Phase transitions and amorphization of $M_2\text{AgF}_4$ (M = Na, K, Rb) compounds at high pressure

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Abstract

We report the results of Raman spectroscopy high-pressure studies of alkali metal fluoroargentates ($M_2\text{AgF}_4$, where $M$=Na, K, Rb) associated with theoretical and x-ray diffraction studies for the K member of the series. Theoretical density functional calculations predict two structural phase transitions for $K_2\text{AgF}_4$: one from low pressure monoclinic $P2_1/c$ (beta) phase to intermediate-pressure tetragonal $I\overline{4}d$2 structure at 6 GPa, and another to high-pressure triclinic $P\overline{1}$ phase at 58 GPa. However, Raman spectroscopy and X-ray diffraction data indicate that both polymorphic forms of $K_2\text{AgF}_4$ as well as two other fluoroargentate phases studied undergo amorphization at pressure as low as several GPa.

Keywords

double perovskite, post-perovskite, silver(II) fluorides, phase transitions, high pressure

1. Introduction

Alkaline metal fluoroargentate $M_2\text{AgF}_4$ family ($M$=Na, K, Rb) [1] are a group of compounds analogous in many properties to important $\text{La}_2\text{CuO}_4$ oxocuprate, [2,3] which is a precursor of the first known oxocuprate superconductor [4]. Specifically, [AgF$_2$] layers are isoelectronic with [CuO$_2$] planes, both hosting formally one hole in the d$^{10}$ set of the transition metal [5–7]. Ambient-pressure crystal structures and magnetic properties of these compounds have been recently explored in thorough experimental and computational studies [8,9].

At ambient pressure, double fluoroargentates crystallize in different space groups depending on the alkali metal cation embedded in the structure. $\text{Na}_2\text{AgF}_4$ adopts a monoclinic $P2_1/c$ post-perovskite structure [10], while $\text{Rb}_2\text{AgF}_4$ adopts an orthorhombic layered double-perovskite structure [11]. Under ambient pressure and room temperature, $K_2\text{AgF}_4$ can – depending on the route of synthesis – adopt either the lower-enthalpy $P2_1/c$ structure ($\beta$-$K_2\text{AgF}_4$ polymorph [12]), or the higher-enthalpy metastable orthorhombic $Cmce$ structure (disordered $\alpha$-$K_2\text{AgF}_4$) [1]. The effect of high-pressure on double fluoroargentates, or an effect of chemical pressure from the smaller alkaline metal cations (Na, K), have been predicted to lead to structural phase transition to more closely-packed $\beta$ structure [12].

The purpose of this study is to determine the behavior of $\text{Na}_2\text{AgF}_4$ and isostructural $\beta$-$K_2\text{AgF}_4$, as well as $\alpha$-$K_2\text{AgF}_4$ and isostructural $\text{Rb}_2\text{AgF}_4$, at high external pressure, using a combination of theoretical and experimental methods.

2. Experimental methods

2.1. Synthesis

Powder samples of K and Rb fluoroargentates were prepared at high temperature using anhydrous alkaline metal fluorides and silver difluoride as described in the literature [1]. Platinum boats enclosed in nickel reactors were used to handle reactive specimen. The solid substrates were loaded in argon-filled glove box, with residual water content lower than 2 ppm. AgF$_2$, which was used as a substrate in
all syntheses, was prepared using a previously described method [13]. β-K₂AgF₄ polymorph was obtained via thermal annealing of the α-form at 180°C for 6 hrs [12].

Sodium analogue was obtained using a somewhat similar synthetic pathway as the one reported for high-purity KAgF₃ [14] i.e. via a trivalent silver intermediate.

$$2 \text{MF} + \text{AgF}_2 \xrightarrow{T} M_2\text{AgF}_4 \quad (M= K, T=480 °C; M=Rb, T=400 °C)$$

$$2 \text{NaF} + \text{AgF}_2 \xrightarrow{\text{aHF, KrF}_2} \text{NaF} + \text{NaAgF}_4 \xrightarrow{400 °C−550 °C, vacuum} \text{Na}_2\text{AgF}_4$$

$$\alpha-\text{K}_2\text{AgF}_4 \xrightarrow{180 °C, 6 hours} \beta-\text{K}_2\text{AgF}_4$$

2.2. Instrumental methods

All Raman spectra were measured using T64000 spectrometer with LN2-cooled CCD detector. A SpectraPhysics Ar,Kr gas laser was used to provide a 514.5 nm excitation line. A confocal microscope with 200 µm aperture was used in all experiments. 300 1/mm diffraction grating was used in every experiment. Laser power lower than 5 mW was used. Rayleigh-scattered light was cut off using low-pass edge filter.

Pressure was determined in all cases using Ruby2020 gauge [15], and in the XRD experiments additionally crosschecked with pressure calculated using position of (111) reflection of gold [16]. Very decent agreement was observed and ruby scale was consistently applied. IIAS diamond anvil pair with 250 µm or 300 µm culets were used. Stainless steel 250 µm thick gaskets were indented by compression up to about 20 GPa, after which 100 µm diameter holes were drilled using tungsten carbide drills. Thin slices of FEP (fluorinated ethylene-propylene) foil were used as pressure medium in all measurements, except for Na₂AgF₄, where tightly pressed dry NaF powder (Sigma Aldrich) was used for this purpose. All samples were loaded in argon-filled glove box, with residual water content lower than 1 ppm. Raman measurements were conducted for samples enclosed in Almax Diacell SymmDAC60, whereas XRD diffraction patterns were obtained for samples enclosed in Almax One20DAC.

Laser heating of the samples was not used, since they tend to decompose with elimination of F₂; moreover, when laser heated, samples are extremely reactive with respect to diamond and gasket.

XRD diffraction patterns were collected at 293 K using SuperNova Single Source Rigaku Oxford diffractometer with laboratory source, an Ag lamp (λ = 0.56087 Å). Due to small intensity of signals from the sample, the scans were conducted for 2θ<45°.

3. Computational methods

Computational exploration of structures of K₂AgF₄ at high pressure was conducted using the following method. First, candidates for high-pressure polymorphs in the 0-100 GPa range were selected by learning algorithms implemented in XtalOpt r11.0 [17,18] and additionally by modifying the proposed high-pressure structures of Ag₃F₄ [19] via substitution of Ag(I) with K(I); such substitution is justified because Pauling ionic radii of silver and potassium cations are quite similar (Ag(I): 1.26 Å, K(I): 1.33 Å). DFT (PBE) geometry optimization with cut-off energy of 950 eV and self-consistent-field convergence criterion of 10⁻⁶ eV per atom was then carried out, yielding a set of candidate structures. (VASP software was utilized for this purpose [20–24].) Further optimization of geometry using DFT+U method (U = 5.5 eV, J = 1 eV) [25] with PBE functional adapted for solids (PBEsol [26]) was carried out for a range of different ferromagnetic and antiferromagnetic models. Finally, one minimum-enthalpy structure was selected for each external pressure point. This structure was then used for additional
single point calculations for several different magnetic models, to estimate the strength of magnetic superexchange using DFT+U method (cf. ESI). A typical density of the k-point grid was 0.04 Å⁻¹.

Since learning algorithms produce P1 structures, symmetry-recognition routines were applied. Space groups for unit cells presented in Supplemental Material (SM) were determined with accuracy of 0.05 Å.

4. Results

4.1. Computational results

We begin by discussing theoretical results obtained for K₂AgF₄. Potassium compound was selected for the theoretical study because it is the only fluoroargentate(II) which exhibits polymorphism in the absence of external pressure. Therefore, it may be used to validate accuracy of computational approach and conclusions from its study may be qualitatively applied to systems with smaller (Na) or larger (Rb) alkali metal cations.

Learning algorithms, used for structure prediction of K₂AgF₄ at ambient and elevated pressure up to 100 GPa, produced a large number of structures. However, many of those corresponded (within error margins) to the same few structure types. Moreover, only a few structures were relevant to the phase diagram in terms of their enthalpy. Therefore, only the most important five polymorph candidates (labeled from A to E) were described here; label of each structure also contains letter f (for ferromagnetic) or af (for antiferromagnetic ordering) as typical for each structure in its magnetic ground state. Their crystal structures and structural parameters are shown and listed in Electronic Supplement (ES).

\textit{Inter alia}, using manual feed of XtalOpt we have considered the Ammm form which was proposed as a high-pressure structure of K₂CuF₄ [27,28], but its enthalpy was always large with respect to those reported here.

The five structures mentioned (cf. ES for .cif files) correspond to:

A – the layered double perovskite corresponding to the lowest-energy ordered variant of the disordered experimental α-K₂AgF₄ polymorph

B – the monoclinic post-perovskite structure corresponding to experimental β-K₂AgF₄ polymorph

C – a chain structure hosting Ag₂F₇ dimers interconnected to another chain via F anions

D – another chain structure with a more complex arrangement of AgF₄ squares and AgF₂ dumbbells

E – structure originating from Ag(I)₂Ag(II)F₄ [19] by Ag(I)→K(I) substitution.

Since only three of these structures (A, B, E) are relevant to experiment in terms of possible phase transitions, they are shown jointly in fig. 1 (structures corresponding to 0 GPa are shown). The unit cell vector and volumes of the high-pressure structures are given as a percent value of the 0 GPa theoretical structures (cf. SM). The relative enthalpy of the five structures in the 0-100 GPa range is presented in fig. 2.
Fig. 1. Crystal structures of three important polymorphs of K$_2$AgF$_4$ derived from DFT computations. Color code: gray = Ag, green = F, purple = K. Green lines indicate presence of Ag-F bonds shorter than or equal to 2.2 Å, whereas yellow lines show Ag-F distances between 2.2 and 2.8 Å. Only AgF$_4$ sublattice is shown in the right panel, with potassium atoms removed for clarity.
Fig. 2. Relative enthalpy of the five important polymorphs of K$_2$AgF$_4$ in the 0-100 GPa pressure range. Enthalpy of the most stable polymorph at any given pressure is taken as reference (0 eV) at that pressure.

DFT calculations correctly grasp the key structural features of the α and β polymorphs of K$_2$AgF$_4$, the associated magnetic properties, as well as their respective stability at 0 GPa [9]. α-K$_2$AgF$_4$ hosts an antiferrodistortive ordering of tilted AgF$_6$ octahedra, which leads to ferromagnetic ground state [9,29]. On the other hand, the β-K$_2$AgF$_4$ polymorph features infinite chains composed of isolated AgF$_4$ units which are stacked in such manner that the magnetic superexchange is very weak, and the antiferromagnetic and ferromagnetic solutions are close in energy [29]. Moreover, β-form is more stable at 0 GPa, as evidenced by the facile structural collapse of metastable α-K$_2$AgF$_4$ in a properly designed experiment [12]. Since β-form is more suited than α-form to accommodate K(II) cation, it is expected that the former should prevail over the latter as pressure is increased. This is indeed what calculations show, the enthalpy of the α-form rising fast with the pressure increase.

β-form is predicted here to be the ground state of K$_2$AgF$_4$ up to ca. 6 GPa, when it should be substituted by Ag$_2$AgF$_4$-type polymorph (E); E form, in turn, should be stable to at least 58 GPa, when C form should prevail in enthalpy. Theoretical calculations predict also that pressure increase should lead to progressive cross-linking of the structural elements features in all polymorphs studied, as it is customary at elevated pressure [30–32].

4.2. Experimental results

We begin our analysis with the case of α-K$_2$AgF$_4$, for which both Raman spectra and x-ray diffraction patterns (XRDPs) were obtained as a function of pressure. An analogous set of results was also obtained for β-K$_2$AgF$_4$. 
Raman spectra of both polymorphs of K$_2$AgF$_4$ are presented in fig. 2, while XRDPs of the α-form are shown in fig. 3.

**Fig. 2.** Raman spectra of α-K$_2$AgF$_4$ (left) and β-K$_2$AgF$_4$ (right) measured with 514 nm laser at increasing pressure, with pressure values labelled next to each spectrum. Red asterisk indicates bands originating from FEP used as pressure medium.

Because the sample of α-K$_2$AgF$_4$ was loaded into DAC along with FEP slices used as an inert hydrostatic medium, the measured Raman spectrum contains bands from both materials. More precisely, the broad, strong band near 760 cm$^{-1}$ is caused by symmetric stretching of C-C-C chains in the polymer, while a shoulder band at 395 cm$^{-1}$ originates from bending of the polymer skeleton – both bands are indicated with red asterisks in respective figures. Further analysis of these FEP bands is omitted here.

Raman spectrum of α-K$_2$AgF$_4$ at a rather low pressure of 2.9 GPa is reminiscent of that at 1 atm (cf. Supporting Information to ref. [12]). The ambient pressure spectrum is predominated by three bands coming from vibrational fundamentals, at 320 cm$^{-1}$ (weak), 415 cm$^{-1}$ (strong) and 476 cm$^{-1}$ (very strong) [[12]]. The weakest of these bands is not seen in the spectrum measured at 2.9 GPa but the strongest two are clearly visible at 427 cm$^{-1}$ and 453 cm$^{-1}$. The upshift of the former band by 12 cm$^{-1}$ and the downshift of the latter by 23 cm$^{-1}$ clearly originate from the impact of external pressure. These bands further migrate to 433 cm$^{-1}$ and 461 cm$^{-1}$ (both showing a small upshift) respectively, at 4.5 GPa. A more dramatic effect is seen at 7.6 GPa, when three bands appear in the spectra, at 413 cm$^{-1}$, 470 cm$^{-1}$, and 547 cm$^{-1}$. While the former two might be reminiscent of the bands seen for α-K$_2$AgF$_4$, the highest-Raman shift band certainly signifies the appearance of a new phase. Its wavenumber is unusually large and it suggests the presence of very short Ag–F bonds, whose stretching mode could give rise to this band.

One is tempted to associate the appearance of the high-wavenumber band with either β-K$_2$AgF$_4$ (which is certainly more stable then α-K$_2$AgF$_4$) or even with the **E** structure, predicted to be minimum of enthalpy at this pressure. However, Raman spectra of the β-K$_2$AgF$_4$ form (fig.2) show that the main
broad Raman doublet detected for this form at 437 and 460 cm\(^{-1}\) (420 and 486 cm\(^{-1}\) at ambient pressure) does not stiffen as pressure is raised, hence it cannot be responsible for the appearance of the band at 547 cm\(^{-1}\). Simultaneously, theoretical analysis of Ag–F bond lengths seen for the A, B and E structures suggest that it is polymorph A, which hosts the shortest Ag–F bonds, that is observed here. Therefore, the appearance of the 547 cm\(^{-1}\) band cannot be explained by the presence of polymorph E. The origin of the latter band is not clear at present.

Unfortunately, further analysis of the evolution of the Raman bands for α-K\(_2\)AgF\(_4\) and β-K\(_2\)AgF\(_4\) at higher pressures was precluded by very low signal-to-noise ratio in the spectra measured at 11.9 GPa and 22.9 GPa, respectively. The disappearance of bands indicative of K\(_2\)AgF\(_4\) phases likely reflects amorphization or even decomposition of both samples.

Fig. 3. X-ray diffraction patterns of α-K\(_2\)AgF\(_4\) at increasing pressure, pressure values being labelled next to each pattern. Radiation with wavelength \(\lambda=0.56087\) Å was applied. The reflexes marked with an asterisk are derived from gold powder used as an additional pressure gauge.

In order to elucidate the nature of the phase transition taking place between 4.5 and 7.6 GPa, we have attempted to obtain additional insight from the evolution of XRDPs of α-K\(_2\)AgF\(_4\) at 2θ > 14° with pressure (fig. 3). Unfortunately, XRDPs are dominated by contributions from DAC elements (diamond, stainless steel gasket) and gold – pressure gauge. Furthermore, due to the size and position of the beamstop in our experimental setup, patterns have been cut off at 2θ < 3°. Therefore, usable information can be extracted from the patterns only for the narrow 3–14° 2θ range. This of course increases the difficulty of the analysis, although some basic information about the crystal structure, \textit{i.e.} cell parameters, could possibly be deduced. This is because for α-K\(_2\)AgF\(_4\) form at 0 GPa, the five strong reflections are expected in the available 2θ range – these are (002), (111), (020), (200) and (113) (fig. 3). Positions of those reflections can be then used to calculate the cell vectors and volume in the orthogonal system.

In the case of α-K\(_2\)AgF\(_4\) sample, our measurement inside DAC at 0 GPa properly reproduced the expected diffraction pattern of this compound at 1 atm [12]. Increasing pressure to 1.2 GPa yielded a
very similar pattern with positions slightly shifted to higher \(2\theta\) values, as expected for pressure-induced compression. Precise calculation of the unit cell vectors is complicated by broadening of the reflections. Diffraction patterns measured at still higher pressures of 3.3, 4.4 and 8.1 GPa do not improve the analysis, as most of the \(\alpha\)-K\(_2\)AgF\(_4\) reflections fade away in intensity, and they are hardly discernible at the largest pressure applied here. This observation is consistent with the Raman data and suggests that \(\alpha\)-K\(_2\)AgF\(_4\) likely undergoes amorphization at pressure above ca. 8 GPa. In view of this discouraging result, and as indicated by equally poor-quality Raman spectra of the \(\beta\)-form, its XRDPs were not studied.

![Raman spectra](image)

**Fig. 4.** Raman spectra of Na\(_2\)AgF\(_4\) (left) and Rb\(_2\)AgF\(_4\) (right) measured with 514 nm laser at increasing pressure, the pressure values being labelled next to each spectrum. Red asterisk indicates bands originating from FEP used as pressure medium.

Two analogs of K\(_2\)AgF\(_4\), i.e. disodium and dirubidium salts, were also studied using Raman scattering spectroscopy.

The most prominent band in the ambient-pressure Raman spectrum of Na\(_2\)AgF\(_4\) ([fig. 4](image)) is present at 450 cm\(^{-1}\). As we have seen, analogous bands are present in Raman spectra of other members of M\(_2\)AgF\(_4\) family, and the 450 cm\(^{-1}\) band corresponds to the totally symmetric vibrations of [AgF\(_4\)]\(^{2-}\) square subunits. Several other, much weaker bands can be found at 153, 222, 273 (sh), 330, 370 (sh) and 524 (sh) cm\(^{-1}\). Compression of the Na\(_2\)AgF\(_4\) sample leads to a clear decrease in spectral quality associated also with band broadening, and disappearance of all weaker features; only the broad 276 and 458 cm\(^{-1}\) features are seen. Between 2.1 GPa and 11.6 GPa the signal-to-noise ratio for all bands decreases even further; two main bands are seen at 463 and 505 cm\(^{-1}\). The appearance of the new band might indicate a structural phase transition. Subsequent measurements at even higher pressures up to 54.5 GPa lead to additional broadening of the bands, indicating a possible amorphization of the fluoroargentate. At the highest recorded pressure for which spectra were recorded, only two
extremely broad bands are seen, at 640 cm\(^{-1}\) and a shoulder at 467 cm\(^{-1}\). They likely correspond to the stretching and deformation vibrations, respectively, of the \([\text{AgF}_4]\)\(^2-\) units in a disordered structure.

Rb\(_2\)AgF\(_4\) spectrum at ambient pressure (fig. 4) contains two strong/very strong bands at 405 and 485 cm\(^{-1}\), as well as several weaker bands at: 193, 320, and 605 cm\(^{-1}\). The former two bands correspond to analogous bands seen at 415 cm\(^{-1}\) (strong) and 476 cm\(^{-1}\) (very strong) in Raman spectrum of \(\alpha\)-K\(_2\)AgF\(_4\). Compression of the sample from 0 to 3.9 GPa leads to substantial stiffening of the main bands from 485 to 538 cm\(^{-1}\) and from 405 to about 443 cm\(^{-1}\). Stiffening of the fundamentals is quite large (> 10%) for a relatively small pressure increment, which together with the fact that the Ag–F bonds are quite incompressible [33] hints at the occurrence of a structural phase transition below 3.9 GPa. Such scenario would be further supported by the appearance of several weaker spectral features in the Ag–F stretching region. Unfortunately, progressive compression up to 37.7 GPa has a similar effect as already seen for the other members of the M\(_2\)AgF\(_4\) family – that is, an immense band broadening which might again suggest amorphization of a sample.

5. Conclusions

Summarizing the research done, there is – at the first glance – an apparent discrepancy between theoretical and experimental results. Theory suggest the occurrence of at least two structural pressure-induced phase transitions in the pressure range up to 60 GPa for K\(_2\)AgF\(_4\). Based on rules of thumb of the high-pressure research [31,32], one may expect that these transitions will be present also for Na and Rb analogues, occurring at higher and lower pressures, respectively, than for potassium salt. On the other hand, experiments point to a progressive amorphization of all samples as pressure is increased.

One explanation for this discrepancy could be that the energy barrier for structural transitions predicted here is too large to be overcome at studied p/T conditions. Indeed, it can be noticed that e.g. the low-pressure \(B \rightarrow E\) structural transition is associated with breaking up of \([\text{AgF}_4]\) infinite chains and reorganization of the local \([\text{AgF}_4]\) square subunits, which adopt a strained (not flat) orientation in the \(B\) polymorph. Since the heavy atom sublattice is also strongly affected by the transition, its energy barrier could be large indeed. Note that our experiments were conducted without laser heating of the samples, since such heating would inevitably lead to reaction between extremely reactive Ag(II) salts and DAC elements. As a consequence, phases observed in experiment may not corresponds to the most thermodynamically stable ones (i.e. ones which are predicted using theoretical approach).

Computations of amorphous systems are certainly possible using programs adapted for periodic systems (e.g. [34]). Regretfully, they require extremely large supercells ("quasi-amorphous periodic systems") and they are currently beyond the possibilities of our supercomputer resources.

It is clear that there are many factors at play which determine high-pressure behavior of fluoroargentates(II), and this will supposedly lead to further experimental and computational studies aimed at elucidating the structural features of the amorphous phases.

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Phase transitions and amorphization of $M_2AgF_4$ ($M = Na, K, Rb$) compounds at high pressure

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SUPPLEMENTARY MATERIAL

Structures and crystallographic information files for five computationally studied polymorphs of $K_2AgF_4$

Color legend: gray = Ag, green = F, purple = K). Green lines indicate presence of Ag-F bonds shorter than or equal to 2.2 Å, whereas yellow lines show Ag-F distances between 2.2 and 2.8 Å. Space groups for unit cells were determined with accuracy of 0.05 Å. The unit cell dimensions and volumes of the high-pressure structures are also given as a percent value of the 0 GPa structures.
### External Pressure [GPa]

| External pressure [GPa] | 0  | 50 |
|-------------------------|----|----|
| Magnetic model          | A.f| A.af1 |
| Z                       | 4  | 4  |
| Symmetry                | $P2_1/c$ | $P2_1/c$ |
| $a$ [Å]                 | 6.328 | 4.800 (75.9%) |
| $b$ [Å]                 | 6.332 | 6.273 (99.1%) |
| $c$ [Å]                 | 12.482 | 9.793 (78.5%) |
| $V$ [Å³]                | 500.08 | 286.23 (57.2%) |
| $\alpha$ [°]           | 90.0 | 90.0 |
| $\beta$ [°]            | 90.0 | 76.1 |
| $\gamma$ [°]           | 90.0 | 90.0 |
| External pressure [GPa] | 0     | 50    |
|--------------------------|-------|-------|
| Magnetic model           | B.af1 | B.af1 |
| Z                        | 4†    | 4†    |
| Symmetry                 | P2_1/c| P-1   |
| a [Å]                    | 7.428 | 5.431 (73.1%) |
| b [Å]                    | 10.218| 8.865 (86.8%) |
| c [Å]                    | 6.377 | 5.941 (93.2%) |
| V [Å³]                   | 483.21| 283.46 (58.7%) |
| α [°]                    | 90.0  | 84.3  |
| β [°]                    | 88.1  | 95.1  |
| γ [°]                    | 90.0  | 91.2  |

†Data presented for the supercell – the antiferromagnetic ordering could not be properly described for the for Z=2 cell.
| External pressure [GPa] | 0     | 50    |
|-------------------------|-------|-------|
| Magnetic model          | C.af1 | C.f   |
| Z                       | 2     | 2     |
| Symmetry                | P-1   | P1    |
| a [Å]                   | 6.033 | 4.697 (77.9%) |
| b [Å]                   | 7.098 | 6.020 (84.8%) |
| c [Å]                   | 7.083 | 6.021 (85.0%) |
| V [Å³]                  | 239.38 | 138.76 (58.0%) |
| α [°]                   | 66.1  | 113.6 |
| θ [°]                   | 67.3  | 103.4 |
| ϱ [°]                   | 63.1  | 105.6 |
### External pressure [GPa]

| External pressure [GPa] | 0       | 50      |
|-------------------------|---------|---------|
| Magnetic model          | D.f     | D.af1   |
| **Z**                   | 2       | 2       |
| **Symmetry**            | P1      | P-1     |
| **a [Å]**               | 4.906   | 4.366 (90.0%) |
| **b [Å]**               | 7.521   | 6.555 (87.1%) |
| **c [Å]**               | 7.530   | 6.277 (83.4%) |
| **V [Å³]**              | 234.85  | 142.38 (60.6%) |
| **α [°]**               | 100.8   | 116.8   |
| **β [°]**               | 100.9   | 95.5    |
| **γ [°]**               | 109.0   | 111.0   |
| External pressure [GPa] | 0     | 50    |
|-------------------------|-------|-------|
| Magnetic model          | E.f   | E.f   |
| Z                       | 4     | 4     |
| Symmetry                | $I-42d$ | $I-42d$ |
| $a$ [Å]                 | 7.296 | 6.450 (88.4%) |
| $b$ [Å]                 | 7.296 | 6.450 (88.4%) |
| $c$ [Å]                 | 8.205 | 6.875 (83.8%) |
| $V$ [Å³]                | 436.70| 286.04 (65.5%) |
| $\alpha$ [°]           | 90.0  | 90.0  |
| $\beta$ [°]            | 90.0  | 90.0  |
| $\gamma$ [°]           | 90.0  | 90.0  |
Figure S1. Investigated magnetic variants of $K_2AgF_4$ structures: ferromagnetic (A.f) and antiferromagnetic ones (A.af1, A.af2 and A.af3). Only Ag-F sublattices are shown. Ag-F bonds are indicated for interatomic distances not longer than 2.2 Å. All visualized example structures are for $p = 0$ GPa.
Figure S2. Investigated magnetic variants of $\text{K}_2\text{AgF}_4\text{B}$ structures: ferromagnetic (B.f) and antiferromagnetic ones (B.af1, B.af2 and B.af3). Only Ag-F sublattices are shown. Ag-F bonds are indicated for interatomic distances not longer than $2.2\ \text{Å}$. All visualized example structures are for $p = 0\ \text{GPa}$.

Figure S3. Investigated magnetic variants of $\text{K}_2\text{AgF}_4\text{C}$ structures: ferromagnetic (C.f) and antiferromagnetic one (C.af1). Only Ag-F sublattices are shown. Ag-F bonds are indicated for interatomic distances not longer than $2.2\ \text{Å}$. All visualized example structures are for $p = 0\ \text{GPa}$.
Figure S4. Investigated magnetic variants of $\text{K}_2\text{AgF}_4$ D structures: ferromagnetic (D.f) and antiferromagnetic one (D.af1). Only Ag-F sublattices are shown. Ag-F bonds are indicated for interatomic distances not longer than 2.2 Å. All visualized example structures are for $p = 0$ GPa.

Figure S5. Investigated magnetic variants of $\text{K}_2\text{AgF}_4$ E structures: ferromagnetic (E.f) and antiferromagnetic ones (E.af1, E.af2 and E.af3). Only Ag-F sublattices are shown. Ag-F bonds are indicated for interatomic distances not longer than 2.2 Å. All visualized example structures are for $p = 0$ GPa.
### Appendix S1. CIF files of structures discussed in this study.

```cif
# DFT(PBEsol)+U K2AgF4 A p=000GPa magn.: f
data_1
_audit_creation_method       'vasp2cif'
_cell_length_a               6.32772727043
_cell_length_b               6.33155419994
_cell_length_c               12.4819750792
_cell_angle_alpha            90.0449569363
_cell_angle_beta             90.0023632874
_cell_angle_gamma            89.9998888167
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label             _atom_site_type_symbol
_atom_site_fract_x           _atom_site_fract_y
_atom_site_fract_z           _atom_site_occupancy
Ag1  Ag  0.005554689763624  0.000090965482804  0.000043499674507   1.0
Ag2  Ag  0.005665989890118  0.499725054385921  0.500064678773409   1.0
Ag3  Ag  0.505551513097716  0.999914760130198  0.499958456800951   1.0
Ag4  Ag  0.505667746933424  0.502895293042880  0.99927112788812   1.0
F5   F   0.563342142504102  0.941477017779963  0.336723580900030   1.0
F6   F   0.447953651766328  0.058403713461015  0.6632138457617   1.0
F7   F   0.449146165633307  0.443622812689357  0.163352895045630   1.0
F8   F   0.5623792555064713  0.556923819186946  0.836501896800705   1.0
F9   F   0.06370479421799  0.598475789602673  0.163277114626166   1.0
F10  F   0.947947325929100  0.941642510989339  0.836792902957445   1.0
F11  F   0.06235461696254  0.443136785965484  0.663493512082365   1.0
F12  F   0.9491588923829334  0.556315371117526  0.336639035019625   1.0
F13  F   0.7334695302252574  0.770042823446273  0.53742519699339   1.0
F14  F   0.276575233997900  0.229850350071465  0.462439573732951   1.0
F15  F   0.23621186297503  0.229851311187315  0.962580369042828   1.0
F16  F   0.776677748459322  0.771121473237880  0.037561861923344   1.0
F17  F   0.27356802645054  0.732905633078529  0.000068350797085   1.0
F18  F   0.73126139144803  0.266923395833647  0.999605399636767   1.0
F19  F   0.773602091871112  0.266978589364888  0.499931620252999   1.0
F20  F   0.23648893267550  0.733205334321255  0.500377859427039   1.0
K21  K   0.528228416492216  0.976651042499370  0.859665888402801   1.0
K22  K   0.529112412982684  0.522678829210753  0.360040371707704   1.0
K23  K   0.482381105182251  0.476928534520197  0.639930185036693   1.0
K24  K   0.482999980106362  0.203656997125161  0.14031072819542   1.0
K25  K   0.983006436289149  0.976339707770550  0.359689805105954   1.0
K26  K   0.028464019493990  0.202348966089451  0.640331400629730   1.0
K27  K   0.982392388543890  0.523050543964653  0.860066413887015   1.0
K28  K   0.029130501556823  0.477377312801842  0.139942686546298   1.0
```

```cif
# DFT(PBEsol)+U K2AgF4 A p=5GPa magn.: f
data_1
_audit_creation_method       'vasp2cif'
_cell_length_a               6.10970065899
_cell_length_b               6.11836679007
_cell_length_c               12.06154274638
_cell_angle_alpha            90.0336466132
_cell_angle_beta             90.0014116733
_cell_angle_gamma            89.9996215016
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label             _atom_site_type_symbol
_atom_site_fract_x           _atom_site_fract_y
_atom_site_fract_z           _atom_site_occupancy
```
|   |   |   |   |   |
|---|---|---|---|---|
| F5  | 0.565273536196829 | 0.93859640230068 | 0.33295866515758 | 1.0 |
| F6  | 0.445476288119992 | 0.06041702143287 | 0.66679077323561 | 1.0 |
| F7  | 0.447316753171630 | 0.44194284507677 | 0.01048418817888 | 1.0 |
| F8  | 0.563610902984997 | 0.565273536196829 | 0.33295866515758 | 1.0 |
| F9  | 0.505597887648245 | 0.99982286788242 | 0.49980233040369 | 1.0 |
| F10 | 0.50668510621848 | 0.500210707241571 | 0.00002141823100 | 1.0 |
| F11 | 0.4415879927451 | 0.44194284507677 | 0.01048418817888 | 1.0 |
| F12 | 0.447316753171630 | 0.44194284507677 | 0.01048418817888 | 1.0 |
| F13 | 0.495494848191877 | 0.93337336155598 | 0.83302609279553 | 1.0 |
| F14 | 0.06310920984998 | 0.4415879927451 | 0.44194284507677 | 1.0 |
| F15 | 0.739205082011094 | 0.765520024973056 | 0.54201977611753 | 1.0 |
| F16 | 0.76932326457019 | 0.2623918319624 | 0.4973668871404 | 1.0 |
| F17 | 0.27228766623736 | 0.26332045067534 | 0.4788672446992 | 1.0 |
| F18 | 0.74197786627598 | 0.26216706729719 | 0.99708788216816 | 1.0 |
| F19 | 0.76932326457019 | 0.2623918319624 | 0.4973668871404 | 1.0 |
| K21 | 0.526424895438936 | 0.97902793285707 | 0.86029388713039 | 1.0 |
| K22 | 0.526321545250046 | 0.521168291220350 | 0.36093293504735 | 1.0 |
| K23 | 0.484671210989019 | 0.74865148942335 | 0.6390893302395 | 1.0 |
| K24 | 0.484538067065757 | 0.232499646010018 | 0.13969136310021 | 1.0 |
| K25 | 0.094193373422343 | 0.786613195963909 | 0.36030208160067 | 1.0 |
| K26 | 0.021495535468053 | 0.737104792737125 | 0.50070908549060 | 1.0 |
| K27 | 0.524624895438936 | 0.7902793285707 | 0.86029388713039 | 1.0 |
| K28 | 0.526321545250046 | 0.521168291220350 | 0.36093293504735 | 1.0 |

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**DFT (PBEsol)+U K2AgF4 A p=10GPa magn.: f**

```
## DFT(PBEsol)+U K2AgF4 A p=20GPa magn.: f

| K|   |   |   |   |
|---|---|---|---|---|
| K21 | K | 0.507138918012257 | 0.963894781043390 | 0.8601649276267927 |
| K22 | K | 0.504148441632879 | 0.536839404595324 | 0.359745664364665 |
| K23 | K | 0.506804222523601 | 0.462909529614885 | 0.64021992805815 |
| K24 | K | 0.503948630362719 | 0.036050461783808 | 0.139781982193256 |
| K25 | K | 0.004129265266668 | 0.963977020980736 | 0.36021992805815 |
| K26 | K | 0.007004608642127 | 0.036082945179800 | 0.639825930583626 |
| K27 | K | 0.006950729605373 | 0.537075076734358 | 0.859731709047254 |
| K28 | K | 0.003956058719825 | 0.463194835838178 | 0.140260839467106 |

## DFT(PBEsol)+U K2AgF4 A p=30GPa magn.: af2

| K|   |   |   |   |
|---|---|---|---|---|
| F5 | F | 0.630808978207563 | 0.175608556629724 | 0.689204210846020 |
| F6 | F | 0.381137459005449 | 0.824385351736100 | 0.310342834204720 |
| F7 | F | 0.471991297419670 | 0.532602189965135 | 0.82900781357768 |
| F8 | F | 0.538650478458544 | 0.46648699210642 | 0.170942724653722 |
| F9 | F | 0.891525265160286 | 0.812255169202033 | 0.807999838622149 |
| F10 | F | 0.118731180493281 | 0.148720252974562 | 0.192117191451945 |
| F11 | F | 0.944002584313083 | 0.49160554336784 | 0.322105019371213 |
| F12 | F | 0.067493838668970 | 0.509288976343666 | 0.678146449494192 |
| F13 | F | 0.687393536692299 | 0.204813435681082 | 0.41381640194089 |
| F14 | F | 0.324402258935907 | 0.795538190513039 | 0.586502311412923 |
| F15 | F | 0.272650219692621 | 0.794517565960626 | 0.11746143433014 |
| F16 | F | 0.737401700234414 | 0.204969420257786 | 0.988038677043642 |
| F17 | F | 0.212737032529822 | 0.226456250757093 | 0.90510126684893 |
| F18 | F | 0.798489234565009 | 0.773040891549449 | 0.09519741427605 |
| F19 | F | 0.8011601775830937 | 0.775315561297206 | 0.51516992802958 |
| F20 | F | 0.21086001925966 | 0.225559229449102 | 0.48506736886718 |
| K21 | K | 0.591184084061196 | 0.094880197570118 | 0.197767434338157 |
| K22 | K | 0.585659662355537 | 0.532993348607432 | 0.638159589615432 |
| K23 | K | 0.425945557027909 | 0.467518238107962 | 0.362005665707303 |
| K24 | K | 0.418932158778879 | 0.904355217940414 | 0.82011470664730 |
| K25 | K | 0.092976923076088 | 0.113401211848115 | 0.674031197876117 |
| K26 | K | 0.919516160506448 | 0.887458451099623 | 0.326143824059993 |
| K27 | K | 0.081291707676241 | 0.521486573497858 | 0.137906265121893 |
| K28 | K | 0.923849259593120 | 0.477844214055948 | 0.862072721272796 |

## DFT(PBEsol)+U K2AgF4 A p=30GPa magn.: f

| K|   |   |   |   |
|---|---|---|---|---|
| K21 | K | 0.507138918012257 | 0.963894781043390 | 0.8601649276267927 |
| K22 | K | 0.504148441632879 | 0.536839404595324 | 0.359745664364665 |
| K23 | K | 0.506804222523601 | 0.462909529614885 | 0.64021992805815 |
| K24 | K | 0.503948630362719 | 0.036050461783808 | 0.139781982193256 |
| K25 | K | 0.004129265266668 | 0.963977020980736 | 0.36021992805815 |
| K26 | K | 0.007004608642127 | 0.036082945179800 | 0.639825930583626 |
| K27 | K | 0.006950729605373 | 0.537075076734358 | 0.859731709047254 |
| K28 | K | 0.003956058719825 | 0.463194835838178 | 0.140260839467106 |
Ag1  Ag   0.005318522709985   0.000080002285181   0.999972824361033   1.0
Ag2  Ag   0.005415516581726   0.499775821053462   0.500022369350084   1.0
Ag3  Ag   0.50564190318038264   0.978427607328121   0.139026057646045   1.0
Ag4  Ag   0.50545106555726276   0.5000186013243254   0.999972824217536   1.0
Ag1  Ag   0.005415516581726   0.499775821053462   0.500022369350084   1.0
Ag2  Ag   0.005415516581726   0.499775821053462   0.500022369350084   1.0
Ag3  Ag   0.50564190318038264   0.978427607328121   0.139026057646045   1.0
Ag4  Ag   0.50545106555726276   0.5000186013243254   0.999972824217536   1.0

## DFT(PBEsol)+U K2AgF4 A p=40GPa magn.: f
| Atom  | Symbol | Fractional X    | Fractional Y    | Fractional Z    | Occupancy |
|-------|--------|----------------|----------------|----------------|-----------|
| Ag1   | Ag     | 0.960131026469753 | 0.928253764098717 | 0.054718094712678 | 1.0       |
| Ag2   | Ag     | 0.960183829808316 | 0.571756837764474 | 0.554713760320585 | 1.0       |
| Ag3   | Ag     | 0.52871394669711    | 0.071568373764474 | 0.445280403531322 | 1.0       |
| Ag4   | Ag     | 0.528670783418563 | 0.42823550921891    | 0.945281822776688 | 1.0       |
| F5    | F      | 0.4194403707026312 | 0.037787627780205 | 0.655933249208286 | 1.0       |
| F6    | F      | 0.641965955715629 | 0.171503828534767 | 0.244079595202308 | 1.0       |
| F7    | F      | 0.641903933783319 | 0.328504834847435 | 0.74407763646034  | 1.0       |
| F8    | F      | 0.419439685175853 | 0.46210597165368 | 0.15953527923261 | 1.0       |
| F9    | F      | 0.0694842316717777 | 0.96220079605809 | 0.844076121806812 | 1.0       |
| F10   | F      | 0.846908484628360 | 0.82409587164768 | 0.25589598693015 | 1.0       |
| F11   | F      | 0.694658243711464 | 0.177555523710537 | 0.55473760320585 | 1.0       |
| F12   | F      | 0.424480370120368 | 0.395457035537157 | 0.317383779964586 | 1.0       |
| F13   | F      | 0.775988308168077 | 0.289911868231791 | 0.494075414070977 | 1.0       |
| F14   | F      | 0.77595161509863 | 0.210094794929584 | 0.994071648076920 | 1.0       |
| F15   | F      | 0.232477791529231 | 0.648325952414767 | 0.937792303733826 | 1.0       |
| F16   | F      | 0.71295885329069 | 0.710354659677667 | 0.00528788174531 | 1.0       |
| F17   | F      | 0.5643184968833 | 0.148262397055465 | 0.662225649685042 | 1.0       |
| F18   | F      | 0.564364692828222 | 0.351725490399183 | 0.562223103586039 | 1.0       |
| F19   | F      | 0.712901424900581 | 0.789954756562218 | 0.505292853676439 | 1.0       |
| K21   | K      | 0.36970418252495 | 0.82513792766427 | 0.193771276014468 | 1.0       |
| K22   | K      | 0.54886678197521 | 0.534171826469985 | 0.369603177458665 | 1.0       |
| K23   | K      | 0.548661789101457 | 0.965824233092165 | 0.869599847008980 | 1.0       |
| K24   | K      | 0.90260459873375 | 0.034207644090809 | 0.630418209674511 | 1.0       |
| K25   | K      | 0.118991034642114 | 0.174755404434121 | 0.306222670650284 | 1.0       |
| K26   | K      | 0.90251284110866 | 0.465794526824784 | 0.130415663755989 | 1.0       |
| K27   | K      | 0.118946589096380 | 0.325260165395845 | 0.806221671587195 | 1.0       |
| K28   | K      | 0.5863796890911    | 0.604261029793575 | 0.317383779964586 | 1.0       |
### DFT(PBEsol)+U K2AgF4 A p=70GPa magn.: af1

data_1

| atom_site_label | atom_site_type_symbol | atom_site_fract_x | atom_site_fract_y | atom_site_fract_z | atom_site_occupancy |
|-----------------|-----------------------|-------------------|-------------------|-------------------|---------------------|
| K2              | K                    | 0.369722467441066 | 0.825016778016849 | 0.193996487783483 | 1.0                 |
| K22             | K                    | 0.369782143827177 | 0.673747665904902 | 0.694001913520919 | 1.0                 |
| K23             | K                    | 0.548275062429090 | 0.532481059300408 | 0.369542807468840 | 1.0                 |
| K24             | K                    | 0.548265471037637 | 0.967515023158531 | 0.869540677408405 | 1.0                 |
| K25             | K                    | 0.940632843359577 | 0.302516517089455 | 0.630462749835690 | 1.0                 |
| K26             | K                    | 0.119176438390050 | 0.174529676265578 | 0.305996745051067 | 1.0                 |
| K27             | K                    | 0.940619467623131 | 0.674869065290729 | 0.130459158789386 | 1.0                 |
| K28             | K                    | 0.119128694576249 | 0.325486290726862 | 0.805996193831044 | 1.0                 |

---

## DFT(PBEsol)+U K2AgF4 A p=70GPa magn.: af1

data_1
| Atom | Symbol | Frac.X | Frac.Y | Frac.Z | Occupancy |
|------|--------|--------|--------|--------|-----------|
| Ag1  | Ag     | 0.960246335226501 | 0.929948852953752 | 0.0595466673637058 | 1.0 |
| Ag2  | Ag     | 0.960274038776697 | 0.570064763106209 | 0.559540876042231 | 1.0 |
| Ag3  | Ag     | 0.528854705976425 | 0.430016669197666 | 0.94042962618318 | 1.0 |
| F    | F      | 0.420630798900446 | 0.037325852824121 | 0.655574995680892 | 1.0 |
| F    | F      | 0.646306385456360 | 0.171214610800708 | 0.236198325836099 | 1.0 |
| F    | F      | 0.646232231634709 | 0.328791751733671 | 0.736195808982752 | 1.0 |
| F    | F      | 0.420640935812173 | 0.46264527419338 | 0.155575849188546 | 1.0 |
| F    | F      | 0.068141254755863 | 0.962460937414235 | 0.844396273614367 | 1.0 |
| F    | F      | 0.84265273033596 | 0.82891687891810 | 0.263828072117728 | 1.0 |
| F    | F      | 0.573548082559470 | 0.34394267907906 | 0.869473438215747 | 1.0 |
| F    | F      | 0.437960456797897 | 0.494241103677465 | 1.0 |
| F    | F      | 0.2109165093660754 | 0.994236428607054 | 1.0 |
| F    | F      | 0.22450398675586 | 0.653758084361443 | 0.937967457019597 | 1.0 |
| F    | F      | 0.706986060463831 | 0.712196815327124 | 0.005791307504322 | 1.0 |
| F    | F      | 0.264304873553176 | 0.153934830345745 | 0.062020743442753 | 1.0 |
| F    | F      | 0.524301638446334 | 0.346048301680010 | 0.562013726285453 | 1.0 |
| K    | K      | 0.119325139580773 | 0.325441847216002 | 0.805710190256075 | 1.0 |
| K    | K      | 0.369797725314138 | 0.531057421364376 | 0.369488412027845 | 1.0 |
K25  K  0.940917762018902  0.02953211309654  0.630611589330098  1.0
K26  K  0.11923003426905  0.17458393265368  0.305285995407843  1.0
K27  K  0.940922750910197  0.470470044396050  0.130691513123598  1.0
K28  K  0.119204280101423  0.325425684387600  0.805281044853323  1.0

## DFT(PBEsol)+U K2AgF4 A p=90GPa magn.: af1
_data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 4.54851737199
_cell_length_b 6.0383678289
_cell_length_c 9.4139188205
_cell_angle_alpha 90.0014766934
_cell_angle_beta 76.8603463811
_cell_angle_gamma 90.000152513
_symmetry_space_group_name_H-M 'P 1'
_loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.960615289394199  0.929730792356059  0.060578835439373  1.0
Ag2 Ag 0.960642678460464  0.570291127690732  0.560582109073928  1.0
Ag3 Ag 0.528477479420107  0.070224097797448  0.439395529198803  1.0
Ag4 Ag 0.528448661934838  0.429755498269671  0.939395031088000  1.0
F5 F  0.420928514973762  0.037304974800918  0.655437335130682  1.0
F6 F  0.647027869611282  0.171221126534174  0.234515169243008  1.0
F7 F  0.469981933074778  0.32878803446945  0.734516800137153  1.0
F8 F  0.420940378139493  0.46285537412240  0.15543126874493  1.0
F9 F  0.06785094930461  0.924997545625168  0.84451578075778  1.0
F10 F  0.91444638076760  0.828923951680849  0.265505761642461  1.0
F11 F  0.06784722107889  0.537510619685292  0.344538032333369  1.0
F12 F  0.841971078179890  0.671067427499663  0.755022354928721  1.0
F13 F  0.222072072667241  0.845583750998294  0.437748007750210  1.0
F14 F  0.784282445558538  0.287358907822896  0.494361995538374  1.0
F15 F  0.784293880503289  0.212465729361864  0.94356080213507  1.0
F16 F  0.22207780825800  0.654438378758298  0.937758288758182  1.0
F17 F  0.704531389905336  0.71279904397706  0.005662443549054  1.0
F18 F  0.266759470864868  0.154575461106868  0.62235241390546  1.0
F19 F  0.266749312724911  0.345399954020704  0.56222230677141  1.0
F20 F  0.704524548263081  0.787183067406680  0.5056682691151  1.0
K21 K  0.370178828847850  0.825646914565122  0.195230291749743  1.0
K22 K  0.37020113053450  0.674341152070500  0.695238145394265  1.0
K23 K  0.547735831099893  0.528094646909983  0.36923265491882  1.0
K24 K  0.547745066875467  0.971903644482805  0.86923339335417  1.0
K25 K  0.941038240480981  0.28056707034728  0.630577590425380  1.0
K26 K  0.118844163839304  0.17459439672457  0.30479794644083  1.0
K27 K  0.914049474885727  0.471945665723098  0.130755850626491  1.0
K28 K  0.118817479337962  0.325418177751822  0.804788013124647  1.0

## DFT(PBEsol)+U K2AgF4 A p=100GPa magn.: af1
_data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 4.49997704578
_cell_length_b 5.98980853074
_cell_length_c 9.35415417477
_cell_angle_alpha 90.007778884
_cell_angle_beta 77.0351168814
_cell_angle_gamma 90.0002012403
_symmetry_space_group_name_H-M 'P 1'
_loop_
_atom_site_label
_atom_site_type_symbol
## DFT(PBEsol)+U K2AgF4 B p=000000 GPa magn.: af1

| atom_site_label | atom_site_type_symbol | atom_site_fract_x | atom_site_fract_y | atom_site_fract_z | atom_site_occupancy |
|-----------------|-----------------------|-------------------|-------------------|-------------------|---------------------|
| Ag1             | Ag                    | 0.500000000000000 | 0.000000000000000 | 0.000000000000000 | 1.0                 |
| Ag2             | Ag                    | 0.000000000000000 | 0.000000000000000 | 0.000000000000000 | 1.0                 |
| Ag3             | Ag                    | 0.499999928000000 | 0.500000024000000 | 0.500000000000000 | 1.0                 |
| Ag4             | Ag                    | 0.500000000000000 | 0.500000024000000 | 0.500000000000000 | 1.0                 |
| F5              | F                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| F6              | F                     | 0.500000000000000 | 0.208867130000000 | 0.509507086999999 | 1.0                 |
| F7              | F                     | 0.780459019999999 | 0.502559060999997 | 0.052559060999997 | 1.0                 |
| F8              | F                     | 0.780459019999999 | 0.502559060999997 | 0.052559060999997 | 1.0                 |
| F9              | F                     | 0.500000000000000 | 0.208867130000000 | 0.509507086999999 | 1.0                 |
| F10             | F                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| K21             | K                     | 0.007174112000000 | 0.874444263000000 | 0.811665327000000 | 1.0                 |
| K22             | K                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| K23             | K                     | 0.500000000000000 | 0.208867130000000 | 0.509507086999999 | 1.0                 |
| K24             | K                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| K25             | K                     | 0.007174112000000 | 0.874444263000000 | 0.811665327000000 | 1.0                 |
| K26             | K                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| K27             | K                     | 0.007174112000000 | 0.874444263000000 | 0.811665327000000 | 1.0                 |
| K28             | K                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| K29             | K                     | 0.007174112000000 | 0.874444263000000 | 0.811665327000000 | 1.0                 |
| K30             | K                     | 0.947440942000000 | 0.477374220000000 | 0.816653527000000 | 1.0                 |
| K31             | K                     | 0.007174112000000 | 0.874444263000000 | 0.811665327000000 | 1.0                 |
## DFT(PBEsol)+U K2AgF4 B p=5GPa magn.: f

```plaintext
 data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 3.58481761052
_cell_length_b 6.2144140457
_cell_length_c 9.68320725887
_cell_angle_alpha 90.0010759972
_cell_angle_beta 90.0000460419
_cell_angle_gamma 89.5800591271
_symmetry_space_group_name_H-M 'P 1'
_loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.99999998999999 0.000000090000002 0.000000030000002 1.0
Ag2  Ag  0.999999999999999 0.499999989999999 0.499999989999999 1.0
F3   F   0.573037359502400 0.217846847137454 0.944368431058741 1.0
F4   F   0.426962660497602 0.782153242862546 0.055631618941262 1.0
F5   F   0.426978895150101 0.282164188201687 0.444364061928229 1.0
F6   F   0.573021014849899 0.717835971798312 0.555635938071771 1.0
F7   F   0.988481778572506 0.133062043913791 0.195257080996895 1.0
F8   F   0.011517961427494 0.866938126086209 0.804742959003101 1.0
F9   F   0.011556946307310 0.366946005470201 0.695261274210651 1.0
K11  K   0.487896011314402 0.421356714335300 0.178385324778735 1.0
K12  K   0.512104238685598 0.578643275664706 0.82161465522163 1.0
K13  K   0.512186770825052 0.078651057248076 0.67836952321023 1.0
K14  K   0.487813269174944 0.921348812751927 0.321610484678978 1.0
```

## DFT(PBEsol)+U K2AgF4 B p=10GPa magn.: f

```plaintext
 data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 3.50089018455
_cell_length_b 6.14886686
_cell_length_c 9.30501143397
_cell_angle_alpha 89.9955634724
_cell_angle_beta 90.0004862263
_cell_angle_gamma 89.9910660488
_symmetry_space_group_name_H-M 'P 1'
_loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.00000312660338 -0.000001335173779 -0.000005534760399 1.0
Ag2  Ag  -0.000001504052230 0.500003332610946 0.499999423281487 1.0
```
| # | # | # | # | # | # | # | # |
|---|---|---|---|---|---|---|---|
| F3 | F | 0.566506805432239 | 0.216536288071983 | 0.941141010995494 | 1.0 |
| F4 | F | 0.433493673249551 | 0.783463077371940 | 0.058859796425863 | 1.0 |
| F5 | F | 0.433496339853342 | 0.283472155713051 | 0.058859796425863 | 1.0 |
| F6 | F | 0.984010528910886 | 0.137489797020841 | 0.200760404735800 | 1.0 |
| F7 | F | 0.01598755044815 | 0.862513229955319 | 0.799242567916040 | 1.0 |
| F8 | F | 0.015981384357716 | 0.362510599723660 | 0.700764582663956 | 1.0 |
| F9 | F | 0.984017890095622 | 0.637488878008991 | 0.299236130891039 | 1.0 |
| K10 | K | 0.484061504234326 | 0.421706914106770 | 0.174973800628102 | 1.0 |
| K11 | K | 0.515937821767612 | 0.578292929073181 | 0.825026685866558 | 1.0 |
| K12 | K | 0.515928327202337 | 0.078282250160894 | 0.674977274748565 | 1.0 |
| K13 | K | 0.484071485624944 | 0.921716864044669 | 0.325023536699573 | 1.0 |

## DFT(PBEsol)+U K2AgF4 B p=20GPa magn.: af2

| data_1 |
|---|
| _audit_creation_method | 'vasp2cif' |
| _cell_length_a | 5.7805905342 |
| _cell_length_b | 6.1673393249 |
| _cell_length_c | 9.53479394639 |
| _cell_angle_alpha | 90.2567596433 |
| _cell_angle_beta | 90.0368347168 |
| _cell_angle_gamma | 82.7993392947 |

## DFT(PBEsol)+U K2AgF4 B p=30GPa magn.: af2

| data_1 |
|---|
| _audit_creation_method | 'vasp2cif' |
| _cell_length_a | 5.563742733 |
| _cell_length_b | 6.0900355833 |
| _cell_length_c | 9.1968517303 |

## DFT(PBEsol)+U K2AgF4 B p=40GPa magn.: af2

| data_1 |
|---|
| _audit_creation_method | 'vasp2cif' |
| _cell_length_a | 5.36742733 |
| _cell_length_b | 6.0900355833 |
| _cell_length_c | 9.1968517303 |
| Atom Site Label | Atom Type Symbol | Fract X | Fract Y | Fract Z | Occupancy |
|----------------|-----------------|---------|---------|---------|-----------|
| Ag1            | Ag              | 0.500   | 0.000   | 0.000   | 1.0       |
| Ag2            | Ag              | 0.000   | 0.000   | 0.000   | 1.0       |
| Ag3            | Ag              | 0.499   | 0.500   | 0.500   | 1.0       |
| Ag4            | Ag              | 0.999   | 0.500   | 0.500   | 1.0       |
| F5             | F               | 0.286   | 0.286   | 0.933   | 1.0       |
| F6             | F               | 0.786   | 0.286   | 0.933   | 1.0       |
| F7             | F               | 0.214   | 0.720   | 0.067   | 1.0       |
| F8             | F               | 0.714   | 0.720   | 0.067   | 1.0       |
| K21            | K               | 0.029   | 0.414   | 0.151   | 1.0       |
| K22            | K               | 0.529   | 0.414   | 0.151   | 1.0       |
| K23            | K               | 0.471   | 0.586   | 0.848   | 1.0       |
| K24            | K               | 0.971   | 0.586   | 0.848   | 1.0       |
| K25            | K               | 0.471   | 0.086   | 0.651   | 1.0       |
| K26            | K               | 0.971   | 0.086   | 0.651   | 1.0       |
| F19            | F               | 0.291   | 0.090   | 0.176   | 1.0       |
| F20            | F               | 0.791   | 0.090   | 0.176   | 1.0       |
| K27            | K               | 0.029   | 0.914   | 0.349   | 1.0       |
| K28            | K               | 0.529   | 0.914   | 0.349   | 1.0       |

## DFT(PBEsol)+U K2AgF4 B p=40GPa magn.: af2

```python
# DFT(PBEsol)+U K2AgF4 B p=40GPa magn.: af2
```

```bash
data_1

_symmetry_space_group_name_H-M 'P 1'
_loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.500000000000000 0.000000000000000 0.000000000000000 1.0
Ag2 Ag 0.000000000000000 0.000000000000000 0.000000000000000 1.0
Ag3 Ag 0.499999948000000 0.500000000000000 0.500000000000000 1.0
Ag4 Ag 0.999999960000000 0.500000000000000 0.500000000000000 1.0
F5 F 0.285890170000000 0.279731980000000 0.932839244000000 1.0
F6 F 0.785890276000000 0.279731980000000 0.932839244000000 1.0
F7 F 0.214109792000000 0.720269810000000 0.067160713000000 1.0
F8 F 0.714109770000000 0.720269810000000 0.067160713000000 1.0
F9 F 0.214528604999999 0.220782051000000 0.432446999999999 1.0
F10 F 0.714528669000000 0.220782051000000 0.432446999999999 1.0
F11 F 0.285471329000000 0.779218186999999 0.567553419999999 1.0
F12 F 0.785471371000000 0.779218186999999 0.567553419999999 1.0
F13 F 0.791425881000000 0.090235044000000 0.176099977000000 1.0
F14 F 0.291425859999999 0.090235044000000 0.176099977000000 1.0
F15 F 0.791425859999999 0.090235044000000 0.176099977000000 1.0
F16 F 0.291425859999999 0.090235044000000 0.176099977000000 1.0
F17 F 0.791425859999999 0.090235044000000 0.176099977000000 1.0
F18 F 0.791425859999999 0.090235044000000 0.176099977000000 1.0
F19 F 0.291425859999999 0.090235044000000 0.176099977000000 1.0
F20 F 0.791425859999999 0.090235044000000 0.176099977000000 1.0
K21 K 0.029 0.414 0.151 1.0
K22 K 0.529 0.414 0.151 1.0
K23 K 0.471 0.586 0.848 1.0
K24 K 0.971 0.586 0.848 1.0
K25 K 0.471 0.086 0.651 1.0
K26 K 0.971 0.086 0.651 1.0
K27 K 0.029 0.914 0.349 1.0
K28 K 0.529 0.914 0.349 1.0
```
## DFT(PBEsol)+U K2AgF4 B p=50GPa magn.: afl

```plaintext
# audit_creation_method 'vasp2cif'
_cell_length_a  5.43088971021
_cell_length_b  5.94098657332
_cell_length_c  8.64506047360
_cell_angle_alpha  84.2887194245
_cell_angle_beta  91.1952507418
_cell_angle_gamma  95.0705461439
_symmetry_space_group_name_H-M 'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_frcxt_x
_atom_site_frcxt_y
_atom_site_frcxt_z
_atom_site_occupancy

Ag1   Ag -0.000000000000000   0.000000000000000   -0.000000000000000   1.0
Ag2   Ag  0.500000000000000   0.000000000000000   0.000000000000000   1.0
Ag3   Ag -0.000000000000000   0.500000000000000   0.000000000000000   1.0
Ag4   Ag  0.500000000000000   0.500000000000000   0.000000000000000   1.0
F5   F   0.228511754114886   0.259643000806500   0.8627751295239   1.0
F6   F   0.728511776114888   0.259643000806500   0.8627751295239   1.0
F7   F   0.740435773193499   0.91372249004758   0.500000000000000   1.0
F8   F   0.28294442015762   0.20187400206202   0.559512529248081   1.0
F9   F   0.78944398015766   0.20187400206202   0.559512529248081   1.0
F10   F   0.798155588984237   0.798126152939801   0.44808745275198   1.0
F11   F   0.798155577894239   0.798126152939801   0.44808745275198   1.0
F12   F   0.25018163196724   0.12503507488225   0.187682586412115   1.0
F13   F   0.12503507488225   0.187682586412115   0.8627751295239   1.0
F14   F   0.79481546803277   0.87498672751177   0.18231372578785   1.0
F15   F   0.87498672751177   0.18231372578785   0.500000000000000   1.0
F16   F   0.348052553591239   0.32157988512010   0.000000000000000   1.0
F17   F   0.348052553591239   0.32157988512010   0.000000000000000   1.0
F18   F   0.717663715523814   0.67734793479299   0.500000000000000   1.0
F19   F   0.565871047653044   0.33744946372229   0.000000000000000   1.0
F20   F   0.881245296297817   0.82017215872354   0.500000000000000   1.0
F21   F   0.82017215872354   0.500000000000000   0.8627751295239   1.0
F22   F   0.228511754114886   0.259643000806500   0.8627751295239   1.0
F23   F   0.728511776114888   0.259643000806500   0.8627751295239   1.0
F24   F   0.740435773193499   0.91372249004758   0.500000000000000   1.0
F25   F   0.28294442015762   0.20187400206202   0.559512529248081   1.0
F26   F   0.78944398015766   0.20187400206202   0.559512529248081   1.0
F27   F   0.798155588984237   0.798126152939801   0.44808745275198   1.0
F28   F   0.798155577894239   0.798126152939801   0.44808745275198   1.0
K21   K   0.474551655330323   0.426492076711447   0.86047624990257   1.0
K22   K   0.025448226666667   0.57350791285525   0.13395233000974   1.0
K23   K   0.500000000000000   0.8627751295239   0.500000000000000   1.0
K24   K   0.798155588984237   0.798126152939801   0.44808745275198   1.0
K25   K   0.348052553591239   0.32157988512010   0.000000000000000   1.0
K26   K   0.348052553591239   0.32157988512010   0.000000000000000   1.0
K27   K   0.717663715523814   0.67734793479299   0.500000000000000   1.0
K28   K   0.565871047653044   0.33744946372229   0.000000000000000   1.0
```

---

**Note:** The above text appears to be a section of a Crystallographic Information File (CIF) format used to describe crystal structures. It includes lattice parameters, atom positions, and additional data such as symmetry operations and atom labels. The CIF format is commonly used in materials science and crystallography to exchange crystal structure information.
# DFT(PBEsol)+U K2AgF4 B p=60GPa magn.: af2

data_1
_audit_creation_method   'vasp2cif'
_cell_length_a    5.35532117074
_cell_length_b    5.88154734445
_cell_length_c    8.74249952677
_cell_angle_alpha    96.2380262316
_cell_angle_beta    88.7294060388
_cell_angle_gamma    94.6518655779
_symmetry_space_group_name_H-M    'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1   Ag    -0.000000000000000   0.000000000000000   0.000000000000000   1.0
Ag2   Ag    0.500000000000000   0.000000000000000   0.000000000000000   1.0
Ag3   Ag    0.999999999000003   0.499999989000003   0.499999997000003   1.0
Ag4   Ag    0.500000032999999   0.499999989000003   0.499999997000003   1.0
F5    F    0.219836791679525   0.299784302021039   0.055344130025403   1.0
F6    F    0.719836813679520   0.299784302021039   0.055344130025403   1.0
F7    F    0.780163213320479   0.700215768978964   0.946655931974595   1.0
F8    F    0.780163213320479   0.700215768978964   0.946655931974595   1.0
F9    F    0.268421855374384   0.241947611878555   0.588625786074426   1.0
F10   F    0.768421877374379   0.241947611878555   0.588625786074426   1.0
F11   F    0.231578197625617   0.499999989000003   0.499999970000003   1.0
F12   F    0.731578242625617   0.758052747412144   0.41374179925571   1.0
F13   F    0.72151689514924   0.602299391702225   0.820801965033463   1.0
F14   F    0.72151689514924   0.602299391702225   0.820801965033463   1.0
F15   F    0.278483967485079   0.939770289829776   0.179197972966539   1.0
F16   F    0.778483900485077   0.939770289829776   0.179197972966539   1.0
F17   F    0.293738321979140   0.371939576655348   0.315502787445723   1.0
F18   F    0.793738299979138   0.371939576655348   0.315502787445723   1.0
F19   F    0.206261700020862   0.628060426344469   0.64497233554282   1.0
F20   F    0.706261678020860   0.628060426344469   0.64497233554282   1.0
K21   K    0.485082300233443   0.397082979418370   0.834825230873466   1.0
K22   K    0.985082300233443   0.397082979418370   0.834825230873466   1.0
K23   K    0.014917599766556   0.602917007581633   0.165174817126538   1.0
K24   K    0.514917630766555   0.602917007581633   0.165174817126538   1.0
K25   K    0.024624471002731   0.736515720333620   0.367974360195543   1.0
K26   K    0.524624444002725   0.736515720333620   0.367974360195543   1.0
K27   K    0.278483967485079   0.939770289829776   0.179197972966539   1.0
K28   K    0.975375518997275   0.26348263966380   0.632025660804456   1.0

## DFT(PBEsol)+U K2AgF4 B p=70GPa magn.: af2

data_1
_audit_creation_method   'vasp2cif'
_cell_length_a    5.29090322805
_cell_length_b    6.34828005505
_cell_length_c    7.9030324044
_cell_angle_alpha    90.0003137565
_cell_angle_beta    89.993641269
_cell_angle_gamma    86.7392774437
_symmetry_space_group_name_H-M    'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
## DFT(PBEsol)+U K2AgF4 B p=80GPa magn.: af2 data_1

| Atom | Symbol | Fractional Coordinates | Occupancy |
|------|--------|------------------------|-----------|
| Ag1  | Ag     | 0.000000000000000     | 1.0       |
| Ag2  | Ag     | 0.500000000000000     | 1.0       |
| Ag3  | Ag     | 0.999999999000003     | 1.0       |
| Ag4  | Ag     | 0.499999970000003     | 1.0       |

| Atom | Symbol | Fractional Coordinates | Occupancy |
|------|--------|------------------------|-----------|
| F1   | F      | 0.16629239278118       | 0.8662254062583 |
| F2   | F      | 0.6662294039718116     | 0.8662254062583 |
| F3   | F      | 0.333707630021880      | 0.8662254062583 |
| F4   | F      | 0.833689547719142      | 0.8662254062583 |
| F5   | F      | 0.166310435280862      | 0.8662254062583 |
| F6   | F      | 0.666310435280862      | 0.8662254062583 |
| F7   | F      | 0.333707630021880      | 0.8662254062583 |
| F8   | F      | 0.833707630021880      | 0.8662254062583 |
| F9   | F      | 0.166310435280862      | 0.8662254062583 |
| F10  | F      | 0.666310435280862      | 0.8662254062583 |
| F11  | F      | 0.166310435280862      | 0.8662254062583 |
| F12  | F      | 0.666310435280862      | 0.8662254062583 |
| F13  | F      | 0.333707630021880      | 0.8662254062583 |
| F14  | F      | 0.833707630021880      | 0.8662254062583 |
| F15  | F      | 0.333707630021880      | 0.8662254062583 |
| F16  | F      | 0.833707630021880      | 0.8662254062583 |
| F17  | F      | 0.166310435280862      | 0.8662254062583 |
| F18  | F      | 0.666310435280862      | 0.8662254062583 |
| F19  | F      | 0.166310435280862      | 0.8662254062583 |
| F20  | F      | 0.666310435280862      | 0.8662254062583 |

| Atom | Symbol | Fractional Coordinates | Occupancy |
|------|--------|------------------------|-----------|
| K1   | K      | 0.403722186234813      | 0.86404201683542 |
| K2   | K      | 0.903722186234813      | 0.86404201683542 |
| K3   | K      | 0.096277705765185      | 0.86404201683542 |
| K4   | K      | 0.596277761765183      | 0.86404201683542 |
| K5   | K      | 0.096277705765185      | 0.86404201683542 |
| K6   | K      | 0.596277761765183      | 0.86404201683542 |
| K7   | K      | 0.096277705765185      | 0.86404201683542 |
| K8   | K      | 0.596277761765183      | 0.86404201683542 |

### Cell Parameters
- **a**: 5.23207592596
- **b**: 6.32886644472
- **c**: 7.78802609232
- **α**: 89.999731689
- **β**: 90.0004627961
- **γ**: 86.0991952525
### DFT(PBEsol)+U K2AgF4 B p=90GPa magn.: af2

data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 5.17801508924
_cell_length_b 6.30532849176
_cell_length_c 7.69332671973
_cell_angle_alpha 89.9997791537
_cell_angle_beta 90.0005076835
_cell_angle_gamma 85.6672551559
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.000000013117052 -0.000000030715845 -0.000000039093649 1.0
Ag2 Ag 0.500000011222850 -0.000000025708357 -0.000000044375240 1.0
Ag3 Ag 0.000000031241019 0.500000030101124 0.4999997753140 1.0
Ag4 Ag 0.49999960321301 0.50000000948343020 0.50000005132886 1.0
F5 F 0.164652008902884 0.248456882369069 0.089483966252565 1.0
F6 F 0.664652033237610 0.248456901613340 0.089483986603641 1.0
F7 F 0.335347970766096 0.751543052327551 0.901516076398277 1.0
F8 F 0.835347968898103 0.751543038982531 0.90151609835621 1.0
F9 F 0.335353072006177 0.251540186410068 0.589483269512136 1.0
F10 F 0.835353102131122 0.251540164108068 0.589483283583186 1.0
F11 F 0.164646995030500 0.748459931632087 0.410516730906082 1.0
F12 F 0.6646469649649651 0.748459931571618 0.410516731822228 1.0
F13 F 0.152326745614881 0.107108216547140 0.792048992443070 1.0
F14 F 0.652326743520245 0.107108247743575 0.792048957790495 1.0
F15 F 0.347673232967641 0.892891873303947 0.207951008359861 1.0
F16 F 0.847673242172248 0.892891859386132 0.207951025204425 1.0
F17 F 0.347674684360454 0.392893280145659 0.292048957790495 1.0
F18 F 0.847674674391613 0.392893287127247 0.292048957790495 1.0
F19 F 0.152326462517634 0.607106646160749 0.707940015104322 1.0
F20 F 0.652326435845034 0.607106724535080 0.707940035781410 1.0
K21 K 0.399446468467518 0.392893192437010 0.8636058093615 1.0
K22 K 0.899446468465240 0.392893122964111 0.8636058093615 1.0
K23 K 0.100553520026905 0.607106818818139 0.131974917274664 1.0
K24 K 0.600553495019093 0.607106832760934 0.131974907659881 1.0
K25 K 0.100556539107557 0.107106539150369 0.36023991614178 1.0
K26 K 0.600556532639839 0.107106547819451 0.36023964352451 1.0
K27 K 0.39944343068607 0.892893456356657 0.631976034790470 1.0
K28 K 0.899443472324032 0.892893440391641 0.631976018182255 1.0

### DFT(PBEsol)+U K2AgF4 B p=100GPa magn.: af1

data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 5.12990963188
_cell_length_b 6.28066052336
_cell_length_c 7.60965154182
_cell_angle_alpha 89.9983249427
_cell_angle_beta 89.997406305
_cell_angle_gamma 94.698560816
### DFT(PBEsol)+U K2AgF4 C p=000GPa magn.: af1

```plaintext
# _audit_creation_method 'vasp2cif'

## symmetry_space_group_name_H-M 'P 1'

loop

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

Ag1 Ag 0.5000000000000000 -0.0000000000000000 -0.0000000000000000 1.0

Ag2 Ag 0.0000000000000000 0.0000000000000000 0.0000000000000000 1.0

Ag3 Ag 0.499999970000002 0.499999950000003 0.5000000000000000 1.0

Ag4 Ag 0.999999980000000 0.999999980000000 0.5000000000000000 1.0

F5 F 0.335582422580979 0.247637614338459 0.909346535239078 1.0

F6 F 0.835582468580976 0.247637614338459 0.909346535239078 1.0

F7 F 0.164417578419024 0.499999995000003 0.5000000000000000 1.0

F8 F 0.664417566419023 0.499999995000003 0.5000000000000000 1.0

F9 F 0.164418745889761 0.252600412978566 0.409344938803026 1.0

F10 F 0.664418722889756 0.252600412978566 0.409344938803026 1.0

F11 F 0.335581204110242 0.754476401767021 0.590655030196976 1.0

F12 F 0.835581274110241 0.754476401767021 0.590655030196976 1.0

F13 F 0.348355342001807 0.108128070127581 0.208846246508553 1.0

F14 F 0.848355273001805 0.108128070127581 0.208846246508553 1.0

F15 F 0.151644566998196 0.89182091872418 0.791153815491445 1.0

F16 F 0.651644578998197 0.89182091872418 0.791153815491445 1.0

F17 F 0.151642114801024 0.39182071873631 0.708846246508553 1.0

F18 F 0.651642091801019 0.39182071873631 0.708846246508553 1.0

F19 F 0.348357886198980 0.608129810812641 0.29115225197633 1.0

F20 F 0.848358025198980 0.608129810812641 0.29115225197633 1.0

K21 K 0.101550314981519 0.393169195735844 0.130626276679147 1.0

K22 K 0.601550297981521 0.393169195735844 0.130626276679147 1.0

K23 K 0.39849819018485 0.606830812641555 0.869373739320854 1.0

K24 K 0.89849772018485 0.606830812641555 0.869373739320854 1.0

K25 K 0.398497085101816 0.106812859468478 0.630624478759581 1.0

K26 K 0.89849105011818 0.106812859468478 0.630624478759581 1.0

K27 K 0.101550906498817 0.893168628053512 0.369372551240419 1.0

K28 K 0.601550910498817 0.893168628053512 0.369372551240419 1.0
```

---

```plaintext
## symmetry_space_group_name_H-M 'P 1'

loop

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_occupancy

Ag1 Ag 0.673409917601150 0.20909597838217 0.13837031258237 1.0

Ag2 Ag 0.414095795884345 0.293391283191945 0.611689178863406 1.0

F3 F 0.79793056664354 0.869105851125474 0.18673122736181 1.0

F4 F 0.289400292850642 0.63399265769111 0.563413651725370 1.0

F5 F 0.854966085437398 0.187738476254667 0.356039705345162 1.0

F6 F 0.543761264884316 0.251504940192091 0.875045223051448 1.0

F7 F 0.23247340548911 0.31540150117190 0.39400386492142 1.0

F8 F 0.404716853973960 0.2514891225319 0.875097058052045 1.0

F9 F 0.522097854972275 0.95585709824289 0.702416286529595 1.0

K11 K 0.323271422913445 0.905701739453220 0.13863492676638 1.0

K12 K 0.046608022822641 0.007445912753590 0.68042050996528 1.0
```
```
K13  K  0.040824132158792  0.495622480032266  0.069624426361725  1.0
K14  K  0.764247734892162  0.597319384894665  0.61144397896119  1.0

## DFT(PBEsol)+U K2AgF4 C p=5GPa magn.: af1
_data1
Audit_creation_method 'vasp2cif'
_cell_length_a  5.67347173553
_cell_length_b  6.9259316359
_cell_length_c  6.91074913849
_cell_angle_alpha  64.3259769006
_cell_angle_beta  66.237320589
_cell_angle_gamma  63.221791696
_symmetry_space_group_name_H-M  'P 1'
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.662457880076017  0.203340027677845  0.150522430001661  1.0
Ag2  Ag  0.42943389003226  0.299717565973584  0.599569740933319  1.0
F3   F  0.807323950727364  0.857140013657078  0.189352890181827  1.0
F4   F  0.280136057482622  0.645893421574517  0.560732505697721  1.0
F5   F  0.87475973471024  0.182456870786834  0.354157256321161  1.0
F6   F  0.543702217412797  0.251524757718237  0.87503505803865  1.0
F7   F  0.21723194086935  0.320586809003303  0.395936943300077  1.0
F8   F  0.40376202345454  0.251536060313681  0.874999713984800  1.0
F9   F  0.543439687700457  0.950787598538867  0.701607900761864  1.0
F10  F  0.540494359024521  0.552286042672024  0.04841947069018  1.0
K11  K  0.317738910528787  0.906352509390755  0.46170305668899  1.0
K12  K  0.042642872143943  0.05414062777867  0.69815070756371  1.0
K13  K  0.04481536265668  0.508476174387989  0.05025116245437  1.0
K14  K  0.769721719625753  0.596701831037658  0.603897178766672  1.0

## DFT(PBEsol)+U K2AgF4 C p=10GPa magn.: af1
_data1
Audit_creation_method 'vasp2cif'
_cell_length_a  5.47508872249
_cell_length_b  6.97496263879
_cell_length_c  6.82850004518
_cell_angle_alpha  62.1417245436
_cell_angle_beta  67.2780835702
_cell_angle_gamma  58.5678405555
_symmetry_space_group_name_H-M  'P 1'
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.655429745869612  0.209617337834960  0.1525591135075  1.0
Ag2  Ag  0.431986260725651  0.29345770726614  0.59876935867270  1.0
F3   F  0.807323950727364  0.857140013657078  0.189352890181827  1.0
F4   F  0.280136057482622  0.645893421574517  0.560732505697721  1.0
F5   F  0.87475973471024  0.182456870786834  0.354157256321161  1.0
F6   F  0.543702217412797  0.251524757718237  0.87503505803865  1.0
F7   F  0.21723194086935  0.320586809003303  0.395936943300077  1.0
F8   F  0.40376202345454  0.251536060313681  0.874999713984800  1.0
F9   F  0.543439687700457  0.950787598538867  0.701607900761864  1.0
F10  F  0.540494359024521  0.552286042672024  0.04841947069018  1.0
K11  K  0.317738910528787  0.906352509390755  0.46170305668899  1.0
K12  K  0.042642872143943  0.05414062777867  0.69815070756371  1.0
K13  K  0.04481536265668  0.508476174387989  0.05025116245437  1.0
K14  K  0.769721719625753  0.596701831037658  0.603897178766672  1.0
| K13 | K   | 0.005406506247410 | 0.529025230284406 | 0.032025795545090 | 1.0  |
| K14 | K   | 0.751106031965985 | 0.600541829029895 | 0.595825841238631 | 1.0  |

## DFT(PBEsol)+U K2AgF4 C p=20GPa magn.: af1

| _audit_creation_method | 'vasp2cif' |
|------------------------|------------|
| _cell_length_a         | 5.20657120292 |
| _cell_length_b         | 6.9199552494  |
| _cell_length_c         | 6.65155084058 |
| _cell_angle_alpha      | 59.671537201  |
| _cell_angle_beta       | 66.2431521174 |
| _cell_angle_gamma      | 57.8698275175 |

| symmetry_space_group_name_H-M | 'P 1' |
| loop |
| _atom_site_label |
| _atom_site_type_symbol |
| _atom_site_frac_x |
| _atom_site_frac_y |
| _atom_site_frac_z |
| _atom_site_occupancy |
| Ag1  | Ag   | 0.651365523495639 | 0.191196616135052 | 0.169747356242096 | 1.0  |
| Ag2  | Ag   | 0.436195114286757 | 0.31893876291158  | 0.580527738288312 | 1.0  |
| F3   | F    | 0.864002301551025 | 0.189870213139614 | 1.0  |
| F4   | F    | 0.223849439043668 | 0.667127646813665 | 0.560047032979999 | 1.0  |
| F5   | F    | 0.914430212162690 | 0.349504168576681 | 1.0  |
| F6   | F    | 0.543134655202292 | 0.875584920392963 | 1.0  |
| F7   | F    | 0.173151067855040 | 0.400646835475972 | 1.0  |
| F8   | F    | 0.043496372687620 | 0.87491129137102  | 1.0  |
| F9   | F    | 0.620128074318176 | 0.7153729257581   | 1.0  |
| F10  | F    | 0.467712303806002 | 0.34330469393260  | 1.0  |
| K11  | K    | 0.358930652205328 | 0.14792029061843  | 1.0  |
| K12  | K    | 0.909535509769768 | 0.729910343132531 | 1.0  |
| K13  | K    | 0.996908494038900 | 0.532931029150765 | 1.0  |
| K14  | K    | 0.728340691874532 | 0.601632892077793 | 1.0  |

## DFT(PBEsol)+U K2AgF4 C p=30GPa magn.: af1

| _audit_creation_method | 'vasp2cif' |
|------------------------|------------|
| _cell_length_a         | 5.01548866811 |
| _cell_length_b         | 6.88841166503 |
| _cell_length_c         | 6.52869620901 |
| _cell_angle_alpha      | 58.0502705109 |
| _cell_angle_beta       | 65.5137012344 |
| _cell_angle_gamma      | 57.4531008618 |

| symmetry_space_group_name_H-M | 'P 1' |
| loop |
| _atom_site_label |
| _atom_site_type_symbol |
| _atom_site_frac_x |
| _atom_site_frac_y |
| _atom_site_frac_z |
| _atom_site_occupancy |
| Ag1  | Ag   | 0.646074242273357 | 0.176887250630981 | 0.185703742503100 | 1.0  |
| Ag2  | Ag   | 0.441386532188265 | 0.326227490266691 | 0.564461424309548 | 1.0  |
| F3   | F    | 0.828520744684459 | 0.827238634253716 | 0.190531748556656 | 1.0  |
| F4   | F    | 0.0204744466481249 | 0.675860609729179 | 0.559603510057344 | 1.0  |
| F5   | F    | 0.94181521796305  | 0.158103779182596 | 0.345029777938797 | 1.0  |
| F6   | F    | 0.543524909888935 | 0.251525754863408 | 0.87519383946281  | 1.0  |
| F7   | F    | 0.145805992132792 | 0.349405951488024 | 0.405001374547888 | 1.0  |
| F8   | F    | 0.043770942449154 | 0.251512773130073 | 0.875096148792609 | 1.0  |
| F9   | F    | 0.6203427054117795 | 0.705370524338849 | 1.0  |
| F10  | F    | 0.467198041635901 | 0.554668101697004 | 0.444307985861950 | 1.0  |
| K11  | K    | 0.37690207123159  | 0.885421221001090 | 0.14208566468969  | 1.0  |
| K12  | K    | 0.901685208110412 | 0.969157572344194 | 0.735990480008248 | 1.0  |
## DFT(PBEsol)+U K2AgF4 C p=40GPa magn.: f

**data_1**

```
_loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy

Ag1  Ag   0.754576176693057   0.115027784792048   0.225932741246652   1.0
Ag2  Ag   0.317712694145222   0.392273213405517   0.524214294130104   1.0
F3   F   0.960310573930571   0.784054317990815   0.193547511016249   1.0
F4   F   0.124977867165470   0.728006137306835   0.545185943270709   1.0
F5   F   0.304425344975911   0.895533890484686   0.324765719066767   1.0
F6   F   0.529456984967389   0.259723803105487   0.853925354291575   1.0
F7   F   0.828419056796803   0.411359005204794   0.424616502736100   1.0
F8   F   0.029563113937464   0.239526308078979   0.901812385512272   1.0
F9   F   0.589174198525543   0.995453528518809   0.662337504405613   1.0
F10  F   0.492526428214056   0.507190418673183   0.092749320523673   1.0
K11  K   0.457632625466900   0.848213549519564   0.122932849870267   1.0
K12  K   0.058191176754988   0.986258414704764   0.73805473966301   1.0
K13  K   0.079534597881815   0.518701712472698   0.00642511571623   1.0
K14  K   0.635679580541769   0.646044036421685   0.634137247358225   1.0
```

## DFT(PBEsol)+U K2AgF4 C p=50GPa magn.: f

**data_1**

```
_loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy

Ag1  Ag   0.398267036119565   0.227538158094896   0.340856175756235   1.0
Ag2  Ag   0.517073105716672   0.518666272545452   0.903986847408478   1.0
F3   F   0.225510632525205   0.206817358767089   0.978813321863925   1.0
F4   F   0.690537525327310   0.53422387930355   0.276593637229969   1.0
F5   F   0.980102691681857   0.327370465905180   0.425943749442384   1.0
F6   F   0.456583248435111   0.85092955632474   0.112870164173081   1.0
F7   F   0.900112726404081   0.424131780923986   0.83117184517302   1.0
F8   F   0.98150901733908   0.893275056413324   0.13578602974449   1.0
F9   F   0.541972506850388   0.668498421272716   0.656152001414099   1.0
F10  F   0.373197687079754   0.080480170428085   0.59586073245248   1.0
K11  K   0.98150901733908   0.893275056413324   0.13578602974449   1.0
K12  K   0.076254353987824   0.747126108742241   0.726657747753781   1.0
```
K13 K 0.837741566893305 0.007568952721957 0.529143084523659 1.0
K14 K 0.196119515933566 0.623997764400886 0.277991054942770 1.0

## DFT(PBEsol)+U K2AgF4 C p=60GPa magn.: f
data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 4.6368754809
_cell_length_b 5.95226560859
_cell_length_c 5.95432605191
_cell_angle_alpha 113.504709613
_cell_angle_beta 103.711545242
_cell_angle_gamma 105.639008089
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.408151359081366 0.237073958414797 0.35627574785517 1.0
Ag2 Ag 0.508647825922821 0.521274712016741 0.90980948479293 1.0
F3 F 0.220748977027185 0.197273807817432 0.975364487831534 1.0
F4 F 0.687982592273890 0.543572946393154 0.27508742545532 1.0
F5 F 0.014526131816979 0.325543656124594 0.425308744047801 1.0
F6 F 0.45080805047549 0.29903828341572 0.13972444244496 1.0
F7 F 0.92404579565624 0.421998435922717 0.82279043532354 1.0
F8 F 0.93419010710431 0.858610856049573 0.11664913465345 1.0
F9 F 0.541952991679715 0.673082153552812 0.657464224127807 1.0
F10 F 0.36662774544689 0.075389417300357 0.594796185186652 1.0
K11 K 0.716995211624697 0.127358158515314 0.976080712900267 1.0
K12 K 0.07783977171013 0.744738513058046 0.67366360503929 1.0
K13 K 0.83143236942937 0.00103270595614 0.52706916769605 1.0
K14 K 0.197488019005640 0.624548960950264 0.27130290046650 1.0

## DFT(PBEsol)+U K2AgF4 C p=70GPa magn.: f
data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 4.58393947221
_cell_length_b 5.89317023134
_cell_length_c 5.8960871193
_cell_angle_alpha 113.471684318
_cell_angle_beta 103.954188382
_cell_angle_gamma 105.651066274
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.408151359081366 0.237073958414797 0.35627574785517 1.0
Ag2 Ag 0.508647825922821 0.521274712016741 0.90980948479293 1.0
F3 F 0.220748977027185 0.197273807817432 0.975364487831534 1.0
F4 F 0.687982592273890 0.543572946393154 0.27508742545532 1.0
F5 F 0.014526131816979 0.325543656124594 0.425308744047801 1.0
F6 F 0.45080805047549 0.29903828341572 0.13972444244496 1.0
F7 F 0.92404579565624 0.421998435922717 0.82279043532354 1.0
F8 F 0.93419010710431 0.858610856049573 0.11664913465345 1.0
F9 F 0.541952991679715 0.673082153552812 0.657464224127807 1.0
F10 F 0.36662774544689 0.075389417300357 0.594796185186652 1.0
K11 K 0.716995211624697 0.127358158515314 0.976080712900267 1.0
K12 K 0.07783977171013 0.744738513058046 0.67366360503929 1.0
K13 K 0.83143236942937 0.00103270595614 0.52706916769605 1.0
K14 K 0.197488019005640 0.624548960950264 0.27130290046650 1.0
| Symbol | Type | x     | y     | z     | Occupancy |
|--------|------|-------|-------|-------|------------|
| Ag1    | Ag   | 0.413097309616901 | 0.231487520678861 | 0.347852291518770 | 1.0 |
| Ag2    | Ag   | 0.486162459463252 | 0.504585167546324 | 0.88698075302661 | 1.0 |
| F3     | F    | 0.223647156641171 | 0.207050107988380 | 0.97755423769710 | 1.0 |
| F4     | F    | 0.996606176743505 | 0.328199515639343 | 0.43462844679997 | 1.0 |
| F5     | F    | 0.459053921179965 | 0.925208425006384 | 0.114356483392342 | 1.0 |
| F6     | F    | 0.89594488047677 | 0.425074358888786 | 0.823910534434397 | 1.0 |
| F7     | F    | 0.889764343501952 | 0.891705742513453 | 0.134749781792309 | 1.0 |
| F8     | F    | 0.551146716775683 | 0.681568025173483 | 0.66140875322570 | 1.0 |
| F9     | F    | 0.366529796639540 | 0.725379364422217 | 0.595641267627173 | 1.0 |
| K1     | K    | 0.716824705830604 | 0.12969167361335 | 0.984747204254660 | 1.0 |
| K2     | K    | 0.081732841432419 | 0.751704727480480 | 0.725582729811713 | 1.0 |
| K3     | K    | 0.839042132803045 | 0.00259396792532 | 0.529965232596396 | 1.0 |
| K4     | K    | 0.195486252699148 | 0.62102551302321 | 0.274862392836702 | 1.0 |

---

| Symbol | Type | x     | y     | z     | Occupancy |
|--------|------|-------|-------|-------|------------|
| Ag1    | Ag   | 0.455934267033396 | 0.495852605764583 | 0.875352062011463 | 1.0 |
| Ag2    | Ag   | 0.225009977607044 | 0.212123394344335 | 0.966059862301939 | 1.0 |
| F3     | F    | 0.687187613093289 | 0.537854172434384 | 0.287094737998163 | 1.0 |
| F4     | F    | 0.032471475264892 | 0.331490416187363 | 0.441071632292804 | 1.0 |
| F5     | F    | 0.456161528970063 | 0.874561758083107 | 0.126451089929629 | 1.0 |
| F6     | F    | 0.880027884289896 | 0.418526771639737 | 0.81196375311307 | 1.0 |
| F7     | F    | 0.956510787483055 | 0.87527893398930 | 0.126620626934352 | 1.0 |
| F8     | F    | 0.553762358087977 | 0.693330875605015 | 0.668335498742858 | 1.0 |
| F9     | F    | 0.358925797919256 | 0.056829166893633 | 0.58471102503938 | 1.0 |
| K1     | K    | 0.725389329168431 | 0.133263048716351 | 0.986779728098878 | 1.0 |
| K2     | K    | 0.084904451403723 | 0.758159933958971 | 0.733031468510742 | 1.0 |
## DFT(PBEsol) + U K2AgF4 C p=100GPa magn.: af1

data_1

_audit_creation_method  'vasp2cif'
_cell_length_a  4.46059922009
_cell_length_b  5.69900371671
_cell_length_c  5.82610045646
_cell_angle_alpha  112.954379784
_cell_angle_beta  105.751027396
_cell_angle_gamma  105.342821034
_symmetry_space_group_name_H-M  'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy

Ag1  Ag  0.920059748660868  0.123213332563819  0.378306097259380  1.0
Ag2  Ag  0.420797795060215  0.379755293755287  0.874626531356601  1.0
F3  F  0.742271546789800  0.755553737181167  0.966805229945816  1.0
F4  F  0.597821991434894  0.747414740013048  0.286237131725046  1.0
F5  F  0.409372467452631  0.109731267869910  0.440531947948704  1.0
F6  F  0.670442217889984  0.25142221387018  0.12670580847482  1.0
F7  F  0.931242693683076  0.393367695249568  0.812707676415972  1.0
F8  F  0.170638255858485  0.251808263458185  0.126549821689809  1.0
F9  F  0.113937842419306  0.974929130491784  0.668090077871254  1.0
F10 F  0.22673544237016  0.528313873547354  0.585089659323738  1.0
K11 K  0.261562203977990  0.853082126140135  0.986528330558793  1.0
K12 K  0.646884782401549  0.974218415988766  0.732290798359257  1.0
K13 K  0.693781371072451  0.52834254981184  0.520817405646222  1.0
K14 K  0.728576666057952  0.774587233667831  0.26599645635531  1.0

## DFT(PBEsol) + U K2AgF4 D p=000GPa magn.: f

data_1

_audit_creation_method  'vasp2cif'
_cell_length_a  4.90613313321
_cell_length_b  7.52063247457
_cell_length_c  7.5299786112
_cell_angle_alpha  100.797300003
_cell_angle_beta  108.894371377
_cell_angle_gamma  109.003038006
_symmetry_space_group_name_H-M  'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy

Ag1  Ag  0.920059748660868  0.123213332563819  0.378306097259380  1.0
Ag2  Ag  0.420797795060215  0.379755293755287  0.874626531356601  1.0
F3  F  0.742271546789800  0.755553737181167  0.966805229945816  1.0
F4  F  0.597821991434894  0.747414740013048  0.286237131725046  1.0
K11 K  0.261562203977990  0.853082126140135  0.986528330558793  1.0
K12 K  0.646884782401549  0.974218415988766  0.732290798359257  1.0
K13 K  0.693781371072451  0.52834254981184  0.520817405646222  1.0
K14 K  0.728576666057952  0.774587233667831  0.26599645635531  1.0
| Code | Atom | Symbol | Fract. X | Fract. Y | Fract. Z | Occupancy |
|------|------|--------|----------|----------|----------|------------|
| **K13** | K | 0.231440694606426 | 0.58715879363679 | 0.004199196243683 | 1.0 |
| **K14** | K | 0.729559842309551 | 0.08555447539835 | 0.502801869667055 | 1.0 |

## DFT(PBEsol)+U K2AgF4 D p=5GPa magn.: f

```plaintext
_data
data

_audit_creation_method 'vasp2cif'
_cell_length_a 4.76227725881
_cell_length_b 7.26482340535
_cell_length_c 7.26565077189
_cell_angle_alpha 101.202380457
_cell_angle_beta 109.047320999
_cell_angle_gamma 109.172912656
_symmetry_space_group_name_H-M 'P 1'

_loop_atom_site_label
_loop_atom_site_type_symbol
_loop_atom_site_fract_x
_loop_atom_site_fract_y
_loop_atom_site_fract_z
_loop_atom_site_occupancy

Ag1 | Ag | 0.981133097507813 | 0.680746332751978 | 0.40707649150092 | 1.0 |
Ag2 | Ag | 0.468640854398579 | 0.180638508502777 | 0.907022879497733 | 1.0 |
F3  | F  | 0.462402028598916 | 0.363801767132888 | 0.724374626793925 | 1.0 |
F4  | F  | 0.19251796848687 | 0.744868686837398 | 0.71978034764366 | 1.0 |
F5  | F  | 0.966655585596845 | 0.180795954429795 | 0.90702633478400 | 1.0 |
F6  | F  | 0.726383174161717 | 0.36743812890301 | 0.3423278955216 | 1.0 |
F7  | F  | 0.480944773137795 | 0.68076866136461 | 0.40703275895002 | 1.0 |
F8  | F  | 0.167936666202229 | 0.99364505828109 | 0.47176558214019 | 1.0 |
F9  | F  | 0.790863961350732 | 0.617211486809017 | 0.09445393183851 | 1.0 |
F10 | F  | 0.455264524383615 | -0.002325010600323 | 0.08978453067744 | 1.0 |
F11 | F  | 0.735686324042920 | 0.87059419493713 | 0.81743963162948 | 1.0 |
F12 | F  | 0.225187950734126 | 0.26931920673796 | 0.30632195710884 | 1.0 |
F13 | F  | 0.974932795205269 | 0.5802554415899 | -0.00342046797816 | 1.0 |
F14 | F  | 0.735241633937250 | 0.09223517124119 | 0.50778428885613 | 1.0 |

## DFT(PBEsol)+U K2AgF4 D p=10GPa magn.: f

```plaintext
_data

_audit_creation_method 'vasp2cif'
_cell_length_a 4.65827333147
_cell_length_b 7.29358329734
_cell_length_c 7.29278491311
_cell_angle_alpha 99.1973140273
_cell_angle_beta 113.633509601
_cell_angle_gamma 113.628092751
_symmetry_space_group_name_H-M 'P 1'

_loop_atom_site_label
_loop_atom_site_type_symbol
_loop_atom_site_fract_x
_loop_atom_site_fract_y
_loop_atom_site_fract_z
_loop_atom_site_occupancy

Ag1 | Ag | 0.975765539730934 | 0.680746332751978 | 0.40707649150092 | 1.0 |
Ag2 | Ag | 0.468640854398579 | 0.180638508502777 | 0.907022879497733 | 1.0 |
F3  | F  | 0.462402028598916 | 0.363801767132888 | 0.724374626793925 | 1.0 |
F4  | F  | 0.19251796848687 | 0.744868686837398 | 0.71978034764366 | 1.0 |
F5  | F  | 0.966655585596845 | 0.180795954429795 | 0.90702633478400 | 1.0 |
F6  | F  | 0.726383174161717 | 0.36743812890301 | 0.3423278955216 | 1.0 |
F7  | F  | 0.480944773137795 | 0.68076866136461 | 0.40703275895002 | 1.0 |
F8  | F  | 0.167936666202229 | 0.99364505828109 | 0.47176558214019 | 1.0 |
F9  | F  | 0.790863961350732 | 0.617211486809017 | 0.09445393183851 | 1.0 |
F10 | F  | 0.455264524383615 | -0.002325010600323 | 0.08978453067744 | 1.0 |
F11 | F  | 0.735686324042920 | 0.87059419493713 | 0.81743963162948 | 1.0 |
F12 | F  | 0.225187950734126 | 0.26931920673796 | 0.30632195710884 | 1.0 |
F13 | F  | 0.974932795205269 | 0.5802554415899 | -0.00342046797816 | 1.0 |
F14 | F  | 0.735241633937250 | 0.09223517124119 | 0.50778428885613 | 1.0 |
```
### DFT(PBEsol)+U K2AgF4 D p=20GPa magn.: af1

|   |   |   |   |   |
|---|---|---|---|---|
| K13 | K | 0.223969841609149 | 0.597857656944920 | 0.989561667979582 | 1.0 |
| K14 | K | 0.726702003237117 | 0.078703524926492 | 0.509297102131161 | 1.0 |

## DFT(PBEsol)+U K2AgF4 D p=30GPa magn.: af1

|   |   |   |   |   |
|---|---|---|---|---|
| K11 | K | 0.7561730712552226 | 0.680726808510253 | 0.407039661190718 | 1.0 |
| K12 | K | 0.194708857483233 | 0.237795300353519 | 0.288297428891516 | 1.0 |
| K13 | K | 0.975487259483233 | 0.407097292573796 | 0.481196680491835 | 1.0 |
| K14 | K | 0.756306769557020 | 0.123689534757050 | 0.525816700519744 | 1.0 |

```python
# DFT(PBEsol)+U K2AgF4 D p=20GPa magn.: af1
data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 4.52910056368
_cell_length_b 6.97156519213
_cell_length_c 6.97062123804
_cell_angle_alpha 106.85931494
_cell_angle_beta 108.954497962
_cell_angle_gamma 109.006580669
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.975622712552226  0.680726808510253  0.407039661190718  1.0
Ag2  Ag  0.475177739935575  0.180726790582565  0.907028158235516  1.0
F3   F  0.47546126283771  0.39279103267975  0.695046204534658  1.0
F4   F  0.167914977038548  0.753322127750519  0.718663176650850  1.0
F5   F  0.75120413197512  0.180774550396036  0.907082155761253  1.0
F6   F  0.7562383841617  0.680755760217275  0.407097292573796  1.0
F7   F  0.168378382527566  0.481196680491835  0.907028158235516  1.0
F8   F  0.783170560584245  0.608133715809385  0.907028158235516  1.0
F9   F  0.475413272400692  0.680754833273448  0.907039661190718  1.0
F10  F  0.474475057207956  0.968711437274422  0.119073777560703  1.0
K11  K  0.7561730712552226  0.680726808510253  0.407039661190718  1.0
K12  K  0.475177739935575  0.180726790582565  0.907028158235516  1.0
K13  K  0.47546126283771  0.39279103267975  0.695046204534658  1.0
K14  K  0.167914977038548  0.753322127750519  0.718663176650850  1.0
```

```python
# DFT(PBEsol)+U K2AgF4 D p=30GPa magn.: af1
data_1
_audit_creation_method 'vasp2cif'
_cell_length_a 4.42221645251
_cell_length_b 6.85613617315
_cell_length_c 6.81941708933
_cell_angle_alpha 107.484374964
_cell_angle_beta 108.413710125
_cell_angle_gamma 109.335015044
_symmetry_space_group_name_H-M 'P 1'
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.975413272400692  0.680754833273448  0.907039661190718  1.0
Ag2  Ag  0.475177739935575  0.180726790582565  0.907028158235516  1.0
F3   F  0.47546126283771  0.39279103267975  0.695046204534658  1.0
F4   F  0.167914977038548  0.753322127750519  0.718663176650850  1.0
F5   F  0.75120413197512  0.180774550396036  0.907082155761253  1.0
F6   F  0.7562383841617  0.680755760217275  0.407097292573796  1.0
F7   F  0.168378382527566  0.481196680491835  0.907028158235516  1.0
F8   F  0.783170560584245  0.608133715809385  0.907028158235516  1.0
F9   F  0.475413272400692  0.680754833273448  0.907039661190718  1.0
F10  F  0.474475057207956  0.968711437274422  0.119073777560703  1.0
K11  K  0.7561730712552226  0.680726808510253  0.407039661190718  1.0
K12  K  0.475177739935575  0.180726790582565  0.907028158235516  1.0
K13  K  0.47546126283771  0.39279103267975  0.695046204534658  1.0
K14  K  0.167914977038548  0.753322127750519  0.718663176650850  1.0
```
### DFT(PBEsol)+U K2AgF4 D p=40GPa magn.: f

```plaintext
data_1

_audit_creation_method 'vasp2cif'
_cell_length_a 4.68054241982
_cell_length_b 6.93859875308
_cell_length_c 5.86099037487

_symmetry_space_group_name_H-M 'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1   Ag   0.97531068831861 0.680570912779707 0.407204174875169 1.0
Ag2   Ag   0.475528254863683 0.180852544618233 0.906871379986519 1.0
F3    F   0.679322385553611 0.404152457943894 0.683581001069243 1.0
F4    F   0.298321974859050 0.812513677638790 0.73709119239248 1.0
F5    F   0.975754035667343 0.181056739093208 0.90678586674223 1.0
F6    F   0.863453413421192 0.350788892255700 0.275562204971870 1.0
F7    F   0.475136876423349 0.680453514203990 0.40799750667200 1.0
F8    F   0.114043542728915 0.010322403214786 0.53838720634153 1.0
F9    F   0.652697093504628 0.549070112941990 0.07725107001693 1.0
F10   F   0.271691855765120 0.97567649570043 0.130373279277627 1.0
K11   K   0.76091208046504 0.776452363495572 0.806916457685958 1.0
K12   K   0.2641239338928 0.280703585758822 0.311079301454576 1.0
K13   K   0.475136876423349 0.689322385553611 0.255040538500923 1.0
K14   K   0.686229430403147 0.80359858504266 0.502723093743100 1.0

## DFT(PBEsol)+U K2AgF4 D p=50GPa magn.: af1

data_1

_audit_creation_method 'vasp2cif'
_cell_length_a 4.36644319958
_cell_length_b 6.55461964231
_cell_length_c 6.276685092

_symmetry_space_group_name_H-M 'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1   Ag   0.712118273622815 0.744220162087384 0.255040538500923 1.0
Ag2   Ag   0.698606994229697 0.188764269301419 0.292294724566219 1.0
F3    F   0.892692427299597 0.408469962289481 0.65763151555859 1.0
F4    F   0.51794263120117 0.524400628329855 0.889721515739506 1.0
F5    F   0.117771166945407 0.123021351365922 0.333850645735804 1.0
F6    F   0.421156563639804 0.30142322502440 0.112865817195797 1.0
F7    F   0.292850466230443 0.809904692131069 0.21353982571925 1.0
F8    F   0.808740466230443 0.97628565631046 0.616920849005466 1.0
F9    F   0.504955252700036 0.631585009505618 0.434611446899403 1.0
F10   F   0.601832316731267 0.956582619871395 0.930441416817955 1.0
K11   K   0.0373043417949 0.840999013742923 0.889678130885602 1.0
K12   K   0.98063210157233 0.373757273541986 0.99977268966502 1.0
```
## DFT(PBEsol)+U K2AgF4 D p=60GPa magn.: af1

### loop
- **atom_site_label**
- **atom_site_type_symbol**
- **atom_site_fract_x**
- **atom_site_fract_y**
- **atom_site_fract_z**
- **atom_site_occupancy**

**Ag1** Ag 0.715495676053985 0.746249901490913 0.242451481345869 1.0
**Ag2** Ag 0.69164291125460 0.186636753080424 0.30492976447931 1.0
**F3** F 0.907528718037279 0.419039552326410 0.673288123353892 1.0
**F4** F 0.503020566145818 0.513902372711853 0.874109766929024 1.0
**F5** F 0.13003923265106 0.132271705730584 0.336325645114344 1.0
**F6** F 0.429493068113148 0.301582737994436 0.10829456564969 1.0
**F7** F 0.280639506425959 0.800606397283565 0.211020855256193 1.0
**F8** F 0.817775368145449 0.98150516182657 0.612790916621559 1.0
**F9** F 0.976308143500260 0.631373303765439 0.439138405813194 1.0

## DFT(PBEsol)+U K2AgF4 D p=70GPa magn.: af1

### loop
- **atom_site_label**
- **atom_site_type_symbol**
- **atom_site_fract_x**
- **atom_site_fract_y**
- **atom_site_fract_z**
- **atom_site_occupancy**

**Ag1** Ag 0.717439215798294 0.745091058106541 0.2258765308530176 1.0
**Ag2** Ag 0.69164291125460 0.186636753080424 0.30492976447931 1.0
**F3** F 0.907528718037279 0.419039552326410 0.673288123353892 1.0
**F4** F 0.503020566145818 0.513902372711853 0.874109766929024 1.0
**F5** F 0.13003923265106 0.132271705730584 0.336325645114344 1.0
**F6** F 0.429493068113148 0.301582737994436 0.10829456564969 1.0
**F7** F 0.280639506425959 0.800606397283565 0.211020855256193 1.0
**F8** F 0.817775368145449 0.98150516182657 0.612790916621559 1.0
**F9** F 0.976308143500260 0.631373303765439 0.439138405813194 1.0
K13  K  0.425600907312806   0.578986831248195   0.529105374126695   1.0
K14  K  0.381263475627934   0.079375947538953   0.657136841939948   1.0

## DFT(PBEsol)+U K2AgF4 D p=80GPa magn.: af1
data_1
_audit_creation_method 'vasp2cif'
cell_length_a  4.37218832545
cell_length_b  6.25618938211
cell_length_c  5.8699948305
cell_angle_alpha  115.006091407
cell_angle_beta  97.963587135
[cell_angle_gamma  111.191247283

_symmetry_space_group_name_H-M  'P 1'
loop
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.717265088640230   0.742508996465642   0.214732790525779   1.0
Ag2  Ag  0.693001444371980   0.190527074825966   0.339632456308880   1.0
F3   F  0.932856914782475   0.442896424781336   0.706005598239799   1.0
F4   F  0.479721396819333   0.490182721836765   0.841385902872807   1.0
F5   F  0.146496564310331   0.148790913380591   0.340944502541645   1.0
F6   F  0.455547392555337   0.303971965678010   0.102275099483364   1.0
F7   F  0.263737928628210   0.784128592561217   0.206380224366838   1.0
F8   F  0.836548351760954   -0.000011540182070   0.600464630979400   1.0
F9   F  0.955616762387407   0.628868903741368   0.449447367061777   1.0
F10  F  0.574916957380143   0.94704959823530   1.0
K11  K  0.027479778700336   0.859978766959021   0.89146232472696   1.0
K12  K  0.984380475030834   0.346594154072391   0.202423497225579   1.0
K13  K  0.382997076810323   0.072774111637797   0.65579192274618   1.0

## DFT(PBEsol)+U K2AgF4 D p=90GPa magn.: af1
data_1
_audit_creation_method 'vasp2cif'
cell_length_a  4.35205244864
cell_length_b  6.18417881155
cell_length_c  5.80465209888
[cell_angle_alpha  114.871652973
[cell_angle_beta  98.3166255241
[cell_angle_gamma  111.134450988

_symmetry_space_group_name_H-M  'P 1'
loop
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.717953908600773   0.740390250595090   0.207652402061259   1.0
Ag2  Ag  0.692811986659894   0.192462954152233   0.339632456308880   1.0
F3   F  0.932856914782475   0.442896424781336   0.706005598239799   1.0
F4   F  0.479721396819333   0.490182721836765   0.841385902872807   1.0
F5   F  0.146496564310331   0.148790913380591   0.340944502541645   1.0
F6   F  0.455547392555337   0.303971965678010   0.102275099483364   1.0
F7   F  0.263737928628210   0.784128592561217   0.206380224366838   1.0
F8   F  0.836548351760954   -0.000011540182070   0.600464630979400   1.0
F9   F  0.955616762387407   0.628868903741368   0.449447367061777   1.0
F10  F  0.574916957380143   0.94704959823530   1.0
K11  K  0.027479778700336   0.859978766959021   0.89146232472696   1.0
K12  K  0.984380475030834   0.346594154072391   0.202423497225579   1.0
K13  K  0.382997076810323   0.072774111637797   0.65579192274618   1.0
## DFT(PBEsol)+U K2AgF4 D p=100GPa magn.: af1

```plaintext
_data_1
_audit_creation_method 'vasp2cif'
_cell_length_a  4.46063020429
_cell_length_b  5.73288033334
_cell_length_c  5.82656981224
_cell_angle_alpha  114.671407494
_cell_angle_beta  105.752434609
_cell_angle_gamma  103.838224661
_symmetry_space_group_name_H-M  'P 1'
_loop_
_atom_site_label  _atom_site_type_symbol
_atom_site_fract_x  _atom_site_fract_y  _atom_site_fract_z  _atom_site_occupancy
Ag1  Ag  0.481734752006825  0.435410876123862  0.153811087556267  1.0
Ag2  Ag  0.725792625644151  0.178899422544729  0.393764933532057  1.0
F3   F  0.603974837243718  0.307725303796986  0.774199870304816  1.0
F4   F  0.103325754266123  0.306723821621337  0.772947362969597  1.0
F5   F  0.223145882372065  0.165457624384597  0.317894850108775  1.0
F6   F  0.672641860253648  0.503316166038101  0.109902569614392  1.0
F7   F  0.985016464224322  0.449088018309156  0.229352893463409  1.0
F8   F  0.824418217628248  0.584107145979598  0.591967737559335  1.0
F9   F  0.536217017410060  0.811150965750048  0.437415543534937  1.0
F10  F  0.383902118889145  0.306895245744104  0.955661665177788  1.0
K11  K  0.850131383299295  0.29896225035966  0.890632215192537  1.0
K12  K  0.094379473396147  0.705613621559630  0.30203682271320  1.0
K13  K  0.357851334497543  0.58455322029195  0.65677499471321  1.0
```

## DFT(PBEsol)+U K2AgF4 E p=000GPa magn.: f

```plaintext
_data_1
_audit_creation_method 'vasp2cif'
_cell_length_a  7.29552613033
_cell_length_b  7.29559583315
_cell_length_c  8.20470904155
_cell_angle_alpha  90.0
_cell_angle_beta  90.0
_cell_angle_gamma  90.0000117875
_symmetry_space_group_name_H-M  'P 1'
_loop_
_atom_site_label  _atom_site_type_symbol
_atom_site_fract_x  _atom_site_fract_y  _atom_site_fract_z  _atom_site_occupancy
Ag1  Ag  0.000000000000000  0.999999490000000  0.000000260000000  1.0
Ag2  Ag  0.000000012999997  0.499999410000000  0.750018114977003  1.0
Ag3  Ag  0.499999329999999  0.499999410000000  0.500013999999997  1.0
Ag4  Ag  0.999994100000001  0.999999490000000  0.249979735022997  1.0
F5   F  0.431323123396055  0.277080934817619  0.20314924573970  1.0
F6   F  0.568676846603942  0.722918545182381  0.20314924573970  1.0
F7   F  0.277049864817741  0.56865206604182  0.796852855426032  1.0
F8   F  0.7229050095182256  0.431343283395819  0.796850435426030  1.0
F9   F  0.43162348460957  0.22902646008904  0.54643613760665  1.0
F10  F  0.56837621539046  0.77798193991094  0.54643933760665  1.0
F11  F  0.277120238874957  0.931621805610236  0.95355170755216  1.0
F12  F  0.722879721125040  0.068377543489767  0.95355653755211  1.0
```
## DFT(PBEsol)+U K2AgF4 E p=5GPa magn.: f

data_1

## DFT(PBEsol)+U K2AgF4 E p=10GPa magn.: f

data_1
cell_length_a 6.91499294007
_cell_length_b 6.91513645352
_cell_length_c 7.63456028221
_cell_angle_alpha 90.0
_cell_angle_beta 90.0
_cell_angle_gamma 90.0
_symmetry_space_group_name_H-M 'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.000000350000000 0.999994900000000 0.000000260000000 1.0
Ag2 Ag 0.000000129999997 0.499997400000000 0.750018114977003 1.0
Ag3 Ag 0.499992999999999 0.499997400000000 0.500013399999997 1.0
Ag4 Ag 0.499994100000000 0.999994900000000 0.249979735022979 1.0
K21 K 0.749976471367559 0.397416371450815 0.125087079133688 1.0
K22 K 0.250021376437554 0.749976471367559 0.874915590866314 1.0
K23 K 0.749976471367559 0.250021376437554 0.374916577283980 1.0
K24 K 0.250021376437554 0.749976471367559 0.625080052716025 1.0
K25 K 0.749976471367559 0.250021376437554 0.95919836691962 1.0
K26 K 0.749976471367559 0.250021376437554 0.95919836691962 1.0
K27 K 0.250021376437554 0.749976471367559 0.95919836691962 1.0
K28 K 0.749976471367559 0.250021376437554 0.95919836691962 1.0

## DFT(PBEsol)+U K2AgF4
E p=20GPa magn.: f

---

audit_creation_method 'vasp2cif'
_cell_length_a 6.74624748247
_cell_length_b 6.74645957172
_cell_length_c 7.33811592226
_cell_angle_alpha 90.0
_cell_angle_beta 90.0
_cell_angle_gamma 90.0
_symmetry_space_group_name_H-M 'P 1'

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.000000350000000 0.999994900000000 0.000000260000000 1.0
Ag2 Ag 0.000000129999997 0.499997400000000 0.750018114977003 1.0
Ag3 Ag 0.499992999999999 0.499997400000000 0.500013399999997 1.0
Ag4 Ag 0.499994100000000 0.999994900000000 0.249979735022979 1.0

---
## DFT(PBEsol)+U K2AgF4 E p=30GPa magn.: f

data_1
_audit_creation_method 'vasp2cif'
_loop_
_cell_length_a 6.62626697711
_cell_length_b 6.62653483829
_cell_length_c 7.14047185947
_cell_angle_alpha 90.0
_cell_angle_beta 90.0
_cell_angle_gamma 90.0
_symmetry_space_group_name_H-M 'P 1' 
_atoms
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1 Ag 0.0000000350000000 0.9999994900000000 0.000000129999997 1.0
Ag2 Ag 0.4999997400000000 0.4999997400000000 0.500000139999997 1.0
Ag3 Ag 0.4999997400000000 0.4999997400000000 0.500000139999997 1.0
Ag4 Ag 0.4999994100000000 0.9999994900000000 0.24999735022997 1.0
F5 F 0.424863289812914 0.295784010084622 0.210542809256925 1.0
F6 F 0.575136680187083 0.704215469915377 0.210537979256923 1.0
F7 F 0.295129577814146 0.575116034794150 0.789459870743077 1.0
F8 F 0.704247002218581 0.424834552058551 0.789457450743075 1.0
F9 F 0.424999158338024 0.204207628338680 0.539216040593443 1.0
F10 F 0.575000201661980 0.79573211661319 0.539214840593443 1.0
F11 F 0.295125273911451 0.924997822706066 0.960718007193317 1.0
F12 F 0.704184686085845 0.075001527293997 0.539214840593443 1.0
F13 F 0.478903836124800 0.295827256545102 0.960773349406551 1.0
F14 F 0.295815273911451 0.924997822706066 0.539214840593443 1.0
F15 F 0.704184686085845 0.075001527293997 0.539214840593443 1.0
F16 F 0.424863289812914 0.295784010084622 0.210542809256925 1.0
F17 F 0.925012476387521 0.704215469915377 0.210537979256923 1.0
F18 F 0.074988303612480 0.295827256545102 0.960773349406551 1.0
F19 F 0.795800919027642 0.425014504656505 0.460773349406551 1.0
F20 F 0.204197680972356 0.574986335343494 0.460773349406551 1.0
K21 K 0.749985798846583 0.398144276245032 0.125091327380587 1.0
K22 K 0.250010161153414 0.601855203754968 0.125091327380587 1.0
K23 K 0.398157620129348 0.250004881509995 0.874909542619413 1.0
K24 K 0.601843699706467 0.749995958490004 0.874910752619414 1.0
K25 K 0.750008049249276 0.101835411906358 0.625086100696294 1.0
K26 K 0.249999107505727 0.898164208093459 0.625086100696294 1.0
K27 K 0.898152691977779 0.750014269605842 0.374910529037081 1.0
K25  K   0.749995618166231   0.101945758038921   0.625090570482558   1.0
K26  K   0.250004341833773   0.898053861961076   0.625090570482558   1.0
K27  K   0.898042343617743   0.750001838498401   0.374906059517477   1.0
K28  K   0.101956406382260   0.249999001501597   0.374906059517477   1.0

## DFT(PBEsol)+U K2AgF4 E p=40GPa magn.: f
data_1
_audit_creation_method   'vasp2cif'
cell_length_a    6.53020644913
cell_length_b    6.53052237003
cell_length_c    6.99228012213
cell_angle_alpha  90.0
_cell_angle_beta  90.0
_cell_angle_gamma 90.0
_symmetry_space_group_name_H-M    'P 1'
loop_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy

Ag1   Ag   0.000000350000000   0.999999490000000   0.000000260000000   1.0
Ag2   Ag   0.000000129999997   0.499999740000000   0.750018114977003   1.0
Ag3   Ag   0.499999299999999   0.499999740000000   0.500001339999997   1.0
Ag4   Ag   0.499994100000001   0.999994900000000   0.249979735022997   1.0
F5    F    0.423211616105331    0.301251480872866   0.211834981750256   1.0
F6    F    0.576783599394667    0.69874999127134    0.211830151875025   1.0
F7    F    0.301220432408234    0.576771711481875    0.788167698249475   1.0
F8    F    0.698779536591763    0.423231778518125    0.788165278249474   1.0
F9    F    0.42331589947992    0.198756619960896    0.537907186859775   1.0
F10   F    0.576688371052012    0.801244220039103    0.537905865859775   1.0
F11   F    0.301262771732021    0.923096502625008    0.962080654453005   1.0
F12   F    0.698733682826795    0.076689979374975    0.962085444530000   1.0
F13   F    0.923239242612173    0.801217113829688    0.711850661803359   1.0
F14   F    0.076760037387832    0.198723661703132    0.711848241803365   1.0
F15   F    0.801246446365058    0.076780734975042    0.288152018196635   1.0
F16   F    0.198753153634946    0.923219155024963    0.28815080196642   1.0
F17   F    0.923324306997489    0.698721215077121    0.03792721554699   1.0
F18   F    0.076676473002511    0.301278264922886    0.37925964556499   1.0
F19   F    0.801251922289392    0.423326332213006    0.426022021340221   1.0
F20   F    0.198746677101066    0.576674507789992    0.426087033140223   1.0
K21   K    0.75001278273828    0.397714224627297    0.125103393473036   1.0
K22   K    0.249987181726168    0.602285255372702    0.125103393473036   1.0
K23   K    0.957275268208045    0.4249981902023109    0.87499276652695   1.0
K24   K    0.602273757191950    0.750018937976890    0.874900486652695   1.0
K25   K    0.749985069820311    0.101265463524272    0.625096366929643   1.0
K26   K    0.250014890177973    0.897734156475725    0.625096366929643   1.0
K27   K    0.897722634656477    0.749991290118956    0.374900263070362   1.0
K28   K    0.101276115343526    0.250009549881042    0.374900263070362   1.0

## DFT(PBEsol)+U K2AgF4 E p=50GPa magn.: f
data_1
_audit_creation_method   'vasp2cif'
cell_length_a    6.45023004
cell_length_b    6.45023004
cell_length_c    6.87494378
cell_angle_alpha  90.0
cell_angle_beta   90.0
cell_angle_gamma  90.0
_symmetry_space_group_name_H-M    'P 1'
loop_atom_site_label
_atom_site_type_symbol
|     |     |     |     |     |
|-----|-----|-----|-----|-----|
| F17 | F   | 0.695619993173557 | 0.07783706924717 | 0.03754623688901 | 1.0 |
| F18 | F   | 0.304379326826443 | 0.92214893075280 | 0.03754183688907 | 1.0 |
| F19 | F   | 0.39640258455496  | 0.249977800000001| 0.12499899999998 | 1.0 |
| F20 | F   | 0.75000149999998 | 0.396946948455495 | 0.87500319999997 | 1.0 |
| K21 | K   | 0.396940258455496 | 0.249998900000001| 0.624997620000002| 1.0 |
| K22 | K   | 0.603062721544509 | 0.749998100000001| 0.125000300000001| 1.0 |
| K23 | K   | 0.89640928455494  | 0.74999889999998 | 0.625000100000001| 1.0 |
| K24 | K   | 0.89640928455494  | 0.74999889999998 | 0.625000100000001| 1.0 |

## DFT(PBEsol)+U K2AgF4 E p=70GPa magn.: f
| data_1 |     |     |     |     |
|--------|-----|-----|-----|-----|
| _audit_creation_method  | 'vasp2cif' |
| _cell_length_a         | 6.32172145287 |
| _cell_length_b         | 6.32172145287 |
| _cell_length_c         | 6.6918356557 |
| _cell_angle_alpha      | 90.0 |
| _cell_angle_beta       | 90.0 |
| _cell_angle_gamma      | 90.0 |

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Ag1  Ag  0.99999927999997  0.99998830000003  0.000000499999999  1.0
Ag2  Ag  0.49999189999997  0.000000620000002  0.749999170000002 | 1.0 |
Ag3  Ag  0.49999400000000  0.50000829999999 | 0.500002199999997 | 1.0 |
Ag4  Ag  0.99999840000001  0.49999789999997  0.249998769999998 | 1.0 |
F5   F   0.305560242885351  0.578287680693276  0.212591294701972 | 1.0 |
F6   F   0.69439627114652  0.421716219306728  0.212589874701969 | 1.0 |
F7   F   0.578286310693276  0.694440187114649  0.787411425298025 | 1.0 |
F8   F   0.42171199306726  0.305560722885348  0.787406555298027 | 1.0 |
F9   F   0.194439267114651  0.57828640693273  0.537412215298027 | 1.0 |
F10  F   0.805560102885347  0.421712519306727  0.537407445298030 | 1.0 |
F11  F   0.921712299306730  0.694439827114648  0.962589824701972 | 1.0 |
F12  F   0.078286560693275  0.305560682885352  0.962592764197019 | 1.0 |
F13  F   0.805560252885352  0.70827750693274  0.712590584701971 | 1.0 |
F14  F   0.194439837114649  0.921712529306727  0.712598594701974 | 1.0 |
F15  F   0.78526520693272  0.194439587114649  0.28741305298030 | 1.0 |
F16  F   0.921713499306729  0.805560662885350  0.287406355298025 | 1.0 |
F17  F   0.694439307114653  0.708286340693272  0.037412285298025 | 1.0 |
F18  F   0.305560282885347  0.921712259306726  0.307405425298031 | 1.0 |
F19  F   0.421713619306723  0.194439417114649  0.462589674197019 | 1.0 |
F20  F   0.578285920693272  0.805560872885346  0.462591204701972 | 1.0 |
K21  K   0.396605945551140  0.249997780000001  0.12499893999998 | 1.0 |
K22  K   0.603062721544509  0.749998810000001  0.125000300000001 | 1.0 |
K23  K   0.249999610000003  0.60339399448868  0.874999940000002 | 1.0 |
K24  K   0.75000149999998 | 0.396612635551139 | 0.87500313999997 | 1.0 |
K25  K   0.103397294448866  0.249999800000001  0.624997620000002 | 1.0 |
K26  K   0.896606615551138  0.749998899999998 | 0.625000100000001 | 1.0 |
K27  K   0.749999570000000  0.103386874448863  0.375000115999997 | 1.0 |
K28  K   0.249999860000003  0.896608505551138  0.375000115999997 | 1.0 |

## DFT(PBEsol)+U K2AgF4 E p=80GPa magn.: f
| Atom Label | Element | Fractional X | Fractional Y | Fractional Z | Occupancy |
|------------|---------|--------------|--------------|--------------|------------|
| Ag1        | Ag      | 0.999999279999997 | 0.999988300000003 | 0.0000000499999999 | 1.0       |
| Ag2        | Ag      | 0.499991899999997 | 0.000000620000002 | 0.749991700000002 | 1.0       |
| Ag3        | Ag      | 0.499994000000000 | 0.500000829999998 | 0.500000219999997 | 1.0       |
| Ag4        | Ag      | 0.999999840000001 | 0.499997899999997 | 0.249997869999998 | 1.0       |
| F5         | F       | 0.30651431792701  | 0.57866274448761  | 0.212704204385709 | 1.0       |
| F6         | F       | 0.693458438207302  | 0.421338125551243  | 0.212702784385705 | 1.0       |
| F7         | F       | 0.578660804448761  | 0.693458998207299  | 0.787298151614289 | 1.0       |
| F8         | F       | 0.421337505551241  | 0.306541911792699  | 0.787293645614291 | 1.0       |
| F9         | F       | 0.193458078207301  | 0.578662134448757  | 0.53729305614291  | 1.0       |
| F10        | F       | 0.806541291792697  | 0.421338025551242  | 0.537294353614294 | 1.0       |
| F11        | F       | 0.921337805551245  | 0.693458638207297  | 0.9627023485708   | 1.0       |
| F12        | F       | 0.078661054448760  | 0.306541871792702  | 0.962703674385707 | 1.0       |
| F13        | F       | 0.193458648207298  | 0.921338033551242  | 0.712703494385707 | 1.0       |
| F14        | F       | 0.578661014448757  | 0.193458638207299  | 0.28729395614293  | 1.0       |
| F15        | F       | 0.921339005551244  | 0.806541851792701  | 0.287294353614294 | 1.0       |
| F16        | F       | 0.693457848207303  | 0.078660834448756  | 0.03729375614289  | 1.0       |
| F17        | F       | 0.306541471792698  | 0.921337765551241  | 0.037294353614295 | 1.0       |
| F18        | F       | 0.421338675551239  | 0.193458228207299  | 0.462702584385709 | 1.0       |
| F19        | F       | 0.578660414448757  | 0.806542061792697  | 0.462704114385708 | 1.0       |
| F20        | F       | 0.396309509034550  | 0.249997800000001  | 0.124998399999998 | 1.0       |
| K21        | K       | 0.6036947965455    | 0.749998810000001  | 0.125000530000001 | 1.0       |
| K22        | K       | 0.750000149999998  | 0.396316199034549  | 0.875003139999997 | 1.0       |
| K23        | K       | 0.103693730965453  | 0.624997620000002  | 0.624997620000002 | 1.0       |
| K24        | K       | 0.749999570000000  | 0.103683310965453  | 0.375000120000003 | 1.0       |
| K25        | K       | 0.249999860000003  | 0.896310269034548  | 0.375001159999997 | 1.0       |
## DFT(PBEsol)+U K2AgF4 E p=100GPa magn.: f data_1

### _audit_creation_method 'vasp2cif'

- **_cell_length_a**: 6.1753690001
- **_cell_length_b**: 6.1753690001
- **_cell_length_c**: 6.49468370629
- **_cell_angle_alpha**: 90.0
- **_cell_angle_beta**: 90.0
- **_cell_angle_gamma**: 90.0

### _symmetry_space_group_name_H-M  'P 1'

#### loop_

- **_atom_site_label**, **_atom_site_type_symbol**, **_atom_site_fract_x**, **_atom_site_fract_y**, **_atom_site_fract_z**, **_atom_site_occupancy**

| Atom | Type | Fract X | Fract Y | Fract Z | Occupancy |
|------|------|---------|---------|---------|-----------|
| Ag1  | Ag   | 0.999999279999997 | 0.999998300000003 | 0.000000049999997 | 0.749999700000002 |
| Ag2  | Ag   | 0.499991899999997 | 0.000000620000002 | 0.749999170000002 | 0.749999700000002 |
| Ag3  | Ag   | 0.499994000000000 | 0.500000829999998 | 0.500000219999997 | 0.749999170000002 |
| Ag4  | Ag   | 0.499998400000001 | 0.499997899999997 | 0.749998769999997 | 0.749998769999997 |
| F5   | F    | 0.308091862510026 | 0.579234673149415 | 0.212845282947997 |
| Ag5  | Ag   | 0.999995134941497 | 0.999997830000003 | 0.000000499999997 | 0.749999700000002 |
| Ag6  | Ag   | 0.499991899999997 | 0.000000620000002 | 0.749999170000002 | 0.749999700000002 |
| Ag7  | Ag   | 0.499994000000000 | 0.500000829999998 | 0.500000219999997 | 0.749999170000002 |
| Ag8  | Ag   | 0.499998400000001 | 0.499997899999997 | 0.749998769999997 | 0.749998769999997 |

F9  F   0.192633884746589   0.578951157591633   0.537218376330466   1.0
F10 F   0.807365485253409   0.421049002408366   0.537213606330469   1.0
F11 F   0.921048782408369   0.692634444746585   0.962783636695932   1.0
F12 F   0.078950077591636   0.30760605253414   0.962784603669532   1.0
F13 F   0.807365635253414   0.078951267591635   0.962784426695931   1.0
F14 F   0.19263454746586   0.92104912408367   0.712784426695931   1.0
F15 F   0.078950037591633   0.192634204746587   0.287214663304649   1.0
F16 F   0.921049982408369   0.807366045253413   0.712784426695931   1.0
F17 F   0.691907654746591   0.789498755161362   0.737184463304649   1.0
F18 F   0.3076565253414   0.921048742408366   0.73713706330470   1.0
F19 F   0.421049652408363   0.192634034746587   0.462783513669534   1.0
F20 F   0.578949473591633   0.807366255253409   0.462785043669533   1.0
K21 K   0.395676305886173   0.249997780000001   0.124989399999998   1.0
K22 K   0.60430567413832   0.749998810000001   0.125000530000001   1.0
K23 K   0.249999610000003   0.604302634113829   0.874999400000002   1.0
K24 K   0.750000149999998   0.395973995886172   0.875003139999997   1.0
K25 K   0.104305934113830   0.749999570000000   0.375001159999997   1.0
K26 K   0.895679755886171   0.749998899999998   0.625000100000001   1.0
K27 K   0.749999570000000   0.1042551413830   0.787157491075198   1.0
K28 K   0.249998600000003 | 0.895679865886172 | 0.375001159999997 | 1.0

| K21   | K    | 0.395676305886173 | 0.249997780000001 | 0.124989399999998 | 1.0
| K22   | K    | 0.60430567413832   | 0.749998810000001 | 0.125000530000001 | 1.0
| K23   | K    | 0.249999610000003 | 0.604302634113829 | 0.874999400000002 | 1.0
| K24   | K    | 0.750000149999998 | 0.395973995886172 | 0.875003139999997 | 1.0
| K25   | K    | 0.104305934113830 | 0.749999570000000 | 0.375001159999997 | 1.0
| K26   | K    | 0.895679755886171 | 0.749998899999998 | 0.625000100000001 | 1.0
| K27   | K    | 0.749999570000000 | 0.1042551413830 | 0.787157491075198 | 1.0
| K28   | K    | 0.249998600000003 | 0.895679865886172 | 0.375001159999997 | 1.0

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### end

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**Note:** The data represents the atomic positions and labels for K2AgF4, including cell parameters and symmetry information. The structure data includes both Ag and F atoms, with their respective coordinates and occupancies.