847
O	19.580439947	27.684677543	6.245945861
O	17.733776425	26.138851014	2.261035988
O	19.605799197	24.346098966	2.828629337
Mg	10.690007389	27.555184846	5.292058968
Mg	10.689650512	29.634907659	7.402806276
Mg	13.207216304	31.257372045	7.890641772
Mg	13.216501736	29.139785923	5.741861694
O	7.655521870	28.127283945	8.845282861
H	7.941330118	27.479578991	9.498714385
H	8.391172513	30.609517979	6.423980780
O	8.693164091	29.941620224	7.049436611
Mg	8.172293792	30.098796457	9.031507002
Mg	8.162864733	27.981388786	6.881374926
Mg	5.632788973	26.329835050	6.367663480
O	5.144667065	24.352674880	6.153732120
H	5.420641201	23.695912977	6.802535234
H	5.819118738	26.832613558	3.753044548
O	6.130220582	26.171006620	4.380314638

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Atom	x	y	z
Mg	5.632428851	24.195830785	4.177183456
Mg	8.079852097	25.858924102	4.748417000
Mg	5.658305817	28.461608862	8.516874620
O	12.686229207	29.278802860	7.704918527
H	12.988872132	28.642760188	8.362371773
H	13.440227502	31.764189466	5.278073221
O	13.724841707	31.100530761	5.915853281
Mg	15.744870176	28.648894518	4.084310298
Mg	15.737535454	26.496999874	1.910541967
Mg	13.294144834	27.040006718	3.586482370
O	15.244112312	26.666902227	3.891417505
H	15.555155207	26.025568658	4.539526551
H	15.952496749	29.130878530	1.458129877
O	16.228404318	28.468399350	2.101107943
Mg	13.286314499	24.838374735	1.338792674
O	15.433932510	33.137832496	3.892593169
Mg	15.721388128	30.767312868	6.246082252
Mg	18.228460675	28.137248006	2.433127711
Mg	15.744898539	24.347925147	-0.267504325
O	12.678543818	22.894638651	1.202963290
H	12.997229725	22.212097174	1.804685237
H	13.479800185	25.338084902	-1.266409202
O	13.747747445	24.687141993	-0.608755373
Mg	13.211910876	22.717878184	-0.796899628
Mg	10.685980364	23.142711219	0.804463570
H	8.372881501	24.152582701	-0.112720334
O	8.693241820	23.542722585	0.561768574
Mg	8.085240126	23.648986127	2.509708401
O	7.624189980	21.704961624	2.329299315

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Atom	x	y	z
H	7.891135590	21.039051401	2.972168821
Mg	8.163529819	21.547166258	0.356472386
O	5.363904251	24.433810437	-0.346549059
Mg	5.626947434	22.053126917	1.994581578
Mg	3.144909350	24.689254470	5.829249561
Mg	5.656435323	19.922876655	-0.160047685
H	5.884607690	20.420349775	-2.778154691
O	6.180411387	19.771844736	-2.129828903
Mg	8.172387702	19.432444505	-1.804116325
O	10.170534890	19.102336894	-1.475117722
H	10.465449219	18.444007987	-0.836475933
H	10.914631726	21.567485489	-3.919184603
O	11.208797167	20.920977161	-3.268220221
Mg	10.689268390	21.061783832	-1.307007607
Mg	13.206780338	20.588190273	-2.943635819
H	15.495842951	19.601223272	-1.969711720
O	15.198713612	20.258283648	-2.608760329
Mg	15.720901097	22.224395388	-2.428156450
O	17.726656270	24.027219780	0.071628650
H	18.023991384	23.367093654	0.707377807
Mg	18.226713613	25.999447642	0.259370126
O	20.228219343	27.800668634	2.757610055
H	20.504192527	27.143906512	3.406413384
Mg	18.231062707	30.276450579	4.603971432
O	17.712482969	30.426585177	6.572218041
H	18.007083488	29.777931901	7.220814759
Mg	15.719520363	32.891737607	8.401236368
O	15.197994710	33.048511878	10.377151997
H	15.495124050	32.391450800	11.016199894

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Atom	x	y	z
Mg	13.206062389	33.378418720	10.042276293
H	10.913912825	34.357713719	9.066727724
O	11.208079218	33.711205609	9.717691891
O	10.169816941	31.892565342	11.510794390
H	10.464730317	31.234236217	12.149436394
Mg	10.689368617	31.741024090	9.538826918
Mg	8.171668801	32.222672034	11.181795290
H	5.883888789	33.210578005	10.207757636
O	6.179692485	32.562072966	10.856083424
Mg	5.658317121	30.588865660	10.670595177
H	3.373821286	29.451523180	7.540015260
O	3.667037467	28.792990169	8.179196354
Mg	3.147510430	26.828456826	8.000093496
H	0.868944471	25.682884777	4.854251941
O	1.144852041	25.020405596	5.497230007
Mg	3.143162287	22.551454107	3.655491976
H	3.344662679	23.039348687	1.027213699
O	3.644651818	22.395841341	1.678506706
H	8.578325858	30.769681315	13.916007495
H	13.654721044	31.941162123	12.754615206
H	7.728416364	34.951616014	9.777890475
H	12.796627538	36.125084859	8.624406265
$V_{\text{H}}\text{Er}_{\text{Mg1}}^{3+}$			
Si	16.639154459	-5.324181120	-6.141785987
Er	18.066609148	-4.715253076	-3.324584229
Si	18.281080382	-5.981654715	-8.586431704
Si	15.035606745	-7.436050981	-4.657204736
Si	16.635870946	-2.386389267	-5.024487369
Si	18.277657617	-0.268033186	-6.414157654

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Atom	x	y	z
Si	15.034908734	-1.786563921	-2.510762546
Si	13.420432980	-3.936125464	-1.094937297
Si	15.041482796	1.062670017	-1.424281469
Si	13.421750556	-6.767031110	-2.171721200
Si	11.790658872	-3.254061799	1.380127724
Si	11.791571899	-8.922140069	-0.774526532
Si	15.041803872	-10.287307765	-5.737543394
Si	18.231382433	-11.986533472	-1.321639028
Si	18.239051410	-9.147054255	-0.232301734
Si	19.883614309	-7.024898109	-1.628658147
Si	16.606444874	-8.467307261	2.247430176
Si	14.983099703	-10.623745651	3.642685032
Si	16.604792694	-5.624973234	3.328436716
Si	18.237340377	-3.467531559	1.929721213
Si	14.982460530	-4.939666478	5.804319472
Si	19.880373600	-4.120498501	-0.523308784
Si	18.230722288	-0.621510649	2.999417650
Si	21.492013808	-1.983186276	-1.969618727
Si	21.493626025	-7.669251557	-4.129158232
Si	18.290509148	-8.829074344	-9.643061562
Si	19.915677169	-3.813933588	-9.962895469
H	21.089043976	-4.269154159	-12.094537696
Si	19.914260734	-0.969766481	-8.882807500
H	21.087873916	0.788543393	-10.171795296
Si	18.288870137	2.563672301	-5.313135748
H	19.461660950	4.323000663	-6.604801262
Si	16.663355283	3.227898640	-2.824785752
H	16.467738966	5.560783558	-2.035746751
Si	13.414929549	1.746539017	1.057476659

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Atom	x	y	z
Si	11.789474810	-0.412414445	2.461066313
H	13.224320292	4.087188170	1.848566478
H	10.322162937	0.228609824	4.354106376
Si	10.160629842	-5.405479585	2.784539628
Si	10.162046277	-8.249646692	1.704451659
H	8.685592398	-4.746645219	4.666662606
H	8.688559105	-9.994763324	2.671915005
Si	11.790115074	-11.765011823	-1.853327944
Si	13.414458747	-12.446725839	-4.336885122
H	10.321639120	-13.501880908	-0.865015706
Si	16.662228757	-10.975430886	-8.223622578
H	19.461617592	-9.283705421	-11.777642286
Si	23.112327567	-5.507777680	-5.550599609
H	24.580328353	-6.148791190	-7.433767044
Si	23.110506982	-2.656097207	-4.466948970
Si	21.485678183	-10.510968718	-5.215088148
H	22.952248850	-11.145104208	-7.108943332
Si	19.860096622	-12.667538622	-3.804238311
Si	16.604803217	-14.141205587	0.080836589
Si	14.980008266	-13.464200753	2.562451545
H	13.810745706	-15.227472405	3.852830298
Si	13.358697291	-9.943490505	6.116746782
Si	13.356876090	-7.091810311	7.200398157
Si	14.979802520	-2.098683488	6.882328685
Si	16.605059086	0.057330756	5.478514945
H	13.810968858	-1.638871222	9.018359232
H	16.796644632	2.328583933	6.441388449
Si	19.861058457	1.534977460	1.594486936
H	20.054605497	3.801801288	2.558299941

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Atom	x	y	z
Si	21.485509493	0.860883397	-0.893529241
H	22.952916807	2.592505833	-1.887239750
H	24.579388166	-0.926188222	-5.447556874
H	12.191953258	-11.710513516	7.416768766
H	12.189429248	-6.635364486	9.345276111
O	17.951567420	-5.768931651	-5.276362244
O	17.039007690	-5.405317773	-7.706370030
O	15.424025596	-6.324964516	-5.785237212
O	16.264387670	-3.792883436	-5.747422441
O	17.947418040	-2.631998401	-4.081759912
O	17.035794538	-1.283838054	-6.138857514
O	15.422598642	-1.871889081	-4.092103637
O	13.817632894	-2.788122478	-2.164258160
O	16.327644579	-2.119890572	-1.580464679
O	14.545145667	-0.266133497	-2.203678187
O	14.667449896	-4.289132719	-0.114947048
O	12.897972099	-5.271257738	-1.844892099
O	12.204597251	-3.358706855	-0.178566782
O	14.669414119	-7.160890800	-1.208046854
O	12.205069740	-7.805540953	-1.867518608
O	13.819505913	-6.912891956	-3.733568746
O	14.544395901	-8.777795741	-5.433982935
O	16.328811491	-7.808437048	-3.742308171
O	18.740587418	-10.656770290	-0.547017741
O	19.479146413	-8.131959516	-0.519038591
O	16.962029599	-8.788087440	-1.168637197
O	17.816119690	-9.037472612	1.329208567
O	15.322824056	-8.115024217	1.320641207
O	16.193627495	-9.588818083	3.343810601

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Atom	x	y	z
O	17.113205931	-7.133165988	3.017818308
O	17.815580216	-4.590651282	3.020304474
O	15.321428470	-5.264839383	2.404441031
O	16.191154250	-5.518637362	4.893140656
O	19.478759080	-4.033163154	1.041834999
O	16.961264574	-3.106991420	0.992815554
O	18.737607018	-2.131251302	2.699990125
O	18.592224752	-3.681932579	-1.411008356
O	20.318457273	-5.639126240	-0.900799431
O	21.102499122	-3.111268434	-0.866179649
O	18.596557929	-6.759324625	-2.583663697
O	21.106174673	-7.554233139	-2.554343066
O	17.780989002	-7.319080075	-9.348384240
O	18.709041299	-4.859076102	-9.672873351
O	19.555837858	-6.338891018	-7.641782441
O	21.188784872	-4.176117137	-9.020988940
O	20.337622503	-3.911244925	-11.522377971
O	19.400062034	-2.311665836	-9.634716977
O	21.187116646	-1.331083697	-7.940120890
O	20.336270353	0.141191865	-9.981721409
O	18.706784882	-0.381975087	-7.972005112
O	19.553174325	-0.633585224	-5.473149867
O	17.777922212	1.238442619	-6.094484138
O	18.704084033	3.685438112	-6.405574735
O	19.569224143	2.197936918	-4.383433544
O	17.083450399	3.128103310	-4.388008462
O	17.946876094	2.879966806	-1.892096376
O	15.461932098	2.185188388	-2.518497319
O	16.145210343	4.731480029	-2.513586623

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Atom	x	y	z
O	16.320021362	0.712346127	-0.484976607
O	13.833083289	1.636302196	-0.505436666
O	14.693166304	1.390010182	1.994138978
O	12.205715183	0.711282027	1.368546732
O	12.909849964	3.256349707	1.368029423
O	11.279851820	-1.746857807	1.696667415
O	13.068225737	-0.767584249	3.397603908
O	10.580399166	0.155263637	3.380435802
O	10.582639461	-4.294521239	1.685625718
O	13.061848565	-3.607888353	2.329017162
O	11.433485754	-5.766796801	3.727226238
O	9.646431142	-6.747378941	2.032630151
O	8.953153991	-4.817688191	3.695342015
O	10.583992227	-8.346957749	0.144968421
O	11.435154596	-8.611829962	2.646357452
O	8.955410407	-9.294789206	1.994473777
O	11.281155941	-10.259516323	-1.538786268
O	13.062695709	-9.295138862	0.167164170
O	12.206500847	-11.876889986	-3.416496761
O	13.068917199	-12.128694541	-0.920307139
O	10.579297183	-12.797639567	-1.541592720
O	14.692606462	-12.809205660	-3.402559694
O	12.909385094	-13.781141702	-5.108678378
O	13.832262691	-11.324176156	-5.430189996
O	16.320815278	-10.655805412	-4.805944657
O	15.462097274	-10.396257483	-7.301579760
O	17.945444622	-11.342056213	-7.297711238
O	16.144746089	-12.306011099	-8.990295161
O	17.082746301	-9.862036161	-9.325047558

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Atom	x	y	z
O	18.703899334	-8.939866608	-11.205158301
O	19.570547183	-9.178892934	-8.707075302
O	21.838278501	-5.154439488	-6.494616649
O	24.322425025	-6.084083188	-6.459396094
O	22.691406304	-6.623876385	-4.450946090
O	23.606707522	-4.167803666	-4.782150383
O	21.995872050	-9.177853357	-4.442471477
O	20.208387070	-7.318839872	-5.062449759
O	20.208039929	-10.152310585	-6.150107974
O	22.692971688	-11.081699113	-6.134851372
O	21.065999018	-11.628526796	-4.117570127
O	18.580535828	-12.319393242	-4.740793016
O	20.374831791	-14.174654960	-4.107093337
O	19.440496830	-12.554509192	-2.242361458
O	16.952288109	-11.627389147	-2.254119099
O	17.815701756	-13.108211805	-0.227043868
O	15.325971158	-13.783249829	-0.852895752
O	17.112920352	-15.648490905	-0.227564967
O	16.186940448	-14.036981428	1.644181014
O	13.700036860	-13.105175628	1.630310337
O	15.489804897	-12.131114645	3.330786278
O	14.562399779	-14.580274950	3.662431748
O	13.701977257	-10.266723187	2.711188064
O	14.568794749	-10.519796012	5.207950297
O	14.567459337	-6.057881703	6.904621249
O	13.701744679	-4.580431787	4.872879267
O	15.489775265	-3.605675332	6.572080251
O	13.699554754	-1.741279747	5.949944209
O	16.187575407	-1.061804285	6.575419599

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Atom	x	y	z
O	14.561962744	-1.997334970	8.445985295
O	17.815478244	-0.511141074	4.562482683
O	15.326466746	0.416538835	4.544876652
O	17.113385222	1.389000503	6.249142835
O	19.442263448	0.410389597	2.684643342
O	16.951957048	-0.263770199	2.065776074
O	18.581426595	1.904439758	0.666006995
O	20.375296661	2.862836449	2.369614464
O	21.065289577	0.963351300	0.669335738
O	21.997075518	-0.647633768	-1.203491326
O	20.207656407	1.220359939	-1.828011560
O	22.693674056	1.897305383	-1.201973721
O	22.687454687	-2.556900056	-2.903748392
O	20.206564378	-1.620195797	-2.898136980
O	21.836642144	-2.286636364	-5.404857607
O	24.321090229	-1.622168598	-4.762725879
O	12.084647609	-9.590152593	5.172730479
O	12.937775412	-11.059589489	7.216401038
O	13.853076631	-8.603516770	6.885196744
O	12.083011252	-6.722349468	6.262489521
O	12.933824411	-6.992612881	8.763597999
Mg	16.574742189	-6.875483210	-1.866539941
Mg	16.572003924	-4.067222627	-0.798851002
O	16.247884527	-5.027549910	-2.492858300
O	16.938704108	-5.963755610	-0.040104640
H	17.661192226	-6.190530407	0.554961874
H	21.046401087	-4.644301491	-3.531501380
O	20.268524326	-4.439751049	-4.063912233
H	18.848049236	-3.288922708	-7.080443704

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Atom	x	y	z
O	19.590792330	-3.507071784	-6.506380015
Mg	19.920624226	-5.421415815	-5.847639012
Mg	19.918738210	-2.514774338	-4.743881066
Mg	18.265701106	-7.650594710	-4.425047502
Mg	18.262764863	-10.431541040	-5.484005653
O	17.980297072	-8.549073255	-6.215771058
H	17.211812372	-8.333530494	-6.754788668
H	19.307990479	-9.716109590	-3.125526758
O	18.554622953	-9.508365042	-3.688268622
Mg	18.264129885	-1.790393460	-2.197121133
Mg	18.261956910	0.991365571	-1.143007712
O	17.979151092	0.071331314	-2.939025216
H	17.210552410	0.268301059	-3.484954845
H	19.308822426	-1.111186831	0.145217578
O	18.554925796	-0.893413717	-0.412976786
Mg	16.633762376	-1.198965439	0.250579433
Mg	15.007725875	-3.356149216	1.668925209
Mg	15.008557582	-0.516061448	2.728578117
O	14.726003552	-1.460575933	0.939790711
H	13.970740807	-1.268956718	0.372984832
H	16.057296168	-2.621082411	4.010996527
O	15.299579700	-2.410525540	3.454699411
Mg	13.384231631	-2.671682179	4.134052603
Mg	13.379538187	-5.514973074	3.057003698
Mg	13.381808704	-8.357962034	1.977778934
H	12.348548492	-6.244598926	0.696157927
O	13.085930851	-6.464396242	1.275975271
H	14.429777266	-7.624087327	4.327308154
O	13.669705019	-7.414645106	3.773824736

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Atom	x	y	z
Mg	15.000158259	-6.203072914	0.588647745
Mg	15.007357689	-9.047404323	-0.496574143
Mg	15.010155767	-11.876082657	-1.587889338
O	14.726401409	-9.980433599	-2.298816785
H	13.971213468	-9.748160868	-2.850328427
H	16.057833980	-11.153452813	0.767560193
O	15.300157461	-10.942180029	0.211473609
Mg	16.634013461	-9.718224207	-2.988030332
Mg	19.885400985	-8.252407851	-6.896075401
Mg	13.384889515	-11.198507257	0.892765137
Mg	19.883615818	0.299673149	-3.646890155
Mg	21.513293550	-3.237486903	-7.214394078
H	24.183407542	-3.188374503	-7.340038237
O	23.423335910	-2.978932001	-7.893522392
Mg	21.510575532	-0.382067981	-6.139693164
H	22.552149379	0.335730891	-3.784655487
O	21.792525566	0.546478277	-4.338428673
Mg	19.888832987	3.126631153	-2.565018631
O	20.178347733	4.061196213	-0.768599667
H	20.938218730	3.851693295	-0.214782129
Mg	18.262287310	3.799532598	-0.077475847
H	15.589269171	3.748510062	0.057047759
O	16.348555960	3.538361835	0.611532743
O	16.923599053	2.581939086	3.124906747
H	17.679463182	2.370480076	3.683388242
Mg	16.634988620	1.642666369	1.330613410
Mg	15.008525604	2.322641106	3.807950952
O	13.095496794	2.061631899	4.495518743
H	12.339930906	2.273423676	3.936645974

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Atom	x	y	z
Mg	13.385215053	0.166260989	5.211213126
O	11.468214453	-2.928232126	4.819683824
H	10.718062596	-2.714921082	4.254150039
Mg	11.756944641	-4.817781085	5.527653964
Mg	11.759662658	-7.673200008	4.452953050
O	9.837161439	-7.942784888	5.160967113
H	9.094418344	-7.724635812	4.586903424
Mg	11.757608667	-10.521313057	3.359356144
H	10.719003570	-11.246405042	1.011435268
O	11.468971942	-11.462911237	1.576005525
Mg	13.384053182	-14.035558197	-0.188295558
H	12.339466651	-14.764066518	-2.540062209
O	13.095031923	-14.975859509	-1.981189058
Mg	15.008060733	-14.714850302	-2.668756850
O	16.923134182	-14.455552322	-3.351801054
H	17.678998312	-14.667011332	-2.793319560
H	15.588804300	-13.288981347	-6.419660042
O	16.348091090	-13.499129573	-5.865175058
Mg	16.633467973	-12.560196623	-4.069264828
Mg	18.261823056	-13.237958530	-6.554184385
O	20.177882862	-12.976295196	-7.245307469
H	20.937753859	-13.185798114	-6.691489930
Mg	19.887334738	-11.083481799	-7.967252930
O	21.794293369	-7.977440883	-7.577406521
H	22.554054144	-8.186833971	-7.023309445
Mg	21.511239558	-6.085599953	-8.307990984
H	16.280139131	-13.306703205	-8.970698381
H	13.050098718	-14.781087876	-5.088496063
H	20.248092550	-14.908089895	-4.789816092

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Atom	x	y	z
H	16.982710437	-16.378981860	-0.912786350
V_HEr_{Mg2}³⁺			
Si	6.094563263	-12.896986731	-10.892011466
Si	4.476709796	-10.739577056	-9.455842183
Si	2.838184747	-11.416954236	-6.980237097
Si	4.478346319	-7.900925421	-10.538647055
Si	2.801284751	-14.274169131	-5.876641602
Si	1.244251046	-9.265464586	-5.557148447
Er	6.160770094	-14.036225406	-5.569493332
Si	4.470283652	-16.459265819	-7.309212563
Si	1.219922431	-14.953162510	-3.391535891
Si	4.472887297	-19.288870875	-6.235039056
Si	6.089261043	-15.744348986	-9.798095451
Si	7.697385973	-17.906323957	-11.211608194
Si	7.695004107	-12.226391190	-13.383825264
Si	9.404279324	-14.100632083	-5.409459240
Si	9.319050980	-11.251828026	-6.462124913
Si	10.928251571	-10.583798240	-8.971049148
Si	7.708351930	-9.088306830	-5.055953867
Si	6.105433184	-9.764744549	-2.573347075
Si	7.711255012	-6.245872968	-6.130419895
Si	6.120711981	-12.608757687	-1.504189488
Si	4.495200080	-7.611301452	-1.149626332
Si	4.496536247	-13.298395839	0.985728131
Si	7.747327463	-14.799262403	-2.842928836
Si	7.725358901	-17.633335785	-1.801111947
Si	10.970030020	-16.263554084	-6.826472459
Si	7.703476997	-20.754595942	-10.144988713
Si	9.298872074	-17.227002661	-13.710325314

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Atom	x	y	z
Si	6.091732637	-21.438409589	-7.654444123
H	8.853661051	-22.520753469	-11.446167533
H	5.897899304	-23.774600302	-6.866395587
Si	2.869331455	-19.949645312	-3.733970069
H	2.675189980	-22.285638413	-2.945336640
Si	1.252252310	-17.796973824	-2.313616935
H	-0.200383543	-18.435008486	-0.413168734
Si	-0.360775009	-12.780798504	-1.969016096
Si	-0.354294295	-9.939097097	-3.056022356
H	-1.812900900	-13.413303479	-0.059966780
H	-1.812246471	-8.202546313	-2.055825291
Si	1.255555131	-6.420814689	-6.625022660
Si	2.869535350	-5.744641394	-9.114525857
H	-0.198701572	-4.682770120	-5.621306732
Si	6.089784059	-7.231413857	-13.031691238
Si	7.698093856	-9.386660503	-14.453688553
H	8.853889785	-8.924911957	-16.595996243
Si	9.305352788	-14.385301254	-14.797331573
H	10.450743627	-13.924474707	-16.945689035
H	10.428997782	-19.007621550	-15.010093280
Si	12.554616203	-15.582912644	-9.336036759
H	14.006630689	-17.318624305	-10.344055294
Si	12.541782983	-12.733934570	-10.403420547
H	14.000490488	-12.098271055	-12.299383967
Si	10.927511850	-7.739590705	-10.044592582
Si	10.934018760	-19.104149904	-5.739909708
H	12.383220990	-20.845607442	-6.739749900
Si	9.322320855	-19.783071316	-3.247882135
H	9.516441955	-22.057897529	-2.296377145

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Atom	x	y	z
Si	6.094450161	-18.299128446	0.679453783
H	6.286650211	-20.570037391	1.635622791
Si	4.479827546	-16.136106930	2.087942290
H	3.329566286	-16.600784924	4.232966098
Si	2.894969121	-11.136708487	2.405272459
Si	2.882135900	-8.287730413	1.337888671
H	1.760185405	-11.609427266	4.561398942
H	1.722488054	-6.529596664	2.647005334
Si	4.485201408	-4.769565305	-2.218245784
Si	6.096866029	-4.093633683	-4.707237911
H	3.329992917	-3.005054236	-0.916578816
Si	9.320652479	-5.578944582	-8.627763994
H	12.383330894	-7.100999205	-11.947430202
O	4.892339913	-11.863844772	-10.552314971
O	5.763069902	-10.379920996	-8.533521988
O	3.261300837	-11.314225901	-8.545351092
O	3.967160846	-9.407996290	-10.228626899
O	2.343232596	-12.939106197	-6.670603024
O	4.107731049	-11.039320865	-6.055614839
O	1.618400602	-10.392489111	-6.665204665
O	4.037145351	-13.912038091	-4.885335584
O	3.295306503	-15.399360334	-6.940191283
O	1.585298989	-14.849099891	-4.973753862
O	3.947857302	-17.963656548	-7.015252621
O	4.873745744	-16.293542580	-8.870250827
O	5.786363234	-16.180806013	-6.396646005
O	6.487454785	-16.875726801	-10.886738865
O	7.385230895	-15.404712502	-8.877102872
O	5.592009966	-14.406245453	-10.566195442

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Atom	x	y	z
O	6.485202754	-12.789756268	-12.460261639
O	7.396185143	-12.548490301	-9.986290405
O	9.859239041	-12.576347798	-5.683332986
O	8.042937240	-11.614036420	-7.405727488
O	10.527389905	-10.712032596	-7.407892135
O	8.927537558	-10.093842242	-5.408104668
O	6.415393507	-9.381415421	-5.995296441
O	7.304007562	-9.180217345	-3.491083429
O	8.222065034	-7.573669376	-5.363084719
O	6.587903243	-11.087456567	-1.773821494
O	4.791135038	-10.067264720	-3.478603170
O	5.700713470	-8.641525016	-1.465916036
O	4.823067950	-12.976308772	-2.414241543
O	5.709256779	-12.757908634	0.062220356
O	7.348534819	-13.639628474	-1.793405881
O	8.269368494	-16.126515161	-2.078596952
O	6.413327485	-15.211037227	-3.691665221
O	8.888128300	-14.291748079	-3.881563653
O	8.176829614	-14.467130633	-6.423314198
O	10.614032869	-15.132337010	-5.713170164
O	7.194109850	-19.415743766	-10.903964817
O	8.989087141	-17.562314564	-10.289230531
O	8.094010844	-17.782002799	-12.777469210
O	6.498664677	-21.321504355	-9.219566217
O	8.108391723	-21.867074954	-11.252833552
O	8.990828791	-20.410811865	-9.217250768
O	7.376650158	-21.089503099	-6.724671829
O	5.581422815	-22.944049745	-7.346112590
O	4.884842562	-20.403203662	-7.335902563

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Atom	x	y	z
O	3.273112079	-19.849506398	-5.301895412
O	5.761123340	-18.940159023	-5.306382210
O	4.159050229	-19.601053721	-2.809600991
O	2.355034784	-21.452481384	-3.418041639
O	1.669962068	-18.902756703	-3.424090190
O	0.053501738	-18.375877603	-1.388948321
O	2.539604107	-17.445553357	-1.388805817
O	0.727057919	-16.463733002	-3.072377582
O	2.511280816	-14.606686680	-2.466773309
O	0.022767251	-13.912307828	-3.065388072
O	0.933888391	-12.440364510	-1.051339093
O	-1.565636239	-13.335798642	-1.036159992
O	0.931584380	-9.590364774	-2.128870158
O	0.043779153	-9.829218399	-4.622613263
O	-1.560031879	-8.901546424	-2.739847691
O	2.531817442	-8.913128238	-4.633134965
O	0.736973047	-7.925201432	-6.317040755
O	2.541478270	-6.073065713	-5.697677373
O	1.665641175	-6.313941705	-8.190622213
O	0.055428986	-5.374781905	-6.311696005
O	3.277354959	-6.857529661	-10.221316681
O	4.157218469	-5.392834233	-8.191226477
O	2.355495175	-4.406928029	-9.873499160
O	4.883514435	-7.792778978	-12.105376306
O	5.766602915	-7.552619032	-9.614494614
O	6.495111563	-8.347505970	-14.134927568
O	7.376536264	-6.881597425	-12.105581426
O	5.581883206	-5.898495455	-13.801570465
O	8.984223247	-9.040758395	-13.525507937

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Atom	x	y	z
O	7.184215725	-10.892269090	-14.146931196
O	8.104537541	-9.279747119	-16.019226599
O	8.984161659	-11.877717619	-12.460324019
O	8.099615204	-13.347750581	-14.481156909
O	8.796680917	-15.892250908	-14.479564860
O	10.591231462	-14.036568931	-13.870179376
O	9.703426236	-14.275422556	-16.363922480
O	10.593534864	-16.886568386	-12.792647570
O	9.682414334	-18.358511985	-14.806697289
O	13.759368245	-16.614336168	-9.663658716
O	11.259913796	-15.930429177	-10.252492600
O	13.048676582	-14.071061567	-9.639047197
O	12.166220977	-15.710610343	-7.766393942
O	13.746049926	-12.165469284	-11.324271461
O	11.256489452	-13.081168378	-11.333810450
O	12.130867527	-11.622453514	-9.297626542
O	9.642008665	-10.921390532	-9.904489617
O	11.437333503	-9.075517914	-9.282416019
O	11.459745024	-17.604010846	-6.058933611
O	9.672655191	-16.607615703	-7.744913368
O	12.129314237	-20.154414068	-6.048459020
O	10.517536814	-19.197020627	-4.175279230
O	9.645997573	-19.445947239	-6.668491991
O	8.031702908	-20.123161654	-4.174469803
O	9.840145255	-21.123319951	-2.501025441
O	8.919270001	-18.679089321	-2.130098686
O	7.307845553	-17.743686088	-0.240863296
O	6.437987834	-17.972900965	-2.734981713
O	4.810518513	-18.646479083	-0.253221262

Continued on next page

Atom	x	y	z
O	6.601347975	-19.628562885	1.449367395
O	5.683747448	-17.175216957	1.772492495
O	4.076278797	-16.241819775	3.655329146
O	3.190898046	-16.487294504	1.163859135
O	4.987089766	-14.631629904	1.768480246
O	3.199389425	-13.644299014	0.068907460
O	4.099721162	-12.168132011	2.077650502
O	3.389029499	-9.624857409	2.102262021
O	1.600266713	-11.484225019	1.488816617
O	2.506574504	-11.264406466	3.974914534
O	4.086403453	-7.719265408	0.417037016
O	1.596842370	-8.634964220	0.407498768
O	2.471220444	-7.176249357	2.443682675
O	3.199834481	-7.947606987	-2.072855093
O	4.996825248	-6.100347528	-1.453464158
O	5.689830082	-4.204146492	-3.143083942
O	3.196644024	-5.112443212	-3.145570208
O	4.079468765	-3.652397706	-1.114902755
O	7.303547378	-5.122955416	-5.033025618
O	4.809759659	-4.433015644	-5.638121999
O	6.601808366	-2.583008594	-5.006090480
O	6.422857871	-6.583819824	-7.061701852
O	8.911075359	-5.671755896	-7.062869329
O	10.519531557	-6.624492140	-8.940337330
O	8.032331130	-5.919587514	-9.556110243
O	9.840605646	-4.077765661	-8.956483316
O	12.129829704	-7.168428034	-10.972088980
O	9.640497408	-8.081000115	-10.974528050
Mg	6.093334029	-11.263997129	-6.691722368

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Atom	x	y	z
O	6.339428083	-12.129086130	-4.931436944
O	5.794030662	-13.174161006	-7.596390265
Mg	7.758452297	-13.478939125	-8.216034414
Mg	4.501387324	-11.936027865	-4.212003202
Mg	2.868938767	-9.840718998	-2.807308052
Mg	2.875709214	-12.691714398	-1.738576176
O	3.173583256	-10.802524886	-1.017966057
H	3.942563456	-10.588850285	-0.478209556
H	1.825942888	-11.943362021	-4.080401981
O	2.574540264	-11.732966886	-3.512362624
O	4.772366291	-7.265902328	-4.587148283
H	5.540451392	-7.084471945	-4.034709081
H	3.414295979	-8.420473114	-7.653050668
O	4.178562735	-8.212850501	-7.104940885
Mg	4.484041891	-6.330990556	-6.377044247
Mg	4.476555844	-9.155606299	-5.307880156
Mg	2.869964946	-7.013282909	-3.886918410
Mg	1.268906275	-10.536539511	-0.322009237
O	-0.862966166	-11.446046751	-2.738255642
Mg	4.434093831	-14.879391925	-3.082082107
Mg	4.487648312	-17.709606067	-2.054855148
O	4.755569457	-15.823726702	-1.321141778
H	5.511629591	-15.592936747	-0.770897440
H	3.418787248	-16.985610203	-4.389432484
O	4.188614831	-16.760578010	-3.855361496
Mg	2.847810572	-15.547607837	-0.642167641
Mg	6.094914586	-17.075961617	-4.544080675
O	8.002550021	-17.287328487	-5.272047992
H	8.771846392	-17.100962533	-4.722345819

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Atom	x	y	z
O	7.424883427	-18.260119512	-7.791791939
H	6.666362903	-18.468114331	-8.347780219
Mg	7.740848897	-16.384946119	-7.093765515
Mg	7.706593060	-19.194374967	-5.990152618
Mg	9.334214412	-15.664324669	-9.569035351
Mg	9.327665479	-12.815473044	-10.665911083
H	10.403021255	-13.543003110	-8.332102258
O	9.647685632	-13.767338341	-8.886013487
O	9.017529514	-14.719576220	-11.359546357
H	8.261238890	-14.930640093	-11.917706543
Mg	7.706031987	-10.651038091	-9.214002259
Mg	7.704556332	-7.820722193	-10.291341824
O	8.003418859	-8.761333770	-8.501334086
H	8.757839797	-8.558981824	-7.937165897
H	6.639737020	-9.918858696	-11.558315376
O	7.404192726	-9.711264321	-11.010206745
Mg	6.092464860	-8.477740683	-7.800394468
Mg	9.312216615	-9.978801652	-11.712382527
Mg	10.928553357	-14.982743668	-12.063318454
Mg	1.266641811	-7.688211905	-1.397354054
H	0.201118107	-6.958403037	-3.737916950
O	0.961880134	-6.746229438	-3.186393116
Mg	2.873128002	-4.175798727	-4.956809699
H	-1.398408193	-10.484435935	-0.176397325
O	-0.642117568	-10.273372063	0.381762861
Mg	1.266342938	-13.381618721	0.757240475
H	0.186551540	-15.485593211	-0.496062301
O	0.949452827	-15.276916301	0.053854598
Mg	2.869966271	-18.388023283	0.425246380

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Atom	x	y	z
H	1.811479894	-20.490132725	-0.844072191
O	2.574456301	-20.276863887	-0.295938947
Mg	4.484465522	-20.545236456	-0.992456243
O	6.392989387	-20.809411366	-1.696056575
H	7.155842501	-20.610052053	-1.142544332
Mg	6.096604926	-19.877023138	-3.484453128
H	5.033205804	-21.973975769	-4.755726830
O	5.796976348	-21.760929779	-4.208698815
Mg	7.704725850	-22.030137719	-4.910714606
O	9.611691962	-22.292143299	-5.613776332
H	10.374202789	-22.088452812	-5.061307515
Mg	9.314376341	-21.352049517	-7.404996131
Mg	9.335505554	-18.514432828	-8.486018861
O	11.232443205	-18.776193729	-9.192469586
H	11.998628014	-18.568304482	-8.646696866
Mg	10.925990020	-17.827822879	-10.984068743
O	12.833230339	-15.248729043	-12.759275274
H	13.602210539	-15.035054442	-12.219518774
Mg	10.926288894	-12.134416062	-13.138663272
O	11.218920143	-10.244767863	-12.415461062
H	11.983524806	-10.040557767	-11.866118318
Mg	9.314411440	-7.141647157	-12.785318720
O	9.612152353	-5.246589944	-12.069233853
H	10.374663180	-5.042898522	-11.516765390
Mg	7.705186241	-4.984584363	-11.366172127
H	5.033666195	-4.928422414	-11.211184351
O	5.797436130	-4.715375208	-10.664155949
O	6.393449778	-3.763857076	-8.151514450
H	7.156302892	-3.564497763	-7.598002207

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Atom	x	y	z
Mg	6.096527326	-5.656285049	-8.869742978
Mg	4.484925303	-3.499682820	-7.447913023
H	1.811940285	-3.444578434	-7.299530066
O	2.574916082	-3.231309316	-6.751396081
H	5.053142910	-13.363066993	-8.183878203
H	2.487382870	-3.406066065	-9.842178793
H	5.716548203	-4.897808298	-13.777269173
H	6.462701835	-1.844974844	-5.681409335
H	9.709344201	-3.352224873	-9.646744859
$2V_{\text{H}}\text{Er}_{\text{Mg1}}^{3+}$			
Si	13.128110676	15.091902786	-3.926331618
Si	12.027061323	15.408142499	-1.133440456
Er	14.201674881	15.994945529	1.278656738
Si	10.998615743	13.047456599	0.453374257
Si	12.024506467	18.231716496	0.194982194
Si	13.126846324	20.588667915	-1.339037440
Si	10.997094512	18.518516700	3.025821314
Si	9.954125663	16.123603064	4.572531741
Si	11.007734436	21.275533651	4.330607721
Si	9.955893400	13.384907318	3.283269768
Si	8.879399844	16.467698598	7.401415668
Si	8.879598521	10.987511848	4.823801557
Si	11.009293521	10.286052250	-0.838328037
Si	13.142467107	12.336056298	-5.216589474
Si	14.204823495	17.492437717	-5.463087979
H	14.889589964	17.297118858	-7.834639154
Si	14.203687227	20.243920885	-4.168690645
H	14.888892549	22.197971609	-5.528498182
Si	13.141455644	23.341452174	-0.039003136

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Atom	x	y	z
H	13.823821048	25.302577765	-1.396115681
Si	12.072958360	23.683517545	2.794257088
H	11.861436174	25.931100048	3.798615280
Si	9.943416435	21.623203141	7.164173436
Si	8.878382164	19.218184267	8.699878242
H	9.734382390	23.874905608	8.175786946
H	7.831884740	19.578654097	10.919677026
Si	7.808399951	14.074322046	8.945126730
Si	7.809536219	11.322838878	7.650729396
H	6.755316323	14.433959601	11.161085469
H	6.756400869	9.386040701	8.785275462
Si	8.879343981	8.233278081	3.532951063
Si	9.943332027	7.883314733	0.700991208
H	7.831919082	6.293288559	4.669660196
Si	12.072785448	9.935710413	-3.673356957
H	13.824294291	12.132445170	-7.592594098
Si	17.404732297	18.942434758	2.103940934
Si	17.394055029	21.703837641	3.395643996
H	18.440273735	23.644668252	2.256257971
Si	16.330559847	22.054173316	6.230667221
Si	18.447453320	18.604983821	-0.725954114
Si	16.376285505	16.581751309	3.690759834
H	16.542270807	24.261348027	7.321285952
Si	15.260864949	19.653839070	7.773889094
Si	15.275233596	16.897993828	6.483645030
Si	14.195421028	19.993122113	10.605332622
Si	14.198524733	14.497461360	8.020400855
Si	14.199667002	11.745970266	6.726003926
Si	13.128464073	14.832780326	10.847331740

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Atom	x	y	z
Si	13.128660920	9.352592110	8.269716047
Si	15.276503519	11.401224576	3.896343173
Si	15.261894225	8.648436125	2.596317781
Si	16.378843295	13.758177277	2.362332559
Si	17.406253528	13.471376466	-0.468505271
H	19.504877735	20.542330012	-1.872348900
Si	18.449222887	15.866289541	-2.015214505
H	19.505176065	15.511396873	-4.238452204
Si	17.395615730	10.714358702	-1.773294648
H	18.440367506	10.352967837	-3.995788788
Si	16.330397805	8.306364167	-0.236944887
Si	14.195415015	6.250598855	4.140109488
Si	13.129680322	6.602107953	6.971252608
H	12.447776212	4.638663931	8.324037961
Si	12.053936015	9.696691092	11.098602042
H	11.394203799	7.726848909	12.444493969
Si	12.052166045	12.435384982	12.387863261
H	11.392869872	12.655432554	14.762627419
Si	13.128717187	17.587015731	12.138181101
H	12.447222514	17.794495351	14.513286609
H	14.402821776	22.203553546	11.700808427
O	12.059821794	15.457194427	-2.758867400
O	13.518196780	15.023671207	-0.630757380
O	10.996608500	14.263879996	-0.626621195
O	11.594021464	16.871743749	-0.579566327
O	12.057561993	19.457226327	-0.874801903
O	13.516074616	18.085689244	0.810332602
O	10.994332339	18.572735995	1.399932195
O	9.975691776	17.385616985	3.561038689

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Atom	x	y	z
O	12.486872233	18.274961630	3.624644277
O	10.456655716	19.962242674	3.565038316
O	11.419242209	15.844060148	5.211340070
O	9.388245107	14.795986809	3.838776280
O	8.929455963	16.496483430	5.786413556
O	11.420816887	13.064464370	3.903327753
O	9.976762412	13.360339900	1.666330630
O	8.929921246	12.214197377	3.772868857
O	10.456567892	11.710963982	-0.312492843
O	12.488294341	12.735908547	1.020410575
O	12.588857167	13.764126603	-4.694628011
O	13.190452150	16.318074837	-4.989820803
O	14.611091870	14.807714426	-3.331947166
O	15.690588804	17.209478856	-4.879857998
O	14.254470674	17.527908353	-7.083999629
O	15.689603364	19.968860390	-3.582106065
O	14.253156210	21.474023127	-5.225450490
O	13.189661868	20.628039285	-2.961679447
O	14.610286187	20.306912026	-0.744892706
O	12.588923203	22.027782655	-0.806168648
O	13.188692715	24.580475372	-1.087440877
O	14.626699033	23.061290281	0.550235995
O	12.128948380	23.716406969	1.173382176
O	13.558753381	23.415385502	3.388940473
O	11.061463494	22.515150714	3.281408035
O	11.512281157	25.109867065	3.325574941
O	12.490945130	21.003919270	4.932065811
O	9.995295892	21.659582477	5.543871955
O	11.426894523	21.343244358	7.760370919

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Atom	x	y	z
O	8.928579344	20.453557864	7.648688330
O	9.389725825	23.048700225	7.708136951
O	8.325856749	17.896668787	7.943911791
O	10.362441271	18.941235529	9.295853334
O	7.863650253	19.593453160	9.910285160
O	7.857868934	15.304424288	7.888366885
O	10.360665739	16.193482389	8.006950029
O	9.294316089	13.799261551	9.531711310
O	7.253849427	12.748463495	8.191189558
O	6.794374593	14.458440446	10.152137928
O	9.295301529	11.039880018	8.233959377
O	6.795164875	10.148475998	8.123996572
O	7.859183399	11.358309514	6.029817746
O	8.326460806	9.657050344	4.070984958
O	10.360600277	10.688195736	5.418525491
O	10.363342244	7.943371189	4.122861723
O	8.930252375	8.260694723	1.911026388
O	7.863732275	7.062518805	4.015922673
O	11.426464115	7.594952226	1.293926360
O	9.389421018	6.555487836	-0.050587340
O	9.995693214	9.108383470	-0.359713554
O	11.063217498	10.309313592	-2.462040399
O	12.492440141	9.990074892	-0.248631302
O	13.558447089	9.641320868	-3.090460104
O	11.511976350	8.616655580	-4.433148925
O	12.128783999	11.165003406	-4.730346402
O	13.189861292	12.356817961	-6.839433013
O	14.627557875	12.054120771	-4.627597245
O	17.946783081	20.278929150	2.869804261

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Atom	x	y	z
O	15.910910939	21.999816384	2.805944315
O	18.407654018	22.881506203	2.917029975
O	17.340129841	21.680570606	5.019356713
O	18.426584928	18.629547013	0.890986961
O	17.406738732	17.726012391	3.183938894
O	15.915052783	19.253982982	1.536904251
O	14.844900225	22.348577476	5.647772189
O	16.891378686	23.373219157	6.990452461
O	16.274560488	20.824886783	7.287661727
O	13.775781612	19.935781756	7.184865202
O	15.213479188	19.633077246	9.396730625
O	16.343524630	16.532698086	5.316187179
O	15.212900438	15.671824378	7.547131038
O	13.792253318	17.182177492	5.889258815
O	12.712759531	14.780414745	7.437170766
O	14.754213059	13.071836869	7.479945123
O	14.148879491	14.461984000	9.641312702
O	12.713746505	12.021028814	6.139421135
O	14.150192745	10.515865343	7.782764770
O	15.213683804	11.361848121	5.518979545
O	15.814428578	9.962111256	3.363478410
O	13.793061853	11.682978426	3.302207472
O	16.345789491	12.532667149	3.432114939
O	14.887275657	13.904202159	1.746982492
O	17.409017530	13.417155018	1.157383727
O	16.809325660	15.118152304	3.136883281
O	14.885152578	16.966219463	3.188071684
O	19.473426390	19.775695400	-1.215551987
O	16.982530237	18.925424444	-1.346014204

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Atom	x	y	z
O	19.473891673	15.493408442	-3.229097111
O	16.984105319	16.145829056	-2.654027349
O	18.427657071	14.604275151	-1.003725153
O	17.946693750	12.027650664	-1.007720289
O	15.916477125	13.714928135	-1.067330399
O	15.912403609	10.985974721	-2.374753871
O	18.408054677	10.330309361	-2.986560135
O	17.341890438	9.474740002	-0.724091480
O	14.844600848	8.574509268	-0.831625490
O	16.891073879	6.880006767	-0.768271830
O	16.274403319	8.273479176	1.383932348
O	13.776651536	8.928601557	2.007075825
O	15.214655028	7.409411930	3.644757640
O	12.711616873	6.531285772	3.545901968
O	14.744559239	4.818072070	3.615032018
O	14.144410807	6.226839794	5.760844131
O	11.645621215	6.879058501	6.375278367
O	13.682204122	7.923620971	7.727221945
O	13.079483143	5.366734356	8.022442520
O	11.647394110	9.626809396	7.664181746
O	13.078604398	9.323809603	9.884720264
O	10.588818044	9.976230217	10.459790026
O	12.032369795	8.434676312	12.110092222
O	12.619816061	11.024308812	11.832356735
O	13.078139114	13.606096561	11.898265388
O	10.587242962	12.755825605	11.767803171
O	12.031297652	12.459948174	14.004804335
O	11.647461401	15.132096610	10.252607440
O	13.681602084	16.163244075	11.600145915

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Atom	x	y	z
O	14.144331018	18.757776004	11.655207373
O	11.644719328	17.876922108	11.548269187
O	13.077810112	17.559598402	13.760104888
O	12.711864994	20.278625958	10.012648095
O	14.744863643	21.311284071	11.373757137
Mg	13.092951638	13.624722731	2.840866617
Mg	13.090187406	16.302861792	4.100099451
O	13.780880514	14.411254170	4.645003225
H	14.651352056	14.236038876	5.017388214
O	12.509957992	15.445683645	2.445501413
O	15.893390343	16.544208147	0.111810504
H	13.751994665	17.753853168	-2.460072135
O	14.622465291	17.578635331	-2.087688788
Mg	15.313161548	15.687029393	-1.542783895
Mg	15.310397720	18.365168843	-0.283551888
Mg	14.201387002	18.823358145	2.609019036
O	13.592373990	20.703680087	2.123031439
H	12.708089491	20.828019325	1.762987787
H	15.694055241	19.450421256	4.692779876
O	14.809822341	19.648448788	4.367241955
Mg	14.200524953	21.520569777	3.877363709
O	15.814483150	18.225767549	7.251941959
Mg	13.136544312	19.082407494	5.401716068
O	11.466038282	18.588234901	6.481657653
H	10.591534773	18.729029296	6.102867176
Mg	12.079039266	16.684825869	6.947661086
Mg	12.069330311	19.433232387	8.234553105
O	12.680989041	17.540922202	8.710500205
H	13.560723295	17.361990775	9.059548875

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Atom	x	y	z
Mg	11.003958839	17.029055123	9.772730180
Mg	12.076417627	13.935751036	5.654949871
Mg	11.005279789	11.536895638	7.190630971
Mg	11.002782697	14.283398392	8.480500731
O	10.397006179	13.431709616	6.726225668
H	9.528863571	13.608462902	6.348173222
H	12.479197193	12.211830520	9.322959770
O	11.611056711	12.388584804	8.944905205
Mg	9.931637647	11.884537084	10.016177950
Mg	12.078339163	11.187775564	4.361522738
Mg	12.071403071	8.443262157	3.066747991
O	11.467261264	10.333072478	2.599539383
H	10.592958221	10.534698317	2.248789308
H	13.561498707	9.129048913	5.187034581
O	12.681573008	9.283049956	4.826744690
Mg	14.202826638	10.469321844	-1.320049077
Mg	14.201962760	13.166534724	-0.051704710
O	13.593529655	12.341440507	-1.809929428
H	12.709295543	12.539469585	-2.135463589
H	15.695260378	11.161872593	0.794328561
O	14.810975368	11.286211487	0.434283290
Mg	15.266800256	12.907483222	-2.844408911
Mg	13.137795276	10.849465361	1.530118474
Mg	11.004101925	8.791237395	5.898402386
Mg	15.265553168	21.140425480	1.027195464
O	19.015102933	17.193907262	-1.281459812
O	13.649136703	18.918062334	-4.922627817
Mg	16.326924519	18.054135534	-3.097638598
O	18.006343583	18.558183253	-4.168911342

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Atom	x	y	z
H	18.874484064	18.381428970	-3.790856778
Mg	16.325011110	20.802114933	-1.804208070
O	16.936088094	21.656819096	-0.042224654
H	17.810391137	21.455193258	0.308525421
Mg	15.269315456	23.897336612	2.323383809
H	16.758642471	24.581280710	4.436316381
O	15.877707612	24.746570124	4.083497815
Mg	14.201827083	24.241551982	5.158019510
O	12.525946850	23.736539704	6.232540485
H	11.645009972	23.901823551	5.879724355
H	14.625785588	22.521901418	8.813904344
O	13.743885402	22.686223577	8.463160522
Mg	13.135596587	21.838281505	6.700761902
Mg	12.069854403	22.184193509	9.531485941
O	10.395213479	21.680985008	10.602010807
H	9.516853530	21.848844462	10.244034855
Mg	11.004672116	19.781493133	11.068121156
O	9.326488160	16.537242046	10.844386623
H	8.446563376	16.691244728	10.484097949
Mg	9.929723835	14.632516094	11.309609305
H	7.356707793	11.584254718	10.653744412
O	8.227178420	11.409036882	11.026127760
Mg	9.929021902	9.135466134	8.723470227
H	8.447338895	8.458301009	6.611585249
O	9.327073042	8.279371438	6.960632325
Mg	11.003389051	6.038800679	4.603011008
O	10.394909075	5.187773007	2.843285688
H	9.516548723	5.355632072	2.485310564
Mg	12.069549596	5.690981119	1.772761650

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Atom	x	y	z
O	13.743580595	6.193011188	0.704436230
H	14.625480780	6.028689029	1.055180052
O	12.525642042	7.243327315	-1.526183807
H	11.644705165	7.408612067	-1.878999511
Mg	13.134034306	8.092555352	0.233930092
Mg	14.201522275	7.748339592	-2.600704781
O	15.877402805	8.253357735	-3.675226476
H	16.758337663	8.088068321	-3.322407910
Mg	15.267749812	10.151616106	-4.143450608
O	16.937307121	13.401653306	-3.924342814
H	17.811810118	13.260862187	-3.545552253
Mg	16.324309177	15.305064973	-4.390347148
H	11.741348501	7.639885500	-4.548944550
H	9.621616791	5.578250459	-0.156380686
H	16.661666697	6.167869391	-1.446750056
H	14.509519701	4.104922330	2.939551549
$2V_H \text{Er}_{\text{Mg2}}^{3+}$			
Si	21.368744883	24.765294525	0.240527195
Si	21.339674059	22.032421800	1.586844571
Si	23.561609408	26.759685446	0.856234267
Si	19.138031478	25.468674169	-1.699098647
Si	23.588958230	21.339682371	3.608290288
Er	21.368065849	23.720509439	4.444889725
Si	19.123358284	20.050053844	1.047109752
Si	23.584771212	18.652771809	4.999062539
Si	25.771293370	23.371719388	4.177791908
Si	25.779866836	26.076074137	2.803937830
Si	27.993115869	22.668197092	6.146177361
Si	28.007887094	28.070310502	3.378059903

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Atom	x	y	z
Si	23.574336782	29.474147482	-0.530175402
Si	19.128359749	17.358447361	2.466036424
Si	16.885590863	20.768794892	-0.888309935
Si	21.351542061	16.662589043	4.428394071
H	17.455178616	15.627915219	1.876408692
H	21.425878538	14.376990608	5.373214672
Si	25.799491012	17.959202065	6.969573356
H	25.873650698	15.673872526	7.914002891
Si	28.016850559	19.966067949	7.546803177
H	29.953339297	19.353466029	8.967829817
Si	30.223909042	24.663642388	6.717956326
Si	30.235393294	27.376925205	5.336438030
H	32.163153766	24.028258601	8.125704910
H	32.177401944	28.883558291	5.665602513
Si	28.018014048	30.780500420	2.003360773
H	29.953092367	32.294613497	2.341448703
Si	25.795376367	31.477706719	0.045520290
Si	21.353191907	30.181382059	-2.492269921
Si	19.130593220	28.182172108	-3.072921373
H	17.454547863	28.714675649	-4.823097022
Si	16.897075115	23.482077708	-2.269828231
H	15.220322428	24.001744992	-4.020315709
H	15.202228129	19.047327431	-1.485694756
Si	16.966878367	23.729437152	4.895824270
Si	16.956971631	26.424500128	3.502685536
Si	19.146379289	23.001663603	6.882661933
Si	14.744223055	21.721521268	4.314119479
Si	19.175099671	28.404067268	4.085055083
Si	14.729106173	27.123450245	1.549599900

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Atom	x	y	z
Si	21.368030132	27.733389019	6.062004457
Si	19.163794474	31.115098145	2.694768424
Si	21.395190750	25.043774225	7.495578115
Si	23.599747705	29.718909754	6.628230770
Si	23.612303917	24.327291651	9.419993019
Si	19.152167667	20.302102551	8.246495444
Si	21.386979711	19.600428814	10.193176056
Si	16.937603243	18.298464660	7.655059646
H	16.862455385	16.195780169	8.956692813
Si	14.720594242	19.005013548	5.689374950
H	12.784666940	17.491967942	5.356319025
Si	12.512707668	22.422783341	2.361033529
Si	12.503264900	25.128208962	0.966858583
H	10.572583492	20.909568754	2.054239418
H	10.560057894	25.738561264	-0.447317643
Si	14.719241243	29.822378596	0.154733450
Si	16.942161786	31.818277669	0.734279125
H	12.783934729	30.432628849	-1.270469920
Si	21.386176087	33.118310122	3.270196237
Si	23.608190558	32.420535674	5.230626340
H	25.283077525	34.152859785	5.822287260
Si	25.841582238	29.023056212	8.573124364
Si	25.851025848	26.317630837	9.967299790
H	27.517285839	30.747351619	9.175530513
H	27.534749583	25.795603212	11.713228591
Si	23.608178182	21.602108658	10.775561757
H	25.282318430	21.068611348	12.523630244
H	21.312909220	17.497998911	11.495345609
O	21.572685337	23.161216709	0.449763696

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Atom	x	y	z
O	22.803071284	25.512672969	0.154420340
O	20.463754699	25.404355020	1.413175041
O	20.592770940	24.980399577	-1.183273616
O	22.747711651	21.549686940	2.235933480
O	20.374460512	22.613262057	2.751623636
O	20.586712144	20.743249177	0.935806458
O	23.812743945	19.739140657	3.818269385
O	25.026919642	22.080043015	3.531338101
O	22.767629330	21.890201717	4.894267501
O	24.928280317	23.977723057	5.425514191
O	26.044133008	24.498845894	3.052692643
O	27.219203608	22.874889423	4.742822634
O	24.957862846	26.745922018	4.030306090
O	27.242162572	26.801237256	2.735351078
O	25.030943555	26.331211431	1.391689588
O	22.692293472	27.430742582	2.048512209
O	23.778789621	27.888228225	-0.308797477
O	18.252777384	20.667905099	2.271420365
O	18.332147314	20.270985718	-0.351441073
O	20.587171653	16.910039434	3.017940429
O	18.365627520	16.064292563	1.848884035
O	18.251407925	17.979317214	3.682079505
O	22.811999345	17.365159104	4.380144100
O	20.474664395	17.283601056	5.645465141
O	21.546581585	15.067614555	4.646186929
O	25.036761583	18.190791825	5.558971757
O	22.706330612	19.267029670	6.220664704
O	24.922313365	18.578811470	8.186722422
O	26.003779263	16.366629594	7.190639772

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Atom	x	y	z
O	27.254606946	18.676513719	6.922289618
O	29.477514978	19.510467929	8.090879635
O	27.144201219	20.581560043	8.768718171
O	28.216574377	21.076738678	6.386346488
O	27.134604271	23.288531043	7.377673102
O	29.442955299	23.393812330	6.078361658
O	29.363045680	25.285101882	7.944598482
O	30.439555098	25.783280697	5.565224828
O	31.670465494	24.165833214	7.254825187
O	29.361507539	27.999207480	6.553828668
O	31.686358401	28.095183249	5.268814117
O	29.464927096	27.610732177	3.928042599
O	27.147811701	28.706318938	4.600495879
O	28.222865128	29.190234034	2.221124339
O	27.144010277	31.404921193	3.219648819
O	29.475506695	31.494684730	1.951415507
O	27.255109836	31.028592374	0.592810705
O	25.028667585	30.199321648	-0.587770352
O	24.921943372	32.105584573	1.260630405
O	26.004414984	32.590547919	-1.116485568
O	22.699923028	30.113210963	0.679248290
O	22.809992411	29.730029508	-1.943580170
O	20.584784729	28.900757333	-3.125673560
O	20.475645590	30.809118959	-1.280497965
O	18.252738170	28.806137193	-1.859320166
O	19.331864375	26.589139610	-2.862885450
O	18.363785064	28.435190865	-4.483573875
O	18.259780692	26.100560380	-0.489307315
O	18.348040221	24.200335753	-2.337452144

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Atom	x	y	z
O	17.101236918	21.888433201	-2.041041432
O	16.023189360	24.104359984	-1.052437593
O	16.126609759	23.715884927	-3.678223182
O	16.024727500	21.390254386	0.338332222
O	16.104637119	19.498964834	-1.527904603
O	17.809651359	23.076682299	3.671675033
O	16.697787251	25.302088621	4.640128036
O	17.707857554	23.493238628	6.323010161
O	15.517898670	22.981306121	4.966397561
O	17.777893867	25.826746950	2.238704725
O	17.705596023	27.719592785	4.120930080
O	15.492593489	26.899597507	2.956054027
O	20.044265081	27.834059728	2.841022969
O	19.933687717	28.240549085	5.506694999
O	18.960538194	30.009292333	3.852436982
O	21.163410492	26.626077778	7.240549423
O	22.146294701	29.012287353	6.721860279
O	22.272761172	27.160086331	4.855510299
O	22.148967086	24.821925487	8.922467028
O	22.359267087	24.438302250	6.343196463
O	19.985046513	24.238474225	7.515954494
O	18.921828800	21.895356063	8.058250177
O	19.970797956	22.287418714	5.682959086
O	19.925992097	20.048503579	9.651993155
O	17.701847381	19.575141448	8.295642132
O	20.030337946	19.677372004	7.029905217
O	17.814837316	17.679566643	6.437638960
O	16.732065797	17.187538600	8.817001116
O	15.482510903	18.756368589	7.100856994

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Atom	x	y	z
O	13.261404807	18.294089844	5.742869746
O	15.593237585	18.378370349	4.473090930
O	14.521966212	20.596035948	5.465472276
O	15.602853075	21.089602082	3.088639951
O	13.293084202	22.196326003	3.765345530
O	13.374150813	21.796175416	1.137354251
O	12.298870747	24.012531505	2.127272591
O	11.065293716	21.696864391	2.451104905
O	13.376884550	24.509399925	-0.252435377
O	13.273361703	26.406488410	1.601634562
O	11.050536364	25.598131214	0.424353322
O	15.590206287	26.509859204	0.316370461
O	14.513006238	28.716604186	1.317669804
O	15.593590348	29.206411485	-1.065730863
O	15.483685102	31.109334751	0.780505232
O	13.260962706	30.280591829	-0.393298868
O	17.707925425	31.582185590	2.141748764
O	17.816554986	31.205931734	-0.488262547
O	16.732700676	33.411455790	0.509875752
O	20.038469829	30.513202672	1.466570245
O	19.928837477	32.410154470	3.314594133
O	22.152109933	32.878906977	4.679918817
O	22.264313048	32.508799330	2.049626005
O	21.193965678	34.715690544	3.053255776
O	24.374479650	33.712720572	5.851051382
O	24.485926764	31.807154755	4.011563918
O	23.407444842	31.318615056	6.400171673
O	24.388854544	29.492978710	8.030619583
O	24.478676062	29.113171540	5.405573882

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Atom	x	y	z
O	25.637188084	27.907378755	9.733538372
O	26.715202730	28.404247421	7.353830884
O	26.611679883	30.301335906	9.207900823
O	26.712468993	25.691022913	8.743620512
O	24.403611054	25.591711642	10.057370685
O	26.631402381	26.091173500	11.371611791
O	23.413055271	23.197614610	10.571977653
O	24.484425035	23.699125397	8.201980835
O	24.371755754	21.345898596	12.185861988
O	22.151502483	20.887950022	10.819590582
O	24.485843861	20.984113049	9.558652781
O	22.263183021	18.982199826	8.974440035
O	21.193329957	18.491772218	11.360381116
O	19.959797491	25.182324755	4.113495660
O	22.778803766	24.843183312	3.452117186
Mg	21.369309116	26.247365087	3.151693812
Mg	23.625043899	25.585154307	5.057867291
Mg	21.368844726	28.952671521	1.769430150
Mg	19.110794478	24.317980735	2.575402532
Mg	23.623526525	22.835732306	6.534301689
H	21.761071981	22.043978185	8.286120498
O	22.285099184	21.666052771	7.571781402
H	25.433805780	20.953403407	6.116549372
O	24.922287404	21.292701071	6.858739052
Mg	23.595854916	20.132792334	7.886371707
Mg	21.368434909	20.813603753	5.940210200
Mg	19.112925676	21.513188180	3.949065759
O	17.814440334	20.346649597	5.011815918
H	17.302438193	20.750701740	5.720523378

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Atom	x	y	z
H	20.975726676	19.630694524	3.568018402
O	20.451930984	19.991861765	4.291205358
Mg	19.140692164	18.836551563	5.352830636
O	19.322132667	18.455405994	1.290210354
Mg	16.919957378	19.530235199	3.371179275
Mg	16.931336031	22.252145292	1.997601403
Mg	16.918591242	24.956459267	0.607286952
O	15.607642572	23.783434212	1.673756977
H	15.105828810	24.162340378	2.403632026
O	18.206862728	23.420100578	0.930963390
H	18.771342468	23.068754063	0.234777150
Mg	14.699970188	22.950681598	0.042114758
Mg	16.930697053	27.648635160	-0.765481761
Mg	19.150734218	29.650603450	-0.189650238
Mg	19.159718895	26.952797033	1.191548681
O	17.837789870	28.495719062	0.856079211
H	17.334382345	28.834957762	1.604154456
H	20.995611292	27.734419186	-0.576866753
O	20.459047471	28.129975986	0.118214266
O	22.279627677	29.809214017	3.402277355
H	21.743864124	30.143103549	4.129550287
Mg	23.589479123	30.948792390	2.348033306
Mg	23.577262282	28.251102252	3.730909569
H	25.405323448	29.017865442	1.961972262
O	24.901187753	29.426497637	2.673983237
Mg	25.819632544	27.557761103	5.690398534
Mg	25.805184395	24.851223715	7.074216319
O	24.529722744	26.396719440	6.747774970
H	23.965330876	26.756833759	7.439536171

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Atom	x	y	z
O	27.130439593	26.008598126	6.019239740
H	27.631803669	25.637254588	5.285131153
Mg	25.807443249	30.246323540	4.309903900
Mg	28.038288368	26.845529094	7.648381019
Mg	25.816863590	22.145954246	8.480017489
H	14.293485489	21.742407092	-2.321135108
O	13.792122256	22.113750876	-1.587026040
Mg	14.699757880	20.245955838	1.427460733
H	16.522070798	18.333380005	1.019957718
O	16.002742574	18.693775805	1.746739278
Mg	16.924850283	16.831326870	4.773581883
H	18.757682956	14.922071017	4.380875711
O	18.233663026	15.295465589	5.097624154
Mg	19.146801202	16.130192896	6.735439673
O	20.058019904	16.968502597	8.368570166
H	19.537902972	17.333364415	9.092598576
H	23.200036560	16.218979394	6.917456043
O	22.679659212	16.593681958	7.636175254
Mg	21.369487609	18.127440141	7.312429284
Mg	23.590999299	17.428161544	9.271670581
O	24.503719218	18.268688851	10.906639412
H	23.979453865	18.633143739	11.627850216
Mg	25.813515874	19.429686313	9.848450426
O	26.734653036	22.974716637	10.108134602
H	26.214981270	23.354576364	10.824702232
Mg	28.038076060	24.140803334	9.033726994
O	28.945960752	27.678281708	9.280023238
H	28.444146147	28.057187628	10.009897807
Mg	28.037779245	29.552972134	6.262777533

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Atom	x	y	z
O	26.726558032	31.091965215	5.938749727
H	26.204933768	31.448562532	6.665746298
Mg	25.812575511	32.951626070	2.924317412
O	24.504354939	34.492607177	2.599514072
H	23.980089586	34.857062065	3.320724875
Mg	23.591635020	33.652079870	0.964545241
H	23.200671439	32.442897474	-1.389669778
O	22.680294933	32.817600284	-0.670950086
Mg	21.369179232	31.652520981	0.388489027
O	20.058654783	33.192420676	0.061444346
H	19.538538693	33.557282741	0.785473236
O	21.547217306	31.291531990	-3.660937955
Mg	19.147436923	32.354111222	-1.571685667
O	18.234298747	31.519383914	-3.209501187
H	18.758318677	31.145989343	-3.926249629
Mg	16.924747093	30.354686248	-2.147908196
H	16.533610435	26.439293588	-3.118199742
O	16.011972332	26.821158070	-2.404242108
Mg	14.699461065	25.658124638	-1.343488728
H	21.567957501	35.463050468	2.486084496
H	17.094828409	34.159127643	-0.064537257
H	25.642192343	33.493537719	-1.387602111
H	21.174352434	32.189121212	-3.935538347
$2V_{\text{H}}\text{Er}_{\text{Mg1}}^{4+}$			
Si	7.306101940	-2.631620573	-15.760749503
Si	4.782056370	-2.203625980	-14.145932300
Er	4.773487964	-3.328453166	-11.037108144
Si	2.270371725	-3.821963547	-14.663642885
Si	4.781204643	-0.114082723	-11.827304252

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Atom	x	y	z
Si	7.304852546	1.450900117	-11.230972980
Si	2.271300981	0.235589636	-10.159966590
Si	7.307512017	-4.680340558	-18.005459393
Si	9.822265446	-1.027709042	-15.147713662
Si	12.339014918	-1.447100953	-16.803282480
Si	9.821681595	1.008418135	-12.888708865
Si	12.339412430	2.611556966	-12.299406165
Si	7.306557787	3.469740468	-8.959677782
Si	9.825691176	5.072384768	-8.375330658
Si	4.787514268	3.883015017	-7.298392632
Si	2.272915982	2.267819485	-7.887744619
H	4.680888457	5.669507968	-5.596396795
H	0.189253651	2.783627798	-6.647578379
Si	-0.234483477	-1.380215696	-10.742800275
Si	-0.233970762	-3.410769446	-12.995656011
H	-2.323139783	-0.868275484	-9.499014674
H	-2.323749135	-4.594181441	-13.633151326
Si	2.272157771	-5.869713333	-16.920931884
Si	4.786427127	-6.287057351	-18.589104419
H	0.188095442	-7.049145787	-17.562864941
Si	9.825207092	-5.093757787	-19.661352259
Si	12.336765740	-3.481352752	-19.063000818
H	14.332890144	-3.647769849	-20.523126451
Si	14.858775892	0.163760691	-16.215529931
H	16.844506154	-0.004366755	-17.685640809
Si	14.858263178	2.194314440	-13.962674195
H	16.844741695	3.639096038	-13.641065821
Si	12.337198659	4.647015694	-10.041221842
H	14.333200245	6.082167064	-9.721861064

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Atom	x	y	z
H	9.726099734	6.861821727	-6.668993308
Si	7.274060250	-8.924726525	-14.186471032
Si	7.275675251	-6.892497345	-11.914249804
Si	9.781460662	-5.276690449	-11.331414835
Si	4.765771589	-6.542823648	-10.246910656
Si	12.300310760	-5.693935248	-12.994683510
Si	9.780947298	-3.246137633	-9.078558259
Si	12.300707319	-1.635276215	-8.490805506
Si	7.276604508	-2.834942824	-7.410572022
Si	4.764918910	-4.453280617	-7.928282405
Si	7.274817509	-0.787193934	-5.153283564
Si	2.240873340	-4.025286024	-6.313465201
Si	2.242123990	-8.107807866	-10.843242033
Si	2.240416236	-10.126647921	-13.114538843
Si	-0.274705363	-7.665325176	-9.185506786
Si	4.759461012	-10.539922283	-14.775822815
H	0.240729347	-11.556132962	-13.428465974
Si	9.790277779	-9.342349012	-15.847749435
Si	12.302522971	-7.729391447	-15.252867419
H	14.384451543	-8.248446801	-16.494973249
Si	14.818041291	-4.090795040	-12.405380705
H	16.900758990	-4.625428567	-13.643498518
Si	14.817457745	-2.054667901	-10.146374527
H	16.900029856	-0.878411307	-9.486089962
Si	12.302957147	0.398975848	-6.231088752
H	14.385165922	1.579551484	-5.584631778
Si	9.791196296	0.821636455	-4.564541128
H	9.896911128	2.336389487	-2.607893475
Si	4.760549106	-0.369848351	-3.485109745

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Atom	x	y	z
H	4.866561223	1.137710737	-1.531547958
Si	2.239465472	-1.976566965	-4.068755823
H	0.240736132	-1.814455722	-2.613671006
Si	-0.275287957	-5.629197811	-6.926500811
H	-2.275962765	-5.466520481	-5.475947362
H	-2.275622009	-9.091740665	-9.499041892
O	5.927170142	-1.931210581	-15.257641859
O	5.301167154	-3.420577073	-13.190816059
O	3.396205870	-2.660613492	-14.839203160
O	4.572359465	-0.868403376	-13.248225838
O	5.926059746	1.021014867	-11.979305596
O	5.299446406	-1.194656489	-10.719539534
O	3.396529888	0.529475744	-11.298044804
O	7.037288941	-3.291972359	-17.214860681
O	8.456619396	-1.496849695	-15.886124292
O	7.790625363	-3.784800170	-14.722202278
O	10.312983447	-2.181158118	-14.115428363
O	10.970929682	-0.766566430	-16.259801797
O	9.535772851	0.350406658	-14.342811073
O	10.312335308	-0.143354917	-11.854588771
O	10.969494832	2.143116716	-13.030381811
O	8.456848338	1.695441669	-12.344506791
O	7.789916309	0.293829873	-10.196657281
O	7.034225324	2.828458123	-10.423152164
O	8.447143307	4.612839039	-9.092991424
O	7.800578818	2.313435137	-7.932255638
O	5.933956888	4.138936451	-8.415532602
O	5.284004712	2.738783488	-6.258581372
O	3.418915967	3.407553130	-8.024347474

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Atom	x	y	z
O	4.505065057	5.267942149	-6.506303947
O	2.004925304	1.614818412	-9.344890404
O	2.763549773	1.118031303	-6.850668214
O	0.903553760	2.945766981	-7.342982032
O	0.886403615	-0.220500651	-10.856609568
O	2.777269816	-0.909244731	-9.118267765
O	0.249832749	-2.536120570	-9.704117131
O	-0.523079734	-2.034518998	-12.194653279
O	-1.608833112	-0.711036870	-10.195536029
O	0.250966793	-4.569778230	-11.960728691
O	0.887358430	-3.173762929	-14.135955333
O	-1.609863241	-3.884500923	-13.715737594
O	2.776842383	-4.982188089	-13.639092764
O	3.419995922	-5.611812660	-18.037691879
O	2.763337414	-7.026275244	-15.891625868
O	0.901974007	-6.340088126	-17.650697897
O	5.282701013	-7.446250588	-17.565732268
O	4.504346671	-6.931307277	-20.048909700
O	5.932550385	-5.148762364	-18.725073533
O	8.447780382	-4.426744226	-19.128371656
O	7.801219415	-5.827837374	-16.968233027
O	12.828943935	-4.635965655	-18.032478719
O	12.059523635	-2.101048830	-18.260369473
O	13.481474808	-3.224664361	-20.182283861
O	10.964461080	-3.947918687	-19.788994603
O	12.827875181	-2.604865913	-15.773953338
O	13.482882460	-0.309971012	-16.935611310
O	15.343713447	-0.995248094	-15.180602611
O	15.980104131	0.400766982	-17.355829049

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Atom	x	y	z
O	14.569666920	1.540011138	-15.414527198
O	15.342579403	1.038409566	-12.923991050
O	15.979150269	3.354029485	-14.076483487
O	13.483912589	2.863493041	-13.415409744
O	12.828281577	1.461848453	-11.261244062
O	12.061072597	3.993378493	-11.498316817
O	12.828926589	3.496369288	-9.005947044
O	13.480648213	5.788531113	-10.176869813
O	10.965769865	5.321018002	-9.500031965
O	10.315320373	3.920189389	-7.341158537
O	9.560815534	6.458374304	-7.580042873
O	7.542051881	-8.271725227	-12.729325450
O	6.769706720	-5.747663018	-12.955947248
O	8.660573570	-6.436404825	-11.217604800
O	6.150445088	-7.186380963	-10.776169796
O	11.155808088	-5.945869019	-11.878679314
O	9.297144436	-4.120786245	-12.370098723
O	10.070054710	-4.622386891	-9.879562063
O	11.156837913	-2.772404258	-8.358478386
O	9.296008791	-2.087128405	-10.113484632
O	8.659616546	-3.483143630	-7.938260752
O	6.150769106	-3.996293066	-7.235012925
O	6.770134153	-1.674719659	-8.435122249
O	7.545124818	-2.167670416	-5.954390703
O	4.245809078	-3.236328629	-8.883398105
O	4.974616767	-5.788502326	-8.825988327
O	3.619804834	-4.725696646	-6.816574969
O	4.247529177	-5.462251485	-11.354675276
O	3.620916182	-7.677920531	-10.094909950

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Atom	x	y	z
O	2.512750604	-9.485365125	-11.651064868
O	1.757059275	-6.950737848	-11.877557529
O	1.090127591	-8.352347332	-9.729708755
O	1.746395508	-8.970341959	-14.141958863
O	3.613019041	-10.795842783	-13.658683686
O	1.099831972	-11.269746305	-12.981224024
O	4.262971216	-9.395689820	-15.815634916
O	5.041909269	-11.924848971	-15.567910554
O	6.128059962	-10.064460132	-14.049869558
O	6.783427716	-7.774938157	-15.223546260
O	8.643420263	-9.602673765	-14.731233849
O	10.314458254	-6.246815425	-18.627838144
O	9.560096195	-5.740875347	-21.122648423
O	9.298086780	-8.190631479	-16.881683584
O	10.071156753	-10.722720124	-16.650627118
O	11.159074370	-8.870907979	-15.117221138
O	13.673951764	-8.403395093	-15.794058782
O	11.810796297	-6.578745523	-16.288141783
O	12.578651242	-7.075755172	-13.795772956
O	13.670227750	-5.225491574	-12.263706911
O	11.811441613	-4.544226065	-14.032844870
O	14.327387882	-2.939023364	-13.439500904
O	16.182874245	-4.777817196	-12.949582674
O	15.103950035	-3.432782893	-10.951277754
O	14.326737534	-0.901218568	-11.178660058
O	16.183102234	-1.585526058	-9.407964969
O	13.668791644	-2.315809284	-9.034288845
O	11.811847402	-0.477510953	-9.520137612
O	12.580199251	-0.981327405	-7.033719354

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Atom	x	y	z
O	13.675260550	0.865542934	-5.505094658
O	11.810779255	1.553588712	-7.261609470
O	11.158247775	0.142290173	-5.111804118
O	9.299205329	1.975380800	-5.596458489
O	10.071876092	1.476529527	-3.108021569
O	8.645001922	-0.316817537	-4.423517648
O	6.783637865	0.369367978	-6.182589579
O	6.126979703	-1.045091626	-4.036523562
O	4.264276476	0.789343065	-4.508482948
O	5.042628609	0.274400680	-2.025305004
O	3.614426497	-1.508142405	-3.349141473
O	2.509686338	-3.364934908	-4.859354766
O	1.745756818	-0.829069667	-5.105982623
O	1.099194594	-2.230160994	-2.945842943
O	1.090355580	-5.160056194	-6.188091050
O	1.756351174	-2.872106909	-7.352011992
O	-0.766009120	-4.475748704	-7.958786139
O	0.011203381	-7.007313029	-7.731403835
O	-1.423955010	-5.890339421	-5.814414926
O	-0.765357819	-6.513553275	-10.219627188
O	-1.422518904	-8.800021710	-9.043832992
Mg	2.224485552	-4.965342177	-11.624223082
Mg	2.223430177	-2.913430553	-9.350422028
Mg	-0.260620144	-6.563096827	-12.218622054
Mg	7.323546055	-3.743476488	-12.723793623
Mg	7.322490681	-1.691564195	-10.449991825
Mg	12.320063158	-2.558747524	-13.774023871
Mg	12.319657823	-0.523629832	-11.520065292
Mg	9.807597025	-0.093809280	-9.855594438

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Atom	x	y	z
Mg	9.806181297	1.932915538	-7.598514437
Mg	9.806423965	-6.202616653	-16.626245468
Mg	9.807492807	-4.166123021	-14.377083488
Mg	4.773356741	-7.419667986	-15.578275092
Mg	4.773310862	-5.429611265	-13.369915572
Mg	4.773665371	-1.227295775	-8.704300079
Mg	4.773619491	0.762760945	-6.495940559
Mg	12.319739846	-4.591667953	-16.032751727
Mg	12.319982737	1.509292426	-9.261337737
Mg	7.291858902	0.327302522	-8.183624787
Mg	7.292065790	-5.786581527	-14.969393148
O	2.001851415	-4.489235955	-16.119824205
Mg	2.255116074	-6.984209081	-13.890591298
Mg	2.254910442	-0.870324844	-7.104821759
Mg	-0.261180074	-4.526221242	-9.958880921
Mg	9.808155354	-2.130686024	-12.115334526
Mg	14.831566580	-0.951691105	-13.178754840
H	7.562740200	-1.062727913	-13.077535651
O	7.815052210	-1.753248781	-12.454790390
O	6.771548482	-3.627500466	-10.767202660
O	2.775427446	-3.029406536	-11.307014372
O	1.731923070	-4.903658485	-9.619425057
H	1.984235080	-5.594179353	-8.996679796
O	4.248477670	-1.192876776	-6.755766986
H	4.545362134	-1.880272490	-6.150037253
H	5.001274634	1.381871748	-9.086857276
O	5.298092958	0.708321821	-8.465751857
O	9.282676071	-0.028624663	-7.880310507
H	9.569243894	-0.718909409	-7.272220642

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Atom	x	y	z
H	10.038447543	2.547878310	-10.192971886
O	10.324963416	1.864672666	-9.577192899
O	11.800724701	-2.484347716	-11.797075882
H	12.079723042	-3.168935644	-11.179193083
H	12.559998891	0.086557845	-14.114897027
O	12.838996929	-0.598029375	-13.497014865
O	9.282820861	-6.125634361	-14.647548393
H	9.569365901	-6.801755728	-14.023733668
H	10.038423130	-3.557107206	-16.968489526
O	10.324698864	-4.240080923	-16.352333994
H	5.001614098	-4.776633882	-15.924177655
O	5.298499211	-5.464028661	-15.318448763
H	4.545701598	-8.038778119	-12.987357632
O	4.248883274	-7.365228862	-13.608463794
O	0.264299858	-6.628281001	-14.193905039
H	-0.022267662	-5.937996962	-14.801994265
H	-2.532747763	-3.487972292	-10.895023108
O	-2.253748773	-4.172559285	-10.277141150
Mg	-0.260516879	-2.490783311	-7.697132800
H	-0.022390622	0.144849131	-8.050481036
O	0.264156973	-0.531272189	-7.426669045
Mg	2.254699793	1.159403401	-4.851058225
H	2.481984312	3.802137170	-5.194528759
O	2.775583165	3.120839092	-4.579945870
Mg	4.773847158	2.771171881	-4.265804896
O	6.772111454	2.421503963	-3.951663284
H	7.065709658	1.740204282	-3.337080297
H	7.522001522	4.997326851	-6.271498006
O	7.813343204	4.315506754	-5.656483922

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Atom	x	y	z
Mg	7.293353661	2.355365733	-5.928930729
Mg	9.807729507	3.963962989	-5.340256891
O	11.801740709	3.612624709	-5.024408763
H	12.089826367	2.930052902	-4.408631416
Mg	12.320322764	3.541811415	-7.002942748
O	14.315023719	1.157705396	-8.941755471
H	14.601298803	0.474730745	-8.325599097
Mg	14.832229775	1.083746825	-10.917006719
H	17.076981734	-2.019649217	-12.216553715
O	16.824668771	-1.329128574	-12.839298773
Mg	14.832125558	-2.988566917	-15.438495770
H	14.601274390	-5.630254771	-15.101116737
O	14.314757261	-4.947049314	-15.716896902
Mg	12.319398217	-6.624187432	-18.291144929
O	11.801022322	-8.586624717	-18.567014516
H	12.089107981	-9.269196524	-17.951237169
Mg	9.807010168	-8.235286662	-18.882862441
O	7.812623864	-7.883742898	-19.199089472
H	7.521282183	-7.201922800	-19.814103556
O	6.771392114	-9.777745689	-17.494268834
H	7.064991272	-10.459045144	-16.879686050
Mg	7.292274534	-7.816309554	-17.223155533
Mg	4.773127818	-9.428077770	-17.808410446
H	2.481264972	-8.397111812	-18.737133566
O	2.774863826	-9.078409890	-18.122550677
Mg	2.253621619	-9.012272330	-16.145283975
H	5.133215132	-12.265769839	-16.514238299
H	10.167713013	-11.055707643	-17.599255708
H	4.397957192	-7.837405895	-20.482230105

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Atom	x	y	z
H	9.460755172	-6.647931006	-21.555639638
2V_HEr_{Mg2}⁴⁺			
Mg1	0.002424	0.001968	0.495991
Mg2	0.004188	0.505687	0.496741
Mg3	0.335529	0.002100	0.496074
Mg4	0.335492	0.502670	0.496093
Mg5	0.668609	0.002024	0.496181
Mg6	0.666932	0.505734	0.495681
Mg7	0.170431	0.251757	0.496993
Mg8	0.168927	0.752503	0.496322
Mg9	0.500703	0.251775	0.495433
Mg10	0.502097	0.752510	0.495775
Mg11	0.835530	0.248191	0.496310
Mg12	0.835540	0.753931	0.496045
Mg13	0.169154	0.085267	0.496164
Mg14	0.169434	0.586463	0.496172
Mg15	0.501965	0.085301	0.496069
Mg16	0.501604	0.586485	0.495984
Mg17	0.835534	0.084563	0.496164
Mg18	0.835603	0.590850	0.496096
Mg19	0.169043	0.419462	0.496664
Mg20	0.168980	0.918887	0.496119
Mg21	0.501971	0.419525	0.495754
Mg22	0.502027	0.918920	0.496098
Mg23	0.835518	0.919089	0.496128
Mg24	0.335550	0.335907	0.496124
Mg25	0.335520	0.835624	0.496016
Mg26	0.664206	0.333562	0.496017
Mg27	0.668675	0.835968	0.496073

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Atom	x	y	z
Mg28	0.006798	0.333514	0.496567
Mg29	0.002368	0.835927	0.495979
Mg30	0.002910	0.168101	0.495918
Mg31	0.002299	0.670135	0.496568
Mg32	0.335542	0.168621	0.496194
Mg33	0.335480	0.669377	0.496134
Mg34	0.668197	0.168158	0.496683
Mg35	0.668777	0.670156	0.495782
Si1	0.284426	0.086138	0.644606
Si2	0.284737	0.586724	0.644535
Si3	0.616854	0.086005	0.644702
Si4	0.618469	0.587060	0.644436
Si5	0.951314	0.086052	0.644569
Si6	0.950926	0.587092	0.646022
Si7	0.051750	0.418772	0.347798
Si8	0.054154	0.918082	0.347543
Si9	0.385298	0.418641	0.347558
Si10	0.387014	0.918183	0.347591
Si11	0.716558	0.417757	0.344536
Si12	0.720207	0.918244	0.347680
Si13	0.119765	0.336015	0.646235
Si14	0.117620	0.836403	0.644616
Si15	0.452403	0.336801	0.644073
Si16	0.450639	0.836234	0.644409
Si17	0.784092	0.334522	0.647381
Si18	0.784080	0.836901	0.644633
Si19	0.220833	0.168383	0.347986
Si20	0.219673	0.668257	0.347727
Si21	0.553490	0.167802	0.347494

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Atom	x	y	z
Si22	0.553457	0.668330	0.347068
Si23	0.887385	0.166649	0.346876
Si24	0.886576	0.668734	0.347362
Si25	0.117990	0.169120	0.644903
Si26	0.117832	0.669630	0.645147
Si27	0.450577	0.169798	0.644314
Si28	0.451384	0.669660	0.644441
Si29	0.784073	0.168226	0.645650
Si30	0.784667	0.670122	0.644778
Si31	0.218799	0.335358	0.348245
Si32	0.220564	0.834895	0.347700
Si33	0.551173	0.334630	0.346198
Si34	0.553686	0.835149	0.347510
Si35	0.887046	0.332713	0.345195
Si36	0.887166	0.835573	0.347445
Si37	0.285807	0.419894	0.644685
Si38	0.284251	0.919475	0.644515
Si39	0.619344	0.420434	0.644629
Si40	0.617074	0.919429	0.644539
Si41	0.954426	0.419345	0.647964
Si42	0.951094	0.919473	0.644470
Si43	0.054545	0.084613	0.347653
Si44	0.052666	0.585429	0.347833
Si45	0.387040	0.084793	0.347665
Si46	0.386505	0.585455	0.347646
Si47	0.720097	0.084762	0.347778
Si48	0.720338	0.585623	0.346393
O1	0.115425	0.169035	0.556151
O2	0.115212	0.669581	0.556360

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Atom	x	y	z
O3	0.447939	0.168953	0.555572
O4	0.448271	0.669588	0.555660
O5	0.781542	0.168104	0.556759
O6	0.781616	0.671759	0.555997
O7	0.222161	0.335537	0.437046
O8	0.222942	0.835503	0.436433
O9	0.554478	0.335022	0.435088
O10	0.555929	0.835661	0.436248
O11	0.893421	0.329306	0.434396
O12	0.889675	0.836367	0.436228
O13	0.282242	0.419342	0.555967
O14	0.281667	0.919256	0.555779
O15	0.616446	0.419359	0.555681
O16	0.614699	0.919348	0.555796
O17	0.957282	0.417894	0.558950
O18	0.948498	0.919486	0.555740
O19	0.056473	0.085046	0.436395
O20	0.056701	0.586655	0.436639
O21	0.389445	0.085242	0.436385
O22	0.388973	0.585730	0.436388
O23	0.722693	0.085452	0.436566
O24	0.721261	0.587505	0.434873
O25	0.281704	0.085810	0.555866
O26	0.282112	0.586248	0.555795
O27	0.614665	0.085617	0.555932
O28	0.614318	0.587317	0.555631
O29	0.948421	0.085911	0.555775
O30	0.949987	0.588142	0.557519
O31	0.054587	0.418644	0.436759

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Atom	x	y	z
O32	0.056420	0.918764	0.436292
O33	0.388840	0.418852	0.436284
O34	0.389445	0.918735	0.436329
O35	0.713496	0.417305	0.433533
O36	0.722659	0.919006	0.436407
O37	0.116555	0.335606	0.557331
O38	0.115166	0.836152	0.555868
O39	0.448983	0.336204	0.555270
O40	0.448117	0.836039	0.555663
O41	0.777787	0.330213	0.558155
O42	0.781447	0.836874	0.555858
O43	0.223192	0.168423	0.436741
O44	0.222760	0.669035	0.436515
O45	0.555843	0.168530	0.436248
O46	0.555952	0.669081	0.435850
O47	0.889665	0.167511	0.435725
O48	0.889548	0.671187	0.436172
O49	0.114981	0.002642	0.553693
O50	0.116487	0.503410	0.553995
O51	0.448095	0.002612	0.553712
O52	0.448430	0.502846	0.553551
O53	0.781343	0.002551	0.553772
O54	0.780228	0.508808	0.550972
O55	0.222492	0.502098	0.438711
O56	0.222910	0.001911	0.438517
O57	0.554654	0.502713	0.438382
O58	0.556021	0.002026	0.438562
O59	0.890967	0.508072	0.441445
O60	0.889627	0.001906	0.438501

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Atom	x	y	z
O61	0.282603	0.252607	0.554142
O62	0.281628	0.752890	0.553772
O63	0.612868	0.251374	0.553713
O64	0.614480	0.753301	0.553442
O65	0.948301	0.252299	0.553392
O66	0.948274	0.753817	0.553885
O67	0.058239	0.250628	0.438949
O68	0.056514	0.752583	0.438730
O69	0.388502	0.251908	0.438302
O70	0.389330	0.752165	0.438421
O71	0.722729	0.251719	0.439271
O72	0.722744	0.753107	0.438356
O73	0.126853	0.252505	0.675493
O74	0.126076	0.753399	0.675007
O75	0.459140	0.253454	0.674097
O76	0.458832	0.753222	0.674665
O77	0.791762	0.251459	0.677420
O78	0.792173	0.754018	0.675010
O79	0.212467	0.251608	0.318093
O80	0.212340	0.751427	0.317480
O81	0.544268	0.250718	0.316896
O82	0.545484	0.751678	0.317158
O83	0.879402	0.249359	0.314961
O84	0.879251	0.752234	0.317133
O85	0.293278	0.003052	0.674692
O86	0.292423	0.503508	0.674711
O87	0.624151	0.002988	0.674953
O88	0.624890	0.503856	0.674594
O89	0.960358	0.003045	0.674640

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Atom	x	y	z
O90	0.958990	0.503403	0.676169
O91	0.046461	0.501784	0.317702
O92	0.047058	0.001251	0.317256
O93	0.379140	0.501815	0.317429
O94	0.378037	0.001339	0.317426
O95	0.712549	0.501463	0.316327
O96	0.710854	0.001397	0.317551
O97	0.198095	0.121769	0.674821
O98	0.199088	0.623353	0.674695
O99	0.531219	0.123162	0.674442
O100	0.532184	0.623372	0.674387
O101	0.865049	0.121693	0.674966
O102	0.866068	0.625186	0.675711
O103	0.137125	0.380554	0.318422
O104	0.140040	0.881661	0.317537
O105	0.469765	0.380352	0.316751
O106	0.473344	0.882455	0.317529
O107	0.803178	0.377962	0.320086
O108	0.806640	0.882812	0.317667
O109	0.035011	0.373084	0.678465
O110	0.031346	0.872365	0.674543
O111	0.367241	0.374171	0.674406
O112	0.364595	0.872445	0.674512
O113	0.699525	0.373537	0.676035
O114	0.698127	0.873461	0.674610
O115	0.307005	0.132448	0.317805
O116	0.305439	0.631537	0.317650
O117	0.640332	0.132690	0.317819
O118	0.638315	0.630943	0.316102

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Atom	x	y	z
O119	0.973550	0.130664	0.317313
O120	0.972800	0.632726	0.317617
O121	0.031328	0.134037	0.674532
O122	0.032855	0.632962	0.676249
O123	0.364539	0.134078	0.674518
O124	0.365618	0.633421	0.674547
O125	0.697962	0.132357	0.675082
O126	0.698325	0.634765	0.674567
O127	0.303528	0.372950	0.317793
O128	0.306625	0.870734	0.317627
O129	0.635705	0.371576	0.313859
O130	0.639897	0.870810	0.317572
O131	0.971340	0.371670	0.316381
O132	0.973035	0.871813	0.317388
O133	0.201091	0.382394	0.675500
O134	0.197943	0.884138	0.674563
O135	0.533794	0.382778	0.673918
O136	0.531238	0.883328	0.674520
O137	0.867682	0.380312	0.672805
O138	0.864651	0.884456	0.674450
O139	0.140200	0.121308	0.317854
O140	0.138819	0.621559	0.317844
O141	0.473556	0.119787	0.317555
O142	0.472015	0.621905	0.317450
O143	0.806538	0.119622	0.317468
O144	0.804918	0.623643	0.316484
H1	0.116375	0.002458	0.606320
H2	0.117324	0.504288	0.606608
H3	0.449366	0.002528	0.606337

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Atom	x	y	z
H4	0.450317	0.503463	0.606189
H5	0.782951	0.002220	0.606397
H6	0.220689	0.501986	0.386086
H7	0.221718	0.001245	0.385890
H8	0.553919	0.502901	0.385774
H9	0.554692	0.001238	0.385939
H10	0.888118	0.000964	0.385883
H11	0.284271	0.252896	0.606775
H12	0.283049	0.752920	0.606405
H13	0.613771	0.252434	0.606322
H14	0.616390	0.752622	0.606060
H15	0.950414	0.251617	0.606034
H16	0.949193	0.753552	0.606506
H17	0.057352	0.251049	0.386340
H18	0.054580	0.751123	0.386122
H19	0.387013	0.251518	0.385678
H20	0.387947	0.751548	0.385800
H21	0.720658	0.250335	0.386630
H22	0.721856	0.752122	0.385740
Er1	0.835438	0.422645	0.496061

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