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**ROTATIONAL EXCITATION OF ALUMINIUM MONOFLUORIDE (AlF)
BY He ATOM AT LOW TEMPERATURE**

L.C. Owono Owono¹

*Centre for Atomic Molecular Physics and Quantum Optics, Faculty of Science,
University of Douala, P.O. Box 8580, Douala, Cameroon,*
and

The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy,

N. Gotoum, C. Nkem

*Centre for Atomic Molecular Physics and Quantum Optics, Faculty of Science,
University of Douala, P.O. Box 8580, Douala, Cameroon,*

K. Hammami and N. Jaidane

*Laboratory for Atomic Molecular Spectroscopy and Applications, Department of Physics,
Faculty of Science, University Tunis El Manar, Campus Universitaire 1060 Tunis, Tunisia.*

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¹Regular Associate of ICTP.

Abstract

We report on the calculation of collision induced rotational excitation cross sections and rate coefficients of AlF by He atom at low temperature. These quantities were obtained by first computing the interaction potential energy surface (PES) of the AlF($X^1\Sigma^+$)-He($1S$) van der Waals complex at the *ab initio* Coupled Cluster with Single and Double and perturbative Triple excitations [CCSD(T)] level of theory. The aug-cc-pVQZ gaussian basis, to which was added a set of bond functions, was used for that purpose. The calculations account for basis set superposition errors (BSSE). The interaction potential presents a minimum of $\sim 24 \text{ cm}^{-1}$ below the AlF-He dissociation limit. The PES was fitted on a basis of Legendre polynomial functions to allow for the calculation of cross sections in the close-coupling (CC) approach. By averaging these cross sections over a Maxwell-Boltzmann velocity distribution, rate coefficients were inferred at low temperatures ($T \leq 300 \text{ K}$). From our computations, a propensity towards $\Delta J = 1$ transitions is observed.

1 Introduction

The observation of several metal halide molecules is one of the most unexpected and exciting results that has occurred in interstellar chemistry during the last three decades. In 1987, Cernicharo and Guelin [1] have detected NaCl, KCl, AlCl, and tentatively, AlF toward the asymptotic giant branch (AGB) star envelope IRC+10 216 by measuring 2 and 3 mm rotational lines with the IRAM 30 m telescope. A few years after, i.e., in 1994, Ziurys et al. [2] gave the confirmation that aluminium monofluoride exists in that source. They recorded the following three new transitions of AlF at 0.8 and 1.2 mm, $J = 10 \rightarrow 9$, $J = 8 \rightarrow 7$, and $J = 7 \rightarrow 6$ with the Caltech Submillimeter Observatory (CSO). More recently, Highberger et al. [3] reported the detection of AlF in the circumstellar envelope of the proto-planetary nebula CRL 2688, the so-called Egg Nebula.

Apart from the astrophysical importance of AlF, its electronic spectrum has always been of interest to spectroscopists. This is because this molecule has an electronic structure which is essentially similar to those of the much studied molecules CO and N₂, and, being heavier, it should have many systems in the more accessible regions of the spectrum [4]. Additionally, the knowledge of the spectroscopy of aluminium monohalides is important for monitoring such species in high temperature fast-flow reactors [5, 6, 7]. It should be pointed out that many experimental studies also report on the spectroscopy of AlF, including electron spectroscopy and resonance-enhanced multiphoton ionization (see [6, 8, 9], and references therein). On the theoretical side, efforts have mainly been devoted to the characterization of lower and excitation states of AlF by using *ab initio* calculations [10, 11]. All the above clearly illustrate that aluminium monofluoride is of interest for both astrophysicists and experimentalists. Hence the effort devoted in this study to the determination of rotational excitation parameters of AlF by helium atom at low temperature.

It is well established that the modeling of the interstellar molecular emission requires excitation parameters such as cross sections, collision rates, polarization and depolarization transfer rates of the collisions between the molecules studied and the most abundant perturbers of the interstellar medium (ISM), namely H, He and H₂. Also, the balance between the collisional and radiative excitation and de-excitation of the species of interest in collision with the above perturbers is needed. Note however that the computation of these quantities heavily rely on accurate potential energy surfaces of the interacting particles. In view of the importance of the above cited characteristics, we have undertaken this study for the determination of state-to-state rotational integral cross sections and rate coefficients of AlF collision with He. To this end, a two-dimensional (2D) PES is calculated in Section 2 with the *ab initio* CCSD(T) [12, 13] method of including electron correlation. The aug-cc-pVQZ basis set of Dunning and co-workers [14, 15, 16, 17], to which was added a set of bond functions optimized by Cybulski and Toczyłowski [18] to account for the intersystem correlation energy is used for all atoms. The PES is fitted on a basis of Legendre polynomial functions and the fitting coefficients are utilized in Section 3 to compute the cross sections in the close-coupling approximation for J ranging from 0 to 10 and a total energy up to 1500 cm⁻¹. The same section also discusses results for the rate coefficients for 10 K $\leq T \leq$ 300 K. Our final remarks are given in Section 4.

2 Interaction potential energy surface

The Jacobi coordinate system, described elsewhere [19, 20] was used to calculate the interaction PES for the AlF($X^1\Sigma^+$)-He(1S) van der Waals system. In that coordinate system, r is the AlF internuclear distance, R the distance from the center of mass (c.m.) of AlF to the He atom, and θ the angle between the two distance vectors. The collinear AlF...He

geometry corresponds to $\theta = 0^\circ$. The CCSD(T) method [12, 13] as implemented in the MOLPRO molecular package [21] was used. In the course of the calculation, the AlF bond distance was frozen at its value for the experimental equilibrium geometry of the ground $X^1\Sigma^+$ state, i.e., $r = r_e = 1.654369 \text{ \AA}$ [22]. All the atoms were described with the aug-cc-pVQZ basis set [14, 15, 16, 17]. To this basis, we have added a set of (3s3p2d2f1g) bond functions defined by Cybulski and Toczyłowski [18] and placed at mid-distance between the center of mass (c.m.) of AlF and He atom. These bond functions are very efficient for the correct description of the intersystem correlation energy [20, 23, 24]. Our total basis sets thus include 237 contracted gaussian basis functions. The PES calculations account for basis set superposition error (BSSE) at all geometries within the counterpoise scheme of Boys and Bernardi [25].

The coordinate R was varied from 3.5 to 13.0 bohrs by steps of 0.25 bohr. Other points were computed on the grid from 14.0 to 20.0 bohrs by steps of 1.0 bohr, to allow for the correct description of the asymptotic part of the interaction potential. The grid of θ values was set uniformly from 0° to 180° with a step of 10° . All this resulted in 874 geometries to be treated in the C_S symmetry group.

Fig. 1 displays the contour plot of our PES. That interaction potential presents a global minimum of 24.056 cm^{-1} at $R = 7.75$ bohrs and $\theta = 0^\circ$. We have carefully worked out this value by computing some additional geometries for $7.55 \text{ bohrs} \leq R \leq 7.95 \text{ bohrs}$ and $\theta = 0^\circ$ with a step of 0.05 bohr. It should be mentioned that the global minimum occurred for an approach of He towards F atom. To appreciate the shape of our PES, we have represented in Fig. 2 the three cuts $V(r_e, R_{\text{AlF}\dots\text{He}}, \theta = 0^\circ)$, $V(r_e, R_{\text{AlF}\perp\text{He}}, \theta = 90^\circ)$ and $V(r_e, R_{\text{He}\dots\text{AlF}}, \theta = 180^\circ)$. For $\theta = 90^\circ$, the minimum is located at $R = 7.85$ bohrs and corresponds to 11.35 cm^{-1} while for $\theta = 180^\circ$, it is found for $R = 10.0$ bohrs to be 7.62 cm^{-1} . It is clear that these two values are well above the global minimum.

To allow for the dynamics calculations, the fitting procedure described in details by Nkem et al. [20] and Hammami et al. [26] was used. The PES was further expanded in terms of Legendre polynomial functions as

$$V(R, \theta) = \sum_{\lambda=0}^{\lambda_{max}} V_\lambda(R) P_\lambda(\cos\theta). \quad (1)$$

where $\lambda_{max} = 18$. Fig. 3 shows plots of the first $V_\lambda(R)$ components. An analysis of Fig. 1 to 3 leads us to the conclusion that our collisional calculations may be carried out faithfully for R starting from 3.5 bohrs. This value provides sufficiently repulsive potential for all orientations. In the course of the scattering calculations, an interpolation was carried out with the POTENL module of the MOLSCAT program [27] to obtain $V_\lambda(R)$ at other values of R .

3 Collision dynamics calculations

3.1 Rotational integral cross sections

The quantum mechanical close coupling approach, formulated by Arthurs and Dalgarno [28] in 1960 and implemented in the MOLSCAT code was used to compute state to state rotational integral cross sections for values of J ranging from 0 to 10, and a total energy up to 1500 cm^{-1} . The rotational levels of AlF are computed from the usual expansion with the spectroscopic constants $Be = 0.552479 \text{ cm}^{-1}$ and $De = 1.0464 \times 10^{-6} \text{ cm}^{-1}$ [22]. In order to account for resonances during the calculations, the energy range was carefully spanned as follows. For $E < 20 \text{ cm}^{-1}$, the energy step was set to 0.1 cm^{-1} , from 20 cm^{-1} to 100 cm^{-1} to 0.2 cm^{-1} , from 100 cm^{-1} to 200 cm^{-1} to 1 cm^{-1} , from 200 cm^{-1} to 500 cm^{-1} to 5 cm^{-1} , from 500 cm^{-1} to 1000 cm^{-1} to 10 cm^{-1} , and from 1000 cm^{-1} to 1500 cm^{-1} to 20 cm^{-1} . In addition, we have set $J_{max} = 15$ for $E < 500 \text{ cm}^{-1}$, and $J_{max} = 17$ for $E \geq 500 \text{ cm}^{-1}$. These values were chosen

after we have performed some convergence tests as illustrated in Table 1. They correspond to rotational basis sets of adequate size for a good accuracy in the calculated cross sections. For the integration, the step was lowered such that for $E < 20 \text{ cm}^{-1}$, STEPS = 30, for $20 \leq E \leq 100 \text{ cm}^{-1}$, STEPS = 20, while for $E \geq 100 \text{ cm}^{-1}$, STEPS = 10. The other parameters required as input by the MOLSCAT program are displayed in Table 2. They were also fixed after the above mentioned convergence tests. The maximum value of the total angular momentum J_{tot} was set large enough to ensure the convergence of the cross sections to within 0.01 \AA^2 for diagonal terms and 0.001 \AA^2 for off-diagonal ones. Thus at 100 cm^{-1} , $J_{tot} = 50$, at 500 cm^{-1} , $J_{tot} = 89$, at 1000 cm^{-1} , $J_{tot} = 113$ and at 1500 cm^{-1} , $J_{tot} = 130$. The propagator of Manolopoulos [29] was used to solve the coupled equations.

Fig. 4 presents the collisional excitation cross sections of AlF by He from the first level (panel (a)), for $\Delta J = 1$ (panel (b)) and $\Delta J = 2$ (panel (c)) as a function of the kinetic energy. It is clear that at lower energies, the cross sections present some resonances. This is consistent with similar observations by Nkem et al [20], Lique et al. [30], Hammami et al. [19, 26, 31], Smith et al. [32], and Christoffel and Bowman [33]. Indeed, resonances are due to the global minimum (located at $R = 7.75$ bohrs and $\theta = 0^\circ$ and whose well depth is $\sim 24 \text{ cm}^{-1}$) which allows the He atom to be temporarily trapped into the well and hence quasibond states to be formed before the complex dissociates. A feature that is also readily apparent from Fig. 4 is that the magnitude of the cross sections for the transition $0 \rightarrow 1$ is greater than that of the other transitions displayed. Fig. 5 shows cross sections as a function of J' for selected values of the energy. It is clear from this figure that transitions with $\Delta J = 1$ are superior.

3.2 Downward rate coefficients

The downward rate coefficients are computed following the procedure used in previous works [19, 20, 26], i.e., by averaging the cross sections over a Maxwell-Boltzmann distribution of kinetic energies as

$$q_{J \rightarrow J'}(T) = \left(\frac{8\beta^3}{\pi\mu} \right)^{1/2} \int_0^\infty E_C \sigma_{J \rightarrow J'}(E) e^{-\beta E_C} dE_C. \quad (2)$$

T is the kinetic temperature, $\mu = 3.679807$ amu the reduced mass of the AlF-He collision partners, $\beta = \frac{1}{k_B T}$ where k_B is the Boltzmann constant and $E_C = E - E_J$ the relative kinetic energy. Our results for the transitions involved at selected temperatures are displayed in Table 3. They may be found online from the BASECOL website [34]. Upon request to the authors, additional values may be computed.

Fig. 6 illustrates the variation of downward rate coefficients with J' for different ΔJ values and temperatures. As one can see from the figure, rates of collision exhibit almost the same trends. In addition, the collision rates reflect the already noticed propensity towards $\Delta J = 1$ transitions observed in the analysis of the cross sections. Switching our attention to Fig. 7, it is clear that rate coefficients are smooth varying functions of the kinetic temperature.

4 Final remarks

In this work, we have obtained collisional excitation cross sections and downward rate coefficients for the collision of aluminium monofluoride with helium atom. Prior to the computation of these quantities, a reliable *ab initio* potential energy surface for the AlF($X^1\Sigma^+$)-He($1S$) van der Waals complex was calculated at the CCSD(T) level of theory with the aug-cc-pVQZ basis set. The quantum mechanical close-coupling approach was used to determine the cross sections that were further averaged over a Maxwell-Boltzmann distribution of kinetic energy to work out the downward rate coefficients. A propensity towards $\Delta J = 1$ transition is observed. From all what precedes, it is clear that our numbers

may be very useful for astrophysical observations as well as for experiments. Encouraged by the results thus achieved, we have undertaken the study of AlF collision with H₂ which is by far the most abundant perturber in the ISM justifying therefore the interest to investigate collision dynamics of the molecule studied with H₂. In addition, other metal halides namely AlCl, NaCl and KCl are in the pipe for the collisional studies. The related works are in progress and will be reported in forthcoming papers.

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Table 1: Selected rotational integral cross sections of AlF in collision with He as a function of J_{max} parameter for different energies (in units of \AA^2).

Energy	Transition	$J_{max} = 12$	$J_{max} = 15$	$J_{max} = 17$	$J_{max} = 20$
100 cm^{-1}	0 \rightarrow 1	25.189	25.189	25.189	25.189
	0 \rightarrow 2	12.529	12.529	12.529	12.529
	1 \rightarrow 2	19.482	19.482	19.482	19.482
	1 \rightarrow 3	8.642	8.642	8.642	8.642
	6 \rightarrow 7	15.971	15.971	15.971	15.971
	6 \rightarrow 8	5.089	5.089	5.089	5.089
	8 \rightarrow 9	16.499	16.494	16.494	16.494
	8 \rightarrow 10	4.189	4.193	4.193	4.193
	500 cm^{-1}	0 \rightarrow 1	15.087	15.087	15.087
0 \rightarrow 2		5.093	5.093	5.093	5.093
1 \rightarrow 2		12.262	12.262	12.262	12.262
1 \rightarrow 3		5.541	5.541	5.541	5.541
6 \rightarrow 7		10.131	10.129	10.129	10.129
6 \rightarrow 8		3.888	3.881	3.880	3.880
8 \rightarrow 9		9.389	9.939	9.948	9.948
8 \rightarrow 10		3.827	3.761	3.763	3.763
1500 cm^{-1}		0 \rightarrow 1	10.353	10.351	10.351
	0 \rightarrow 2	3.373	3.379	3.379	3.379
	1 \rightarrow 2	9.300	9.303	9.303	9.303
	1 \rightarrow 3	3.896	3.893	3.894	3.894
	6 \rightarrow 7	7.733	7.733	7.746	7.745
	6 \rightarrow 8	3.213	3.244	3.285	3.284
	8 \rightarrow 9	7.848	7.625	7.518	7.528
	8 \rightarrow 10	4.308	3.310	3.025	3.063

Table 2: MOLSCAT parameters used in the present calculations

INTFLG=6	STEPS=30,20,10	OTOL=0.001	DTOL=0.01
Be = $0.5524798 \text{ cm}^{-1}$	De = $1.0464 \times 10^{-6} \text{ cm}^{-1}$	JMAX=15,17	RMIN=3.5 bohrs, RMAX=40 bohrs

Table 3: Downward rate coefficients (given as $a(b) = a.10^b$) of rotational levels of AlF in collision with He as a function of kinetic temperature (in units of $\text{cm}^3.\text{s}^{-1}$)

Initial level	Final level	Rate Coefficients						
		10K	30 K	50 K	100K	150K	200K	300K
1	0	9.3619(-11)	1.1549(-10)	1.2682(-10)	1.3361(-10)	1.4929(-10)	1.5658(-10)	1.6795(-10)
2	0	1.4678(-11)	2.2999(-11)	2.9277(-11)	3.3449(-11)	4.0083(-11)	4.1206(-11)	4.1764(-11)
2	1	1.2396(-10)	1.4984(-10)	1.6780(-10)	1.8036(-10)	2.1071(-10)	2.2387(-10)	2.4414(-10)
3	0	1.3115(-12)	4.2061(-12)	7.5464(-12)	1.0408(-11)	1.7299(-11)	1.9836(-11)	2.3583(-11)
3	1	2.1602(-11)	3.2736(-11)	4.3069(-11)	5.1306(-11)	7.0391(-11)	7.6553(-11)	8.3735(-11)
3	2	1.3955(-10)	1.6303(-10)	1.7996(-10)	1.9239(-10)	2.2616(-10)	2.4180(-10)	2.6553(-10)
4	0	1.8658(-13)	1.1028(-12)	2.7140(-12)	4.5689(-12)	1.1009(-11)	1.3811(-11)	1.7612(-11)
4	1	2.2576(-12)	6.4953(-12)	1.1646(-11)	1.6436(-11)	3.0102(-11)	3.5772(-11)	4.3870(-11)
4	2	2.4485(-11)	3.6954(-11)	4.7747(-11)	5.6261(-11)	7.6906(-11)	8.4317(-11)	9.3811(-11)
4	3	1.5305(-10)	1.7328(-10)	1.8882(-10)	2.0037(-10)	2.3334(-10)	2.4978(-10)	2.7587(-10)
5	0	3.4413(-14)	2.0656(-13)	6.4468(-13)	1.2709(-12)	4.0946(-12)	5.5088(-12)	7.4072(-12)
5	1	3.4534(-13)	1.7832(-12)	4.2983(-12)	7.3012(-12)	1.8783(-11)	2.4311(-11)	3.2309(-11)
5	2	2.9333(-12)	7.9798(-12)	1.3731(-11)	1.9001(-11)	3.4615(-11)	4.1766(-11)	5.2816(-11)
5	3	2.6910(-11)	4.0138(-11)	5.1200(-11)	5.9746(-11)	8.0050(-11)	8.7454(-11)	9.7326(-11)
5	4	1.6586(-10)	1.8207(-10)	1.9620(-10)	2.0692(-10)	2.3815(-10)	2.5414(-10)	2.8018(-10)
6	0	1.0676(-14)	6.1650(-14)	2.2140(-13)	4.9765(-13)	2.1738(-12)	3.2408(-12)	4.9952(-12)
6	1	5.5256(-14)	3.4573(-13)	1.0614(-12)	2.1197(-12)	7.5473(-12)	1.0736(-11)	1.5658(-11)
6	2	5.0918(-13)	2.2896(-12)	5.2223(-12)	8.6480(-12)	2.1699(-11)	2.8163(-11)	3.7839(-11)
6	3	3.7288(-12)	9.3707(-12)	1.5523(-11)	2.1039(-11)	3.7005(-11)	4.4380(-11)	5.6196(-11)
6	4	2.9468(-11)	4.2859(-11)	5.4041(-11)	6.2612(-11)	8.2581(-11)	8.9776(-11)	9.9562(-11)
6	5	1.7729(-10)	1.8985(-10)	2.0260(-10)	2.1256(-10)	2.4230(-10)	2.5776(-10)	2.8308(-10)
7	0	1.9867(-15)	1.4664(-14)	6.4971(-14)	1.7226(-13)	1.1123(-12)	1.8866(-12)	3.3269(-12)
7	1	1.8273(-14)	1.0399(-13)	3.6363(-13)	8.1838(-13)	3.8025(-12)	5.8847(-12)	9.5363(-12)
7	2	7.5229(-14)	4.5292(-13)	1.3130(-12)	2.5481(-12)	8.7971(-12)	1.2565(-11)	1.8687(-11)
7	3	7.2973(-13)	2.8030(-12)	6.0691(-12)	9.8065(-12)	2.3715(-11)	3.0567(-11)	4.1008(-11)
7	4	4.7519(-12)	1.0770(-11)	1.7201(-11)	2.2889(-11)	3.9004(-11)	4.6332(-11)	5.8116(-11)
7	5	3.2458(-11)	4.5402(-11)	5.6522(-11)	6.5057(-11)	8.4768(-11)	9.1752(-11)	1.0119(-10)
7	6	1.8895(-10)	1.9720(-10)	2.0845(-10)	2.1763(-10)	2.4605(-10)	2.6107(-10)	2.8575(-10)
8	0	3.3015(-16)	3.1495(-15)	1.6644(-14)	5.0353(-14)	4.3312(-13)	8.0174(-13)	1.5562(-12)
8	1	3.6377(-15)	2.5412(-14)	1.0896(-13)	2.8825(-13)	1.9684(-12)	3.4685(-12)	6.4866(-12)
8	2	2.6170(-14)	1.3983(-13)	4.6130(-13)	1.0073(-12)	4.5190(-12)	7.0109(-12)	1.1569(-11)
8	3	1.0491(-13)	5.6593(-13)	1.5519(-12)	2.9293(-12)	9.6597(-12)	1.3636(-11)	2.0100(-11)
8	4	1.0142(-12)	3.3387(-12)	6.8832(-12)	1.0875(-11)	2.5425(-11)	3.2475(-11)	4.3172(-11)
8	5	5.9838(-12)	1.2206(-11)	1.8814(-11)	2.4612(-11)	4.0829(-11)	4.8117(-11)	5.9777(-11)
8	6	3.5609(-11)	4.7838(-11)	5.8769(-11)	6.7211(-11)	8.6682(-11)	9.3513(-11)	1.0262(-10)
8	7	1.9947(-10)	2.0403(-10)	2.1384(-10)	2.2226(-10)	2.4945(-10)	2.6412(-10)	2.8828(-10)
9	0	6.6360(-17)	8.2654(-16)	5.2178(-15)	1.8211(-14)	2.2595(-13)	4.7936(-13)	1.1014(-12)
9	1	6.5096(-16)	5.5608(-15)	2.8228(-14)	8.4966(-14)	7.7528(-13)	1.5017(-12)	3.1366(-12)
9	2	5.5130(-15)	3.4896(-14)	1.4036(-13)	3.5924(-13)	2.3459(-12)	4.1162(-12)	7.7395(-12)
9	3	3.6205(-14)	1.7794(-13)	5.5570(-13)	1.1793(-12)	5.0505(-12)	7.7467(-12)	1.2686(-11)
9	4	1.4773(-13)	6.8825(-13)	1.7881(-12)	3.2909(-12)	1.0434(-11)	1.4559(-11)	2.1171(-11)
9	5	1.3652(-12)	3.9041(-12)	7.6845(-12)	1.1886(-11)	2.6957(-11)	3.4154(-11)	4.4952(-11)
9	6	7.4050(-12)	1.3688(-11)	2.0393(-11)	2.6246(-11)	4.2497(-11)	4.9756(-11)	6.1300(-11)
9	7	3.8923(-11)	5.0233(-11)	6.0875(-11)	6.9171(-11)	8.8377(-11)	9.5097(-11)	1.0398(-10)
9	8	2.0941(-10)	2.1052(-10)	2.1891(-10)	2.2657(-10)	2.5254(-10)	2.6687(-10)	2.9054(-10)
10	0	8.1840(-18)	1.5597(-16)	1.2405(-15)	5.0741(-15)	9.0195(-14)	2.1635(-13)	5.7316(-13)
10	1	1.4138(-16)	1.4926(-15)	8.9246(-15)	3.0736(-14)	3.9399(-13)	8.6190(-13)	2.0789(-12)
10	2	1.0423(-15)	7.8195(-15)	3.7032(-14)	1.0755(-13)	9.3467(-13)	1.8038(-12)	3.8050(-12)
10	3	7.9186(-15)	4.5245(-14)	1.7159(-13)	4.2598(-13)	2.6478(-12)	4.5855(-12)	8.5146(-12)
10	4	4.9172(-14)	2.1949(-13)	6.5049(-13)	1.3445(-12)	5.5253(-12)	8.3740(-12)	1.3516(-11)
10	5	2.0567(-13)	8.2217(-13)	2.0267(-12)	3.6413(-12)	1.1150(-11)	1.5412(-11)	2.2140(-11)
10	6	1.7784(-12)	4.5019(-12)	8.4856(-12)	1.2863(-11)	2.8367(-11)	3.5692(-11)	4.6579(-11)
10	7	8.9600(-12)	1.5209(-11)	2.1949(-11)	2.7816(-11)	4.4038(-11)	5.1271(-11)	6.2758(-11)
10	8	4.2246(-11)	5.2591(-11)	6.2884(-11)	7.1000(-11)	8.9900(-11)	9.6508(-11)	1.0515(-10)
10	9	2.1829(-10)	2.1657(-10)	2.2365(-10)	2.3060(-10)	2.5540(-10)	2.6945(-10)	2.9278(-10)

Figure 1: Contour plot of the potential energy surface (in cm^{-1}) of AlF-He as a function of R and θ . The zero of energy is taken as that of the AlF-He asymptote.

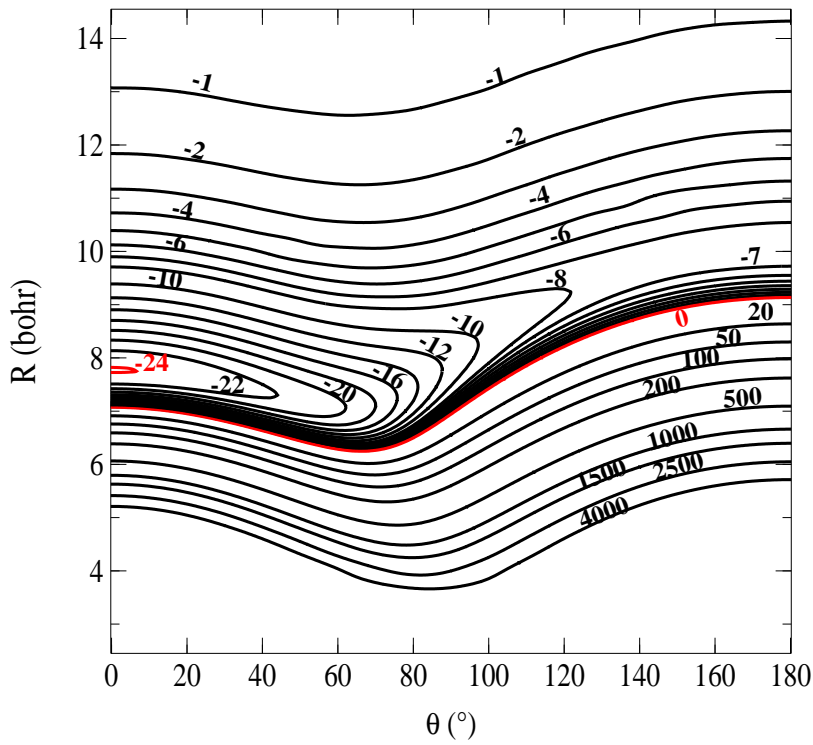


Figure 2: Cuts of the potential energy surface for angle values $\theta = 0^\circ$, $\theta = 90^\circ$ and $\theta = 180^\circ$ as a function of the distance R.

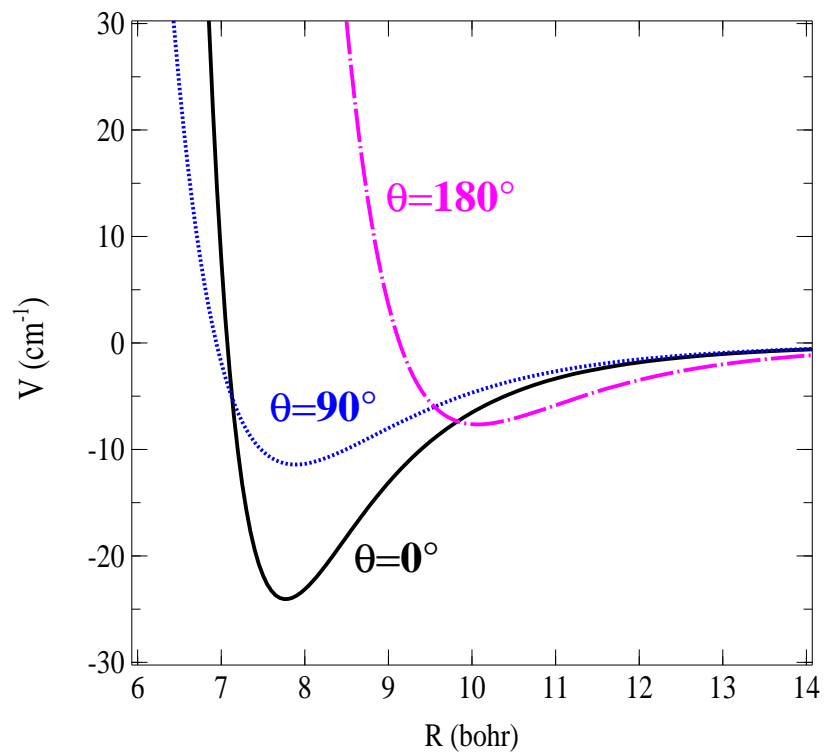


Figure 3: V_λ expansions of the interaction potential energy surface ($\lambda = 0, 1, 2, 3$) as a function of the Jacobi coordinate R .

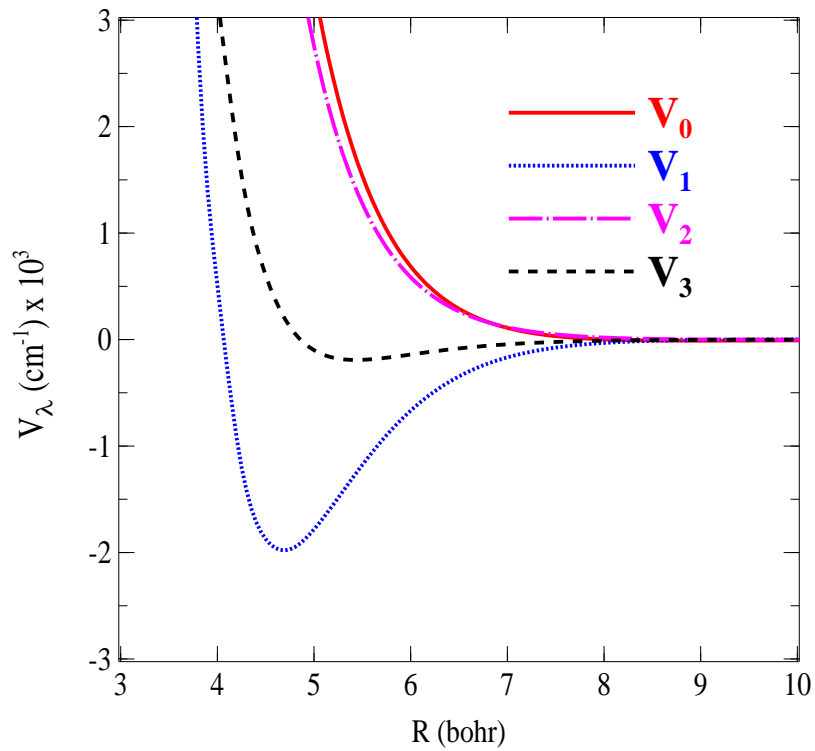
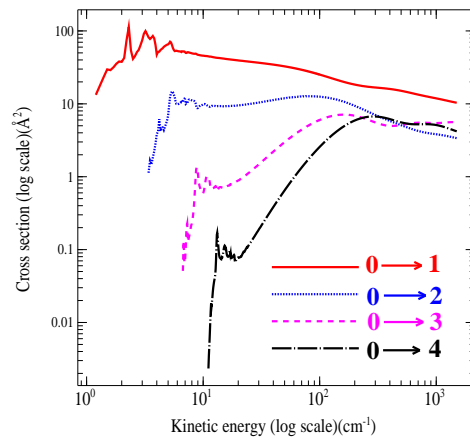
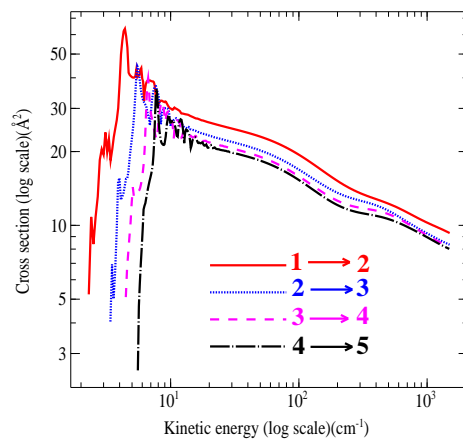


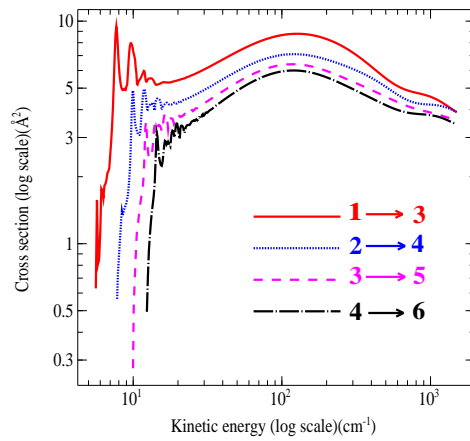
Figure 4: Collisional excitation cross sections of AlF by He from the first level (a) and for $\Delta J = 1$ (b) and $\Delta J = 2$ (c) as a function of the kinetic energy.



(a)

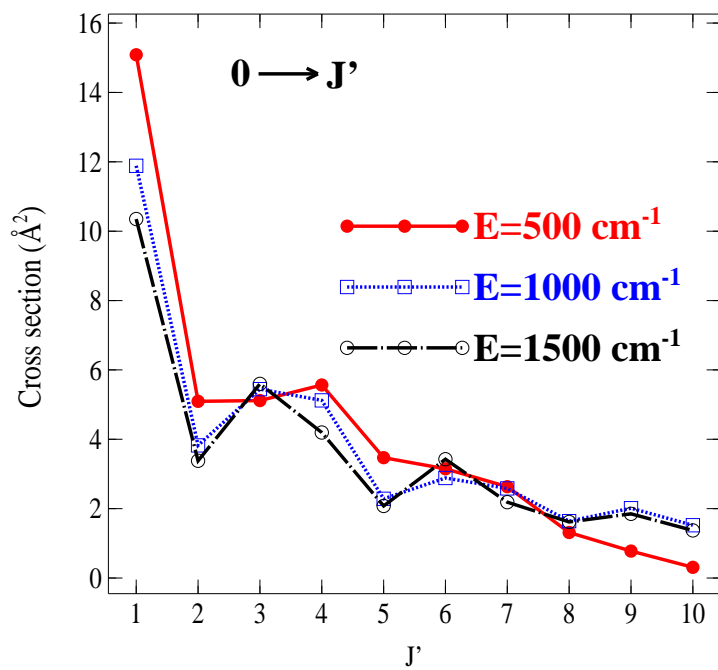


(b)

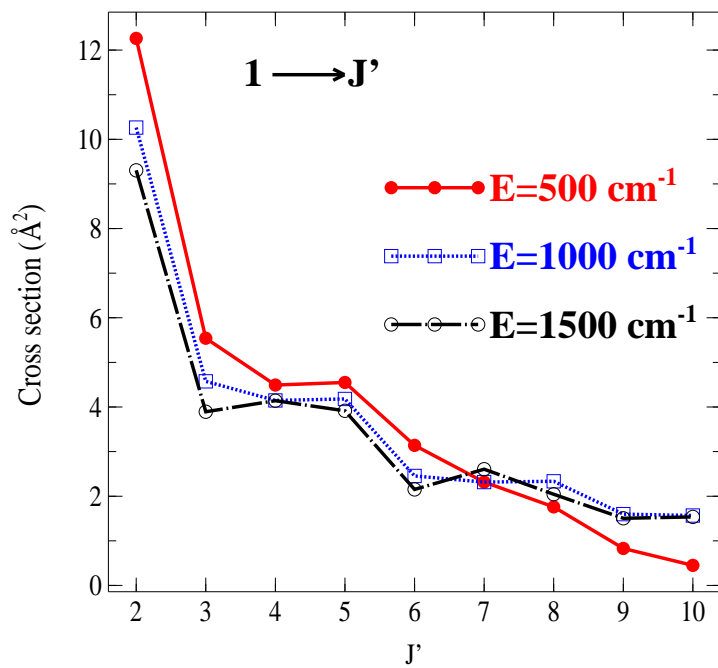


(c)

Figure 5: Collisional excitation cross sections of AlF by He as a function of J' for selected values of energy.

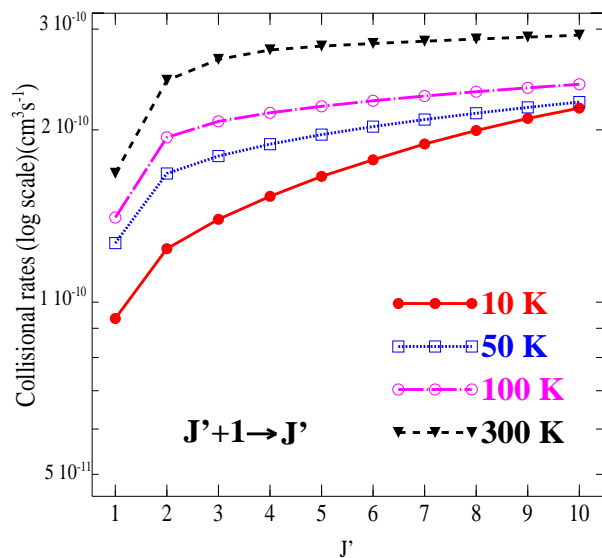


(a)

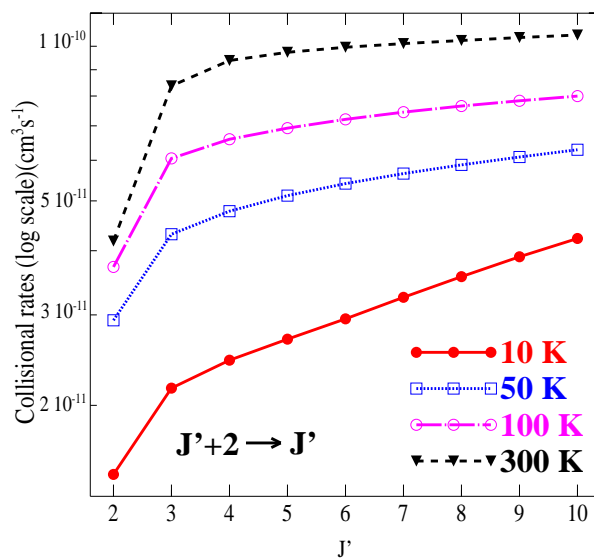


(b)

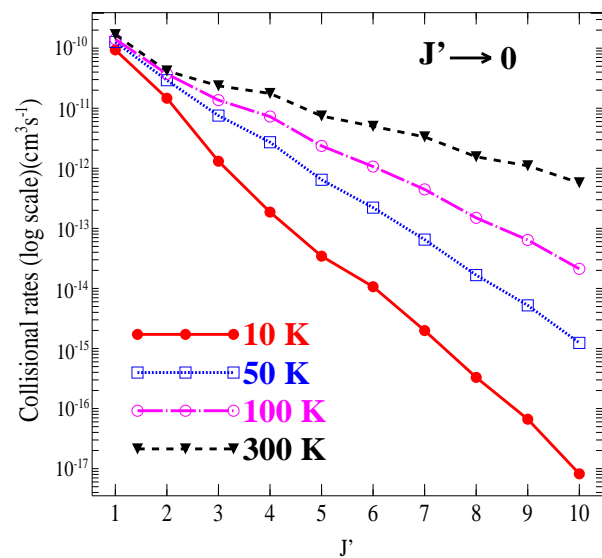
Figure 6: Calculated downward rate coefficients for the collisions of AlF with He for $J' \rightarrow 0$, $J' \rightarrow 1$, $J' + 1 \rightarrow J'$ and $J' + 2 \rightarrow J'$ transitions for selected kinetic temperature.



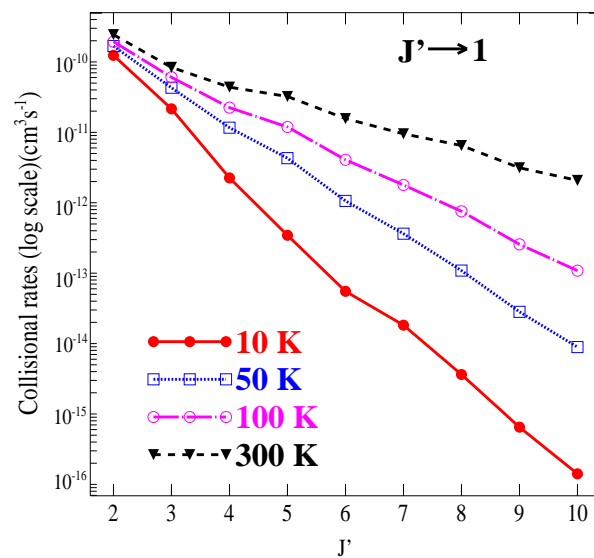
(a)



(b)



(c)



(d)

Figure 7: Calculated downward rate coefficients for the collisions of AlF with He for selected transitions as a function of kinetic temperature.

