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GENERAL PROPERTIES OF ASTATINE

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ABSTRACT

This study represents a compilation of the general physico-chemical properties of astatine atoms and ions. Along with the data a brief account of methods for determining of the properties cited is also given.

The literature search was completed in July 1984.

АННОТАЦИЯ

Дается обзор общих физико-химических свойств астата. Наряду с приводимыми в работе данными, обсуждаются также методы определения основных свойств астата.

Литературный обзор был составлен в июле 1984 года.

KIVONAT

A tanulmányban az asztácium alapvető fizikai-kémiai tulajdonságainak összefoglaló leírását adjuk. Az adatok közlésével együtt röviden tárgyaljuk az asztácium általános tulajdonságainak meghatározására szolgáló módszereket is.

Az irodalom gyűjtését 1984. júliusában fejeztük be.

III.

CONTENTS

5.	GENERAL PROPERTIES OF ASTATINE	1
5.1	Electronic Structure	2
5.2	Electronegativity	2
5.3	Atomic Volume	3
5.4	Atomic Refraction	3
5.5	Polarizabilities	3
5.6	Ionization Energies	3
5.7	Oxidation States	5
5.7.1	Astatine(-I)	5
5.7.2	Astatine(O)	6
5.7.3	Astatine(I)	7
5.7.4	Astatine(III)	8
5.7.5	Astatine(V)	8
5.7.6	Astatine(VII)	9
5.8	Electrochemical Properties	9
5.8.1	Critical Deposition Potentials	9
5.8.2	Standard Electrode Potentials	10
5.9	Thermodynamic Data	11
5.9.1	At ⁻ Ion	11
5.9.2	Astatine Atom	13
5.9.2.1	Thermodynamic Properties	13
5.9.2.2	Electron Affinity	14
5.9.3	Astatine Molecule	15
5.9.3.1	Phase Transition Properties	15
5.9.3.2	Thermodynamic Properties	16
5.9.3.3	Dissociation Energy	17
5.9.4	Positive Molecular Ion of Astatine, At ₂ ⁺	19
5.9.5	At ⁺ and At ²⁺ Ions	19
5.10	Radii	20
5.10.1	Atomic Radius	20
5.10.2	Ionic Radii	20

IV.

5.10.2.1	At ⁻ Ion	20
5.10.2.2	At ⁺ and At ⁷⁺ Ions	21
5.11	Spectroscopic Properties	21
5.11.1	Atomic Absorption Spectrum	21
5.11.2	Mass Spectrometry	21
5.11.3	X-Ray Spectroscopic Properties	22
5.11.3.1	X-Ray Energies	22
5.11.3.2	X-Ray Atomic Energy Levels	23
5.11.3.3	K- and L-Shell Fluorescence Yields	25
5.11.3.4	Natural Widths of Atomic K and L Levels and K _α X-Ray Lines ...	25
5.11.3.5	X-Ray Screening Constants	25
5.11.4	Spectroscopic Constants of At ₂	26
REFERENCES	27

5. GENERAL PROPERTIES OF ASTATINE

Only a very limited amount of direct evidence is available concerning the properties of astatine because it occurs naturally in trace amounts. In view of this, most of the data for astatine have been extrapolated or interpolated by various empirical or theoretical treatments from the values determined for the other halogens, or for the neighboring elements of astatine in the Periodic Table. Recent improvements in the theoretical ab initio computations have also made it possible to calculate some of the basic properties of astatine.

5.1 Electronic Structure

Similarly to the other halogens, the astatine atom lacks one electron to fill its valence shell. The electron configuration of the ground state astatine atom can be assigned as $[\text{Xe}]4f^{14}5d^{10}6s^26p^5(^2P_{3/2})$ [1,2].

The ground state electronic structure of astatine ions is also analogous to that for other halogens. The valence shell of astatide ion has the noble gas configuration of $6s^26p^6(^1S_0)$ [3]. The ground state outer electron configuration of At^+ ion can be assigned as $6s^26p^4(^3P_2)$. For positive atomic ions the electronic structure is given in Table 2 (see Section 5.6).

5.2 Electronegativity

In Pauling's original table the electronegativity (X) of astatine is given as 2.2 [4]. The subsequent improved and more precise electronegativity scales give similar results [1,5,6]. The X values based on a number of scales and calculated by different methods [1,4 to 9] are summarized in Table 1.

Table 1. Electronegativity Values of Astatine Atom

Method of Determination	X Values	Ref.
Pauling Scale	2.2	[4]
Mulliken Scale	2.4	[1]
Gordy Scale	2.2	[5]
Electrostatic Forces	1.9	[6]
	2.42	[8]
Extrapolation by Mendeleev's Rule	2.25	[7]
$X = f(I)$	2.32	[9]

Electronegativities for higher oxidation states of astatine have been calculated on the basis of electrostatic forces and were found to be 1.74 and 2.048 for At^{5+} and At^{7+} ions, respectively [6].

5.3 Atomic Volume

The atomic volume for astatine has been estimated by extrapolation from the plot of atomic volume vs. period of halogens as $27.5 \text{ cm}^3/\text{gatom}$ [10]. More recently the atomic information indices, derived from the known electronic configuration of halogens, have also been used for correlation with their atomic volume. The latter value for astatine was then extrapolated from this dependence and found to be $33.9 - 34.5 \text{ cm}^3/\text{gatom}$ [11].

5.4 Atomic Refraction

The atomic refraction calculated on the basis of the electronegativity of astatine has been found to be $19.3 \text{ cm}^3/\text{gatom}$ [12].

5.5 Polarizabilities

The polarizability of astatide ion has been derived from its ionic radius and was stated to be $8.3 \times 10^{-24} \text{ cm}^3$ [13]. Using theoretical methods of calculation, the total quadrupole polarizabilities have been estimated as $57.03699 \times 10^{-40} \text{ cm}^5$ and $19.78638 \times 10^{-40} \text{ cm}^5$ for the free and for the crystal astatide ions, respectively [14].

Ab initio calculations have also been performed to estimate the static dipole polarizability of neutral astatine atom in the ground state. The values obtained in this way were found to be $4.36 \times 10^{-24} \text{ cm}^3$ [15,16], $7.88 \times 10^{-24} \text{ cm}^3$ [17], and $5.76 \times 10^{-24} \text{ cm}^3$ (38.9 Bohr^3)* [18].

5.6 Ionization Energies

The first ionization energy (I_1) for the element with atomic number 85 was originally derived by Finkelburg as 9.4 eV [19]. In subsequent papers the original value was modified to $9.5 \pm 0.2 \text{ eV}$ [20] and then to $9.2 \pm 0.4 \text{ eV}$ [21], which last value is usually quoted in the review literature [22]. This set of ionization energies was estimated by using regularities in the change of the screening constant ($\Delta\sigma$) from element to element in the Periodic Table. From the estimated value of $\Delta\sigma = 0.7$ for astatine and from the experimental I_1 quantities of adjacent to astatine elements (Po or Rn) the first ionization energy for astatine could be calculated [19 to 21]. From the linear dependence between the experimental parameter Z' for halogens - derived from gas chromatographic retention data of halogenated aliphatic compounds - and

*Originally quoted value is given in parentheses.

their first ionization energy Norseseyev and Nefedov have estimated the value of I_1 as 9.5 eV [23]. From the relationship between the vibrational frequency (ω_e) for halogen molecules and the first ionization energy of halogen atoms the value of I_1 has been estimated to be 10.4 eV by Varshni [24] assuming Clark's predicted value of $\omega_e = 139.4 \text{ cm}^{-1}$ for astatine (see Section 5.11.4). Ozhigov applied Mendeleev's rule of extrapolation to obtain 9.44 eV for the first and 16.71 eV for the second ionization energy of astatine atom [7]. The electron binding energy values of the outermost P_3 ($6p_{3/2}$) subshell for the free At atom - i.e. its first ionization energy - obtained by interpolation (9.3 eV) and by ab initio calculation (8.6 eV), as given in Table 14 (see Section 5.11.3.2), are close to the values of I_1 mentioned above. In Parsons' Handbook of Electrochemical Constants a value of 9.6 eV is given [25]. The estimated first and higher ionization energies for ground state astatine atom are summarized in Table 2.

Table 2. Atomic Ionization Energies of Astatine

I_n	Ionization Energy in eV	Ground State Configuration	Ref.
I_1	9.4	$\text{At}^+ \quad 6p^4 \quad ({}^3P_2)$	[19]
	9.5		[20]
	9.2		[21]
	9.5		[23]
	10.4		[24]
	9.44		[7]
	9.6		[25]
I_2	20.1	$\text{At}^{2+} \quad 6p^3 \quad ({}^4S_{3/2})$	[21]
	17.3		[23]
	18.0		[25]
	16.71		[7]
I_3	29.3	$\text{At}^{3+} \quad 6p^2 \quad ({}^3P_0)$	[21]
	30.0		[25]
I_4	41.0	$\text{At}^{4+} \quad 6p \quad ({}^2P_{1/2})$	[25]
I_5	51.0	$\text{At}^{5+} \quad 6s^2 \quad ({}^1S_0)$	[25]
I_6	78.0	$\text{At}^{6+} \quad 6s \quad ({}^2S_{1/2})$	[25]
I_7	91.0	$\text{At}^{7+} \quad 5d^{10} \quad ({}^1S_0)$	[25]
I_8	138.0	$\text{At}^{8+} \quad 5d^9 \quad ({}^2S_{1/2})$	[25]

The ionization energy for molecular astatine has been estimated by Kiser as 8.3 eV [26] in the same way as was done by Varshni [24]. In the calculation procedure the ionization energy for molecular halogens, as well as an estimated value of $\omega_e = 160 \text{ cm}^{-1}$ for At_2 were used [26]. Norsejev and Nefedov, using extrapolation based on the experimental parameter Z' (see above), estimated the ionization energy for molecular astatine as 8.4 eV [23].

5.7 Oxidation States

From the general trend in the Periodic System, astatine is expected to possess a more electropositive character than the other halogens. Thus, the first investigators considered astatine to be a metal showing a closer resemblance to polonium than to iodine [27 to 29]. On the other hand, the volatility of astatine, its extractability with carbon tetrachloride [29], and its similarity in physiological behavior to iodine [30,31] seemed to be consistent with its halogen character. Further systematic investigation of its aqueous solutions has shown that the valence states of astatine are similar to those of iodine. Johnson et al. described four oxidation states, viz. (-I), zero, and two positive valency states [32]. Appelman has confirmed and characterized (-I), zero, intermediate positive (I or III), and (V) valence states but found no evidence for the (VII) state [33,34]. Later, perastatate was able to be obtained by using XeF_2 as the oxidizing agent [35] and also by other methods [36 to 39]. Methods of preparation for different oxidation states of astatine are described in Section 10.2.1. In the following sections we review briefly the properties of these At species.

5.7.1 Astatine(-I)

The best defined valence state - astatine(-I) - has been found to be stable in acidic and basic solutions containing sufficiently strong reducing agents [32 to 34, 40 to 45]. In acidic solutions without reducing agents the astatide ion may be oxidized to the zero valence state [40,42]. Electromigration experiments [32,46], coprecipitation with insoluble iodides [32 to 34, 42,47,48], paper electrophoresis [38,40 to 42], paper chromatography [36,49], high pressure ion exchange chromatography [43], and free solution electrophoresis [39,45,50] have been used to characterize astatine(-I).

In contrast to the iodide ions, astatide has a strong tendency to adsorb on metallic silver [42,47] and tellurium [29,41,42,51] surfaces from acidic solutions containing reducing agents. Astatide, similarly to iodide, may be completely adsorbed on the reduced surfaces of metallic platinum from sulfuric acid solutions [52], and can also be characterized by the ability to replace halogens in simple halogenated aliphatic and aromatic compounds (see e.g. [53]).

5.7.2 Astatine(0)

At(0) is the expected oxidation state of astatine when it is isolated by dry methods at high temperatures from bismuth after irradiation with α -particles [32 to 34, 44, 54 to 58], and from thorium or uranium targets after bombardment with high energy protons [59 to 61]. At(0) is also assumed to be the oxidation state when astatine is redistilled at 500 °C from silver and platinum surfaces in closed glass ampoules [33, 39, 50, 58].

When elemental astatine is dissolved in pure water [38, 44, 58, 62 to 64], or in nitric acid solutions [32, 33, 65] the retention of the zero oxidation state is expected. The zero valence state of astatine was also supposed when it is prepared from a cyclotron-irradiated bismuth target by conventional dissolution and extraction techniques [43, 44, 62 to 64].

Aqueous solutions of At(0) may be prepared by oxidation of astatide ion with dilute nitric acid, Fe^{3+} , I_2 , VO_2^+ , As^{3+} at $\text{pH} < 5$, or $[\text{Fe}(\text{CN})_6]^{3-}$ at $\text{pH} < 3$ [32 to 34]. On the other hand, the zero oxidation state of astatine may also be formed from the higher oxidation states by reduction with Fe^{2+} , I^- , or VO^{2+} [32 to 34].

The zero oxidation state is characterized by its volatility, a tendency to be adsorbed by various metallic surfaces such as silver, gold, and platinum [32, 33, 38, 58, 60, 61] and less strongly by glass surfaces [33] both from vapours and solutions. At(0) can be extracted either from nitric acid solutions with isopropyl ether [54, 65, 66], CCl_4 , C_6H_6 [32, 33, 54], $n\text{-C}_6\text{H}_{14}$, and $c\text{-C}_6\text{H}_{12}$ [33, 65], or from sulfuric acid solutions with CHCl_3 [43, 44, 63 to 65]. At(0) is also characterized by reduced volatility from solutions as compared with the volatility of iodine, by varying degrees of coprecipitation with metal sulfides and hydroxides [32], and with metallic silver or tellurium *in situ* [33]. From acidic solutions containing SO_2 astatine is partially carried by TlI and AgI as a result of adsorption of At(0) on the surface of precipitates [32, 33].

The exact chemical nature of At(0) in solutions, however, still remains uncertain. Merinis et al. - during their experiments to produce interhalogen compounds of astatine (see KFKI-1984-29) - described the astatine activity, deposited in the gradient thermochromatographic tube at 16 °C, as At_2 [67]. More recently Oozai and Takahashi have claimed to identify the At_2 peak by gas liquid chromatography [68]. However, as several authors have pointed out, the existence of molecular astatine is excluded by its extremely low concentration under ordinary conditions of chemical experiments [33, 69 to 72]. Furthermore, the formation of At_2 does not seem to be realistic because any reaction which tends to split the At_2 molecule becomes thermodynamically favored at these low concentrations [65]. It is also unlikely that the zero valence state of astatine is present as a true At^\cdot radical because of the assumed high reactivity of the latter [33, 71]. Since iodine is always present in excess, Aten supposed that in aqueous solutions At(0) exists as AtI [69].

A similar conclusion has been drawn by Visser and Diemer from their extraction experiments with At(O) [72]. Other authors have assumed that At(O) in aqueous solutions may react with organic impurities forming organic astatine compounds the exact nature of which depends on the medium [33,34,65,71,73].

Meyer et al. have investigated the reactivity of At(O), dissolved in neutral aqueous solutions, with simple aromatic compounds. For benzene and chlorobenzene the hydrogen and chlorine substitution yields did not exceed 1%. A higher hydrogen replacement yield (49%) was observed with aniline [63, 64].

In the presence of elemental chlorine, bromine, and iodine the zero oxidation state of astatine is represented by AtCl, AtBr, and AtI. These diatomic interhalogen compounds have been prepared both in solution and in the gaseous state [33,44,48,63,64,69,74 to 76], and have been characterized by their extractibility with organic solvents [33,48,69,74] and by their deposition temperature [67].

5.7.3 Astatine(I)

The time-of-flight spectrometry measurements of Appelman et al. have demonstrated the existence of At⁺ ions in the gaseous phase (see Section 5.11.2). This is so far the only direct method to identify any of the oxidation states of astatine [75]. The mass spectrum of At⁺ is shown in Fig. 1. Later, Golovkov et al. also detected At⁺, formed in the plasma ion source of a mass separator, by its radioactivity [76].

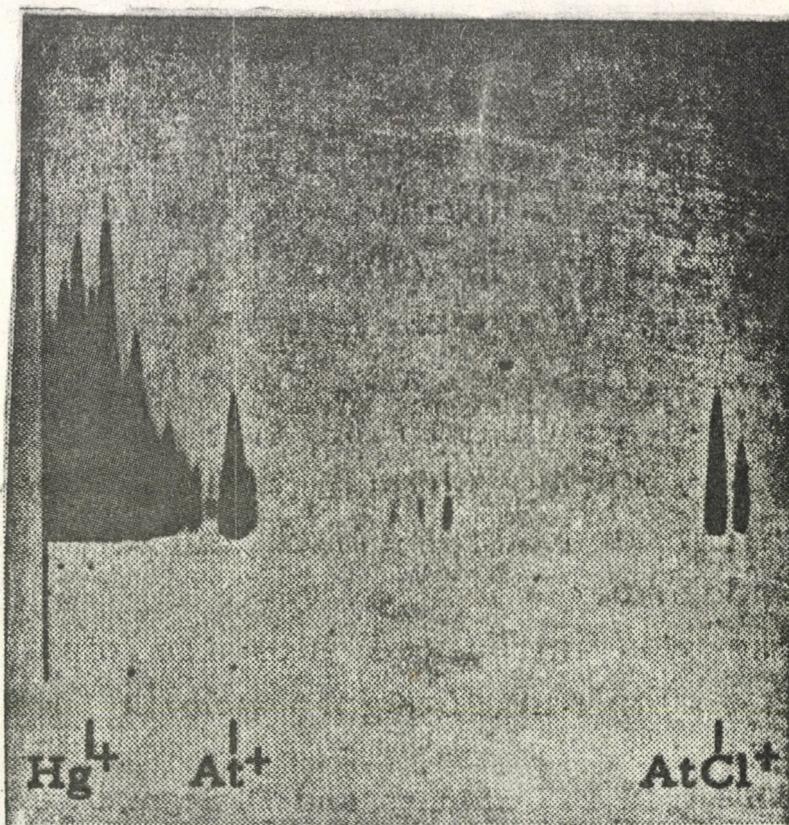


Fig. 1
Mass spectrum of At⁺
and other A-species

The monovalent cationic form of astatine can be obtained and stabilized in nitric acid solutions containing $\text{Cr}_2\text{O}_7^{2-}$ as the oxidizing agent. The positive charge of astatine(I) species has been established by free solution electrophoresis [46,50,77], while its monovalent character by ion exchange chromatography [43,77,78].

The astatine(I) state has been assumed to be responsible for the formation of complex anions AtX_2^- ($X = \text{Cl}, \text{Br}, \text{I}, \text{SCN}, \text{CN}$, thiourea or its derivatives) [54,79 to 84]. From the results of numerous experiments [46,50,77 to 82,85 to 88] Khalkin et al. concluded that astatine(I) in acidic solutions containing $\text{Cr}_2\text{O}_7^{2-}$ can form a stable aquacomplex $[(\text{H}_2\text{O})_x\text{At}]^+$ ($x=1$ or 2) [86 to 88]. This assumption is well in line with the earlier findings of Neumann [54] and with the recent experimental results on the hydrogen substitution reactions of astatine with simple aromatic compounds. From the positive results of aromatic H-replacement the existence of $[\text{H}_2\text{OAt}]^+$, as an electrophilic species, could also be concluded [89].

5.7.4 Astatine(III)

For the anionic species formed by oxidation of astatine with elemental bromine, the probable oxidation state of At(III) has been assumed [32,33]. From the migration rates measured by free solution electrophoresis Dreyer et al. have proposed the existence of AtO^+ or H_2AtO_2^+ , AtO_2^- , and AtOX_2^- ($X = \text{Cl}, \text{Br}$, and I) species. In order to study the mobilities of these ions, At(III) state was obtained by oxidation of At(0) with $\text{S}_2\text{O}_8^{2-}$ in HClO_4 solutions or with XeF_4 in neutral medium [36,39,50,82]. In the course of investigating the properties of inorganic astatine species under oxidative conditions, Visser and Diemer suppose that with *n*-dibutyl ether from $\text{S}_2\text{O}_8^{2-}$ and H_2O_2 solutions, etherates containing the At(III) moiety are extracted. The expressed complex forming ability of astatine(III) is also discussed by these authors [72].

In the compounds of ArAtCl_2 and Ar_2AtCl ($\text{Ar} = \text{C}_6\text{H}_5$ or $p\text{-CH}_3\text{C}_6\text{H}_4$) synthesized by Norsejev et al., the At(III) state was obtained by oxidation of At(-I) with Cl_2 [90,91] (see KFKI-1984-29).

5.7.5 Astatine(V)

The AtO_3^- anion belongs to the well characterized chemical form of astatine(V). This ionic species can be formed from the lower oxidation states under stronger oxidation conditions (i.e. in hot solutions containing the oxidizing agent) [32 to 34,37 to 40,50] or by acidifying the AtO_4^- containing solutions [39].

AtO_3^- ion was originally characterized by its tendency to coprecipitate with AgIO_3 [32 to 34], $\text{Ba}(\text{IO}_3)_2$, and $\text{Pb}(\text{IO}_3)_3$ [33,34]. This interpretation became doubtful when the $\text{At}(\text{I})$ state was also shown to coprecipitate with the insoluble iodates [80]. Identification by paper chromatography, paper electrophoresis [38,40], and by free solution electrophoresis [39,50] made the existence of the AtO_3^- anion certain.

In the organometallic compounds of ArAtO_2 ($\text{Ar} = \text{C}_6\text{H}_5$ or $p\text{-CH}_3\text{C}_6\text{H}_4$) the central astatine atom has an oxidation state of $\text{At}(\text{V})$. These compounds have been prepared by Norsejev et al. by oxidation of ArAtCl_2 with hot NaOCl solution [90,91].

5.7.6 Astatine(VII)

The perastatate ion, AtO_4^- , was first prepared by Khalkin et al. by oxidizing At^- with XeF_2 in a hot alkaline solution [35], in the same way that the formation of perbromate was carried out shortly before [92]. The AtO_4^- anion was identified and characterized by paper electrophoresis and by its coprecipitation with potassium and cesium metaperiodate [35]. Later anodic oxidation [36] or oxidation with KIO_4 in neutral or alkaline solutions were also utilized to prepare AtO_4^- [36 to 39]. For the identification of the perastatate ion, paper chromatography [35,36,38], paper electrophoresis [38], and free solution electrophoresis [39,50] have been applied.

AtO_4^- , similarly to IO_4^- , is stable only in neutral and alkaline solutions. By means of heating in an acidic medium the reduction of perastatate into astatate is completed in several minutes [38,39].

5.8 Electrochemical Properties

5.8.1 Critical Deposition Potentials

The critical deposition potentials of astatine both at the cathode and anode from different aqueous solutions have been determined by Johnson et al. and are summarized in Tables 3 and 4. These values were obtained by extrapolation of deposition rates vs. potential curves to zero rate. The chemical forms of deposited At species in the electrolytic experiments were not determined [32].

Table 3. Critical Deposition Potentials of Astatine at the Cathode [32]

Solution	At Concentration in pM	Potential in V vs. NHE*
0.066 M HNO ₃	0.28	- 1.225
1.0 M HNO ₃	0.05	- 1.240
0.075 M H ₂ SO ₄ +0.1 M Na ₂ Cr ₂ O ₇	0.60	- 1.200
0.006 M HNO ₃ + 3 mg Au	0.10	- 1.220
0.066 M HNO ₃	0.04	- 1.220

*NHE = normal hydrogen electrode.

Table 4. Critical Deposition Potentials of Astatine at the Anode [32]

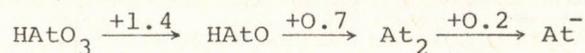
Solution	At Concentration in pM	Potential in V vs. NHE*
0.066 M HNO ₃	0.24	- 1.460
0.066 M HNO ₃	0.53	- 1.450
0.100 M HNO ₃ +0.1 M K ₂ S ₂ O ₈	0.54	- 1.445

*NHE = normal hydrogen electrode.

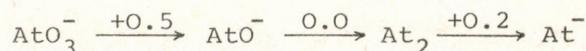
5.8.2 Standard Electrode Potentials

On the basis of potentials of the redox couples employed by Johnson et al. for preparing the oxidation states of At(-I), At(O), At(I), and At(V) [32], Latimer has constructed the first tentative standard electrode potential diagrams (in V) for astatine [93]:

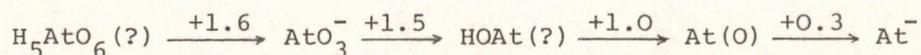
Acidic Solution



Basic Solution



However, the uncertain potentials of the systems studied by Johnson et al. [32], as well as the problematic nature of the chemical form of At(O) (see Section 5.7.2) make Latimer's potential diagram questionable. Later, in a more systematic study with suitably chosen redox couples Appelman determined the following reduction potential diagram for At(-I), At(O), At(I?), At(V), At(VII?) oxidation states in 0.1 M acid at 25 °C:



The exact valence of the positive oxidation state (or states) between At(O) and At(V) could not be determined, and no evidence for At(VII) state was found at that time [33,34].

The standard electrode potential for At(O)/At(-I) couple has been estimated by Mendeleev's rule of extrapolation as 0.457 V [7]. More recently, ion exchange chromatography at a fixed redox potential has also been used to determine standard potentials for different redox couples of astatine. The potential values obtained by this technique were found to be 0.335 V at 323 K and 0.85 V at 332 K for the At(O)/At(-I) and At(x)/At(O) couples, respectively [94]. For the latter couple, At(x) represents an intermediate oxidation state between At(O) and At(V).

5.9 Thermodynamic Data

The thermodynamic properties of astatine species have solely been able to be estimated by various theoretical and empirical calculations. Data on enthalpies, Gibbs free energies, entropies, and other thermodynamic properties of individual inorganic and organic astatine compounds are dealt with in KFKI-1984-29. Here, the thermodynamic data for different astatine species are summarized.

5.9.1 At⁻ Ion

Enthalpies, Gibbs free energies, entropies, and heat capacities at constant pressure for gaseous and hydrated At⁻ ions are summarized in Table 5. The heat of formation for gaseous At⁻ was first evaluated by Ladd and Lee from the ΔH_f° values for gaseous alkali metal astatides by using the Born-Haber cycle [95]. Another ΔH_f° value for gaseous At⁻ has been estimated from the lattice energy of alkali metal halides vs. ΔH_f° for a gaseous halide ions plot [96]. The entropy of gaseous At⁻ was calculated by using the Sackur-Tetrode equation [96]. In Table 5 the thermodynamic data for gaseous At⁻ from the Handbook of Thermal Constants [97] are also given.

Table 5. Thermodynamic Data for Gaseous and Hydrated At^- at 298.15 K

At^-	ΔH_f°	ΔG_f°	S°	C_p°	Ref.
	in kJ/mol (kcal/mol)*		in J K ⁻¹ gatom ⁻¹ (cal K ⁻¹ gatom ⁻¹)*		
Gaseous	-196.6 (-47.0)				[95]
	-190.8 (-45.6)	-255 (-53.8)	175.5 (41.95)		[96]
	-178.66 (-42.7)	-202.47 (-48.391)	175.4 (41.93)	20.79 (4.968)	[97]
Hydrated	-8.4 (-2.0)	-7.95 (-1.9)	125.5 (30.0)		[96]

The heat of formation for hydrated At^- has been deduced from calculated heat of hydration and heat of formation for gaseous At^- [96].

The entropy of astatide ion in a crystalline lattice has been given as 67.78 J K⁻¹ gatom⁻¹ (16.2 cal K⁻¹ gatom⁻¹)* [98].

Krestov has calculated the change of thermodynamic functions on hydration for astatide ion in a series of papers [98 to 100]. The results are given below:

Properties		Values	Ref.
ΔH_{hydr}	in kJ/gatom (kcal/gatom)*	182.42 (43.6)	[99]
ΔS_{hydr}	in J K ⁻¹ gatom ⁻¹ (cal K ⁻¹ gatom ⁻¹)*	-107.95 (-25.8)	[98]
$(\Delta C_p)_{\text{hydr}}$	in J K ⁻¹ gatom ⁻¹ (cal K ⁻¹ gatom ⁻¹)*	-66.94 (-16.0)	[100]

An empirical method, based on the effective charge on the astatide ion, has been used to determine the heats of solvation (ΔH_{solv}) for At^- in different organic solvents [101]. The ΔH_{solv} values for aliphatic alcohols are given below together with the entropy changes on solvation (ΔS_{solv}) in these alcohols evaluated by Krestov [102].

*Originally quoted values are given in parentheses.

Properties	CH ₃ OH	C ₂ H ₅ OH	n-C ₃ H ₇ OH	Ref.
ΔH_{solv} in kJ/gatom	322.4	297.3	288.9	[101]
ΔS_{solv} in J K ⁻¹ gatom ⁻¹ (cal K ⁻¹ gatom ⁻¹)*	-120.5 (-28.8)	-135.14 (-32.3)		[102]

5.9.2 Astatine Atom

5.9.2.1 Thermodynamic Properties

The fundamental thermodynamic properties for the gaseous astatine atom, taken from the literature [96,97,103], are summarized in Table 6 and show good agreement. In addition to the properties given in Table 6, the compilation of data by Stull and Sinke gives also the enthalpy, free energy function, and the logarithm of the equilibrium constant of formation for the temperature range 298.15 K to 3000 K [103].

Table 6. Thermodynamic Properties of Gaseous Astatine Atom at 298.15 K

Properties	[96]	[97]	[103]
$\Delta H_{\text{f}}^{\circ}$ in kJ/gatom (kcal/gatom)*	92 (22)	97.24 (23.24)	92.048 (22.000)
$\Delta G_{\text{f}}^{\circ}$ in kJ/gatom (kcal/gatom)*	54 (13)	59.576 (14.239)	54.400 (13.002)
S° in J K ⁻¹ gatom ⁻¹ (cal K ⁻¹ gatom ⁻¹)*	187 (44.7)	186.98 (44.69)	186.94 (44.68)
C_{P}° in J K ⁻¹ gatom ⁻¹ (cal K ⁻¹ gatom ⁻¹)*		20.79 (4.968)	20.79 (4.97)

The entropy for the solid state astatine atom has been estimated by Krestov as 60.67 J K⁻¹ gatom⁻¹ (14.5 cal K⁻¹ gatom⁻¹)* [96].

*Originally quoted values are given in parentheses.

5.9.2.2 Electron Affinity

The classical method of determining electron affinity (EA) from the selected ΔH_f^O quantities for gaseous astatine atom and At^- [97] results in a value of -276.39 kJ/gatom at 298.15 K. In similar calculations, the value $\Delta H_f^O(At) = 0.5D(At_2) - D(At_2)$ is the dissociation energy of molecular astatine (see Section 5.9.3.3) - was used by Ladd and Lee, instead of the heat of formation for the astatine atom. The EA value given by these authors as -255.22 kJ/gatom (-61 kcal/gatom)* [95] is, therefore, to be considered not quite correct.

The atomic electron affinity of astatine has also been estimated by using different extrapolation methods [3,7,96], semiempirical [23] and empirical relationships [104], and theoretical ab initio calculations [105]. The EA value for astatine recommended by Hotop and Lineberger is given in [106]. The data are summarized in Table 7. With the exception of ab initio calculations, the atomic electron affinity values for astatine estimated by different methods are in reasonable agreement with those determined from thermodynamic data.

Table 7. Calculated Electron Affinity Values for Astatine

Method of Calculation	EA in kJ/gatom	Ref.
From Thermodynamic Data	-276.39 [†]	
	-255.2 (-61.0 kcal/gatom)*	[95]
Horizontal Analysis	-270.2 (-2.80 eV)*	[3]
Mendeleev's Rule of Extrapol.	-267.8 (-64.0 kcal/gatom)*	[7]
EA = f(Z')	-270.2 (-2.8 eV)*	[23]
Extrapol. from EA for Halogens	-284.5 (-68.0 kcal/gatom)*	[96]
EA = f(ω_e , μ)	-268.93 (-2.7872 eV)*	[104]
Theoretical Calculation	-318.4 (-3.3 eV [#])*	[105]
Recommended Value	-270.2 (-2.8 eV)*	[106]

*Originally quoted values are given in parentheses.

[†]Calculated from tabulated data for ΔH_f^O values [97].

[#]Approximated value derived from histogram bars.

The entropy change of atomic electron affinity (ΔS_{EA}) for astatine has been calculated by Krestov who deduced a value $\Delta S_{EA} = -41.99 \text{ J K}^{-1} \text{ gatom}^{-1}$ ($-10.036 \text{ cal K}^{-1} \text{ gatom}^{-1}$)* from the entropies of the gaseous astatine atom and At^- , the entropy of free electronic gas, and the entropy change on mixing [107].

5.9.3 Astatine Molecule

Although the existence of At_2 in typical chemical experiments so far remains uncertain (see Section 5.7.2), many of its thermodynamic properties have been predicted. These data may be useful in further searches for the astatine molecule.

5.9.3.1 Phase Transition Properties

Melting and boiling temperatures (T_m and T_b), enthalpy and entropy changes on phase transitions (ΔH and ΔS) for the astatine molecule are listed in Table 8. Durand's prediction belongs to the first determinations of the physicochemical properties of astatine. His extrapolation was based upon the nearly linear dependence of T_m and T_b for noble gases and H_2 on the melting and boiling temperatures of halogen molecules in the corresponding rows of the Periodic Table. The value of 684 K for T_m however, seems to be unrealistic being higher than that for T_b [108]. Ozhigov's T_m and T_b values have been extrapolated on the basis of Mendeleev's rule [7] and are in reasonable agreement with those given in different compilations [97,103,109,110]. The T_m and T_b values estimated by Norsejev and Nefedov using the empirical parameter Z' are somewhat lower compared with other corresponding data given in Table 8. However, the enthalpy of vaporization at the boiling temperature was found by these authors to be similar [23] to that given in the Handbook of Thermal Constants [97].

Recently, Otozai and Takahashi determined the boiling temperature for At_2 from the GLC absolute retention volume and obtained $503 \pm 3 \text{ K}$ [68]. The T_b value determined by these authors is significantly lower than those given in Table 8 and does not seem to be reliable because of the uncertainty of the existence of At_2 (see Sections 5.7.2 and 10.2.1.3.1), under the given experimental conditions.

The heat of vaporization (ΔH_v) and heat of sublimation (ΔH_s) at the melting point for At_2 have been estimated by correlation of these quantities for halogens with their atomic numbers. The ΔH_v and ΔH_s values obtained in this way, as well as the literature value of the heat of melting (ΔH_m) were then adjusted using the relation $\Delta H_m = \Delta H_s - \Delta H_v$. The data estimated by Gerasimov et al. are given below [111].

*Originally quoted value is given in parentheses.

$$\Delta H_m = 17.57 \text{ kJ/mol} \quad (2.1 \text{ kcal/gatom})^*$$

$$\Delta H_s = 67.78 \text{ kJ/mol} \quad (8.1 \text{ kcal/gatom})^*$$

$$\Delta H_v = 50.21 \text{ kJ/mol} \quad (6.0 \text{ kcal/gatom})^*$$

Table 8. Thermodynamic Data of Phase Transitions for At₂

Phase Transition	T in K	ΔH in kJ/mol (kcal/mol)*	ΔS in J K ⁻¹ mol ⁻¹ (cal K ⁻¹ mol ⁻¹)*	Ref.
Cryst. → Liquid	684			[108]
	505.5			[7]
	473			[23]
	500	20.92 (5.0)	41.84 (10)	[97]
	575	23.85 (5.70)		[103]
	573			[109]
	575			[110]
Cryst. → Gas	0	86.61 (20.7)		[97]
	298.15	83.68 (20.0)	280.75 (67.1)	[97]
Liquid → Gas	572			[108]
	582			[7]
	543	50.21 (12.0)		[23]
	590	54.39 (12.0)	92.05 (22.0)	[97]
	650	90.37 (21.6)		[103]
	608			[109]
	610			[110]

5.9.3.2 Thermodynamic Properties

The thermodynamic functions for molecular astatine have been estimated by Stull and Sinke by comparison with the corresponding thermodynamic properties of other halogens. In their compilation the data of the reference state and ideal gaseous state for At₂ over the entire temperature range from 298.15 K to 3000 K are tabulated [103]. In the Handbook of Thermal Constants

*Originally quoted values are given in parentheses.

the selected and calculated values of the fundamental thermodynamic properties for crystalline solid and ideal gaseous At_2 at 298.15 K are given [97]. The enthalpy and Gibbs free energy of formation, entropy, and heat capacity at constant pressure for crystalline solid and ideal gaseous At_2 at 298.15 K from these two sources [97,103] are given in Table 9. The heat of formation for At_2 has also been estimated by Kaganyuk on the basis of the effective charge on astatine; he has obtained the value $\Delta H_f^\circ = 87.9 \text{ kJ/mol}$ [101].

Table 9. Thermodynamic Properties of At_2 at 298.15 K

Properties	Cryst. Solid		Ideal Gas	
	[97]	[103]	[97]	[103]
ΔH_f° in kJ/mol (kcal/mol)*	0	0	83.68 (20.0)	90.37 (21.6)
ΔG_f° in kJ/mol (kcal/mol)*	0	0	40.145 (9.595)	44.217 (10.568)
S° in $\text{J K}^{-1} \text{mol}^{-1}$ (cal $\text{K}^{-1} \text{mol}^{-1}$)*	121.34 (29.0)	121.34 (29.0)	267.36 (63.9)	276.14 (66.0)
C_P° in $\text{J K}^{-1} \text{mol}^{-1}$ (cal $\text{K}^{-1} \text{mol}^{-1}$)*	54.39 (13.0)	58.58 (14.0)	37.07 (8.86)	33.47 (8.0)

Similar results were obtained by Kharitonov et al. using a statistical thermodynamic approach for determining the thermodynamic functions for gaseous molecular astatine. Estimated values of interatomic distance and vibrational frequency (see Section 5.11.4) were used to calculate the enthalpy ($H_T^\circ - H_O^\circ$), internal energy ($U_T^\circ - U_O^\circ$), reduced isobar potential Φ , absolute entropy, and heat capacity at constant pressure for the temperature range from 298.15 K to 1000 K [112]. These data are given in Table 10.

5.9.3.3 Dissociation Energy

From the decreasing tendency of dissociation energy (D) with increasing atomic number for molecular halogens (with the exception of F_2), the D value for At_2 is expected to be the lowest in this group of elements. Most of the dissociation energy data for At_2 have been estimated by using various

*Originally quoted values are given in parentheses.

Table 10. Thermodynamic Functions for At_2 Calculated by Statistical Thermodynamic Approach [112]

T in K	$H_T^{\text{O}} - H_O^{\text{O}}$ in J/mol	$U_T^{\text{O}} - U_O^{\text{O}}$ in J/mol	$\Phi = - \frac{G_T^{\text{O}} - H_O^{\text{O}}}{T}$ in $\text{J K}^{-1} \text{mol}^{-1}$	S_T^{O} in $\text{J K}^{-1} \text{mol}^{-1}$	C_p^{O} in $\text{J K}^{-1} \text{mol}^{-1}$
298.15	10 416	7 937	241.2	276.1	37.1
400	14 203	10 878	251.6	287.8	37.2
500	17 931	13 774	259.5	295.4	37.3
600	21 663	16 675	266.1	302.2	37.3
700	25 398	19 578	271.7	307.9	37.4
800	29 135	22 483	276.5	312.9	37.4
900	32 872	25 389	280.8	317.1	37.4
1 000	36 611	28 296	284.7	321.3	37.4

empirical correlations connecting the D values for halogens with their other properties, such as ionization energy (*I*) [26], atomic number (*Z*) [113], period [113,114], and experimental parameter (*Z'*) [23] (see Section 5.6). Theoretical calculations of dissociation energy for At₂ have also been performed [115]. The D values from these sources are summarized in Table 11.

Table 11. Calculated Values of Dissociation Energy for At₂

Method of Calculation	Dissociation Energy in kJ/mol	Ref.
lg D = f (lg <i>I</i>)	115.78 (1.2 eV)*	[26]
D = f (<i>Z</i>)	77.19 (0.8 eV)*	[113]
D = f (Period)	77.19 (0.8 eV)*	[113]
	96.23 (23.0 kcal/mol)*	[114]
D = f (<i>Z'</i>)	112.13 (26.8 kcal/mol)*	[23]
Theoretical	75.31 (18.0 kcal/mol)*	[115]
Thermodynamic	108.78 (26 kcal/mol)*	[97]

5.9.4 Positive Molecular Ion of Astatine, At₂⁺

For this ionic species the enthalpy of formation has been deduced from the ionization energy of At₂ (see Section 5.6) as 887 kJ/mol (212 kcal/mol)* [97].

The dissociation energy for At₂⁺ has been derived from the thermodynamic cycle of dissociation and ionization and was found to be 231.56 kJ/mol (2.4 eV)* [26]. A similar estimation with selected values for the dissociation energy of At₂, and the atomic and molecular ionization energies of astatine gave a value of 193.966 kJ/mol (46.359 kcal/mol)* [97].

5.9.5 At⁺ and At²⁺ Ions

The heat of formation for gaseous At⁺ and At²⁺ ions has been deduced from their ionization energies [96,97], and is given below.

*Originally quoted values are given in parentheses.

Species	ΔH_F^O in kJ/mol (kcal/mol)*	
	[96]	[97]
At ⁺	1 004 (240)	983 (235)
At ²⁺	2 761 (660)	2 084 (498)

5.10 Radii

5.10.1 Atomic Radius

The atomic radius (R) for astatine has been evaluated as 0.146 nm using Mendeleev's rule of extrapolation [7]. Estimation from the linear plot of atomic radii for halogens vs. their experimental parameter Z' (see Section 5.6) leads to a value of 0.145 nm [23]. The values of 0.119 nm [17] and 0.127 nm [116] have been obtained by theoretical ab initio calculations.

5.10.2 Ionic Radii

5.10.2.1 At⁻ Ion

The radius (r) for the gaseous astatide ion has been estimated from the constancy of the ratio of radii for the isoelectronic ion pairs. The value of 0.197 nm calculated in this way by Krestov [96] seems to be low compared with those for other halogens given by Krasnov as 0.112 nm for F⁻, 0.1683 nm for Cl⁻, 0.1864 nm for Br⁻, and 0.2119 nm for I⁻ gaseous ions [117].

Different methods have been applied to estimate the ionic crystal radius for At⁻ [7,23,96,118 to 121]. The methods and the results of these calculations are summarized in Table 12.

Table 12. Calculated Values of Ionic Crystal Radius for At⁻

Method of Calculation	Radius in nm	Ref.
From Interionic Distance	0.227	[117]
Mendeleev's Rule	0.226	[7]
r = f (lg Z)	0.234	[118]
	0.261	[119]
r = f (r _{X-}) X = Halogen	0.230	[96]
r = f (Z')	0.229	[23]
r = f (Lattice Energy)	0.222	[120]

*Originally quoted value are given in parentheses.

5.10.2.2 At⁺ and At⁷⁺ Ions

Extrapolation according to Mendeleev's rule has been used to determine the radius of the gaseous At⁺ ion. The value obtained in this way was found to be 0.061 nm [7]. From the ratio $r_{\text{At}^+}/R_{\text{At}} = 0.28$ determined by Korablev [122], the radius of At⁺ can be estimated as 0.041 nm if one uses Ozhigov's value for the atomic radius of 0.146 nm [7].

The radius of At⁷⁺ has been evaluated by making use of the smooth regularity between radius and charge for isoelectronic ions. From the sequence Au⁺, Hg²⁺, Tl³⁺, Pb⁴⁺, and Bi⁵⁺ the extrapolated value for At⁷⁺ was found to be 0.062 nm [123]. Norsejev and Nefedov estimated the radius of At⁷⁺ as 0.06 nm [23]. In Parsons' Handbook of Electrochemical Constants a value of 0.062 nm is given [25].

5.11 Spectroscopic Properties

5.11.1 Atomic Absorption Spectrum

The ability to detect the atomic absorption spectrum is one of the very few ways of obtaining direct information on astatine. Using a highly sensitive spectroscopic detection method, McLaughlin was able to measure the absorption spectrum of astatine atoms. His method included the adaptation of capillary-absorption-cell spectroscopy, which allowed the detection of as little as 0.2 ng of gaseous astatine. The temperature of the quartz capillary absorption cell was kept at 600 °C to enhance the decomposition of molecules that might have contained astatine. In order to prove which of the recorded lines belongs to astatine, the intensities were monitored as a function of time. The decrease of line intensities for 244.401 nm and 216.225 nm were found to be consistent with the radioactive decay of astatine. The two astatine lines were assigned by extrapolation from the lowest absorption lines for lighter halogens. The lines 224.401 nm and 216.225 nm were assigned to the transitions $^2P_{3/2} \rightarrow ^4P_{5/2}$ and $^2P_{3/2} \rightarrow ^4P_{3/2}$, respectively, between electron configurations $6p^5 \rightarrow 6p^47s$ [124].

5.11.2 Mass Spectrometry

Using a highly sensitive (~ 40 atom/cm³) time-of-flight spectrometer, Appelman et al. have directly detected the mass spectra of some astatine containing ions, such as At⁺, HAt⁺, CH₃At⁺, and AtX⁺ - X = Cl, Br, I - even though no evidence for At₂⁺ and AtF⁺ ions could be obtained [75].

More recently Golovkov et al. - using a mass separator with plasma ion source - detected the following ionic species: AtH⁺, AtOH⁺, AtOH₂⁺, AtX⁺ (X = Cl, Br, I), and At₂⁺ from their radioactivity. The formation of At₂⁺

was explained as the result of a heterolytic reaction between At^+ and $\text{At}(\text{O})$ at the outlet of the plasma ion source. The existence of At_2^+ in this mass spectroscopic study was interpreted by means of its higher dissociation energy value compared with that of At_2 [76].

When introducing chlorine or bromine into the ion source in both cases two lines of AtCl^+ and AtBr^+ could be observed with relative intensities corresponding to the relative abundance of stable halogen isotopes in question [75,76].

5.11.3 X-Ray Spectroscopic Properties

5.11.3.1 X-Ray Energies

In the electron capture branch of neutron-deficient radon isotopes, e.g. ^{208}Rn , ^{209}Rn , ^{210}Rn , ^{211}Rn , X-ray emission from the daughter astatine isotopes is to be expected. Indeed, X-rays with energies characteristic for astatine ($K_{\alpha_2} = 78.945$ keV, $K_{\alpha_1} = 81.516$ keV, and $K_{\beta_1} = 92.30$ keV) have been detected in the low energy region of γ -spectra [125,126]. Besides the experimental results, X-ray data for astatine can be found in a number of tables with computed values of X-radiation energies for the heavier elements (see e.g. [127 to 129]). The X-ray energies of the principal K and L spectral lines for astatine, determined by interpolation - taken from the most frequently cited source, i.e. Bearden's X-Ray Wavelengths compilation [129], - are summarized in Table 13. The relative intensities of these lines are also given in this table [127]. A complete tabulation of K and L X-ray energies and of their relative intensities for astatine can be found in [127].

Table 13. The K and L X-Ray Energies for Astatine

Designation	X-Ray Energy in keV [129]	Relative Intensities in % [127]
K - S e r i e s		
α_2 KL_2	78.95	60.3
α_1 KL_3	81.52	100.0
β_3 KM_2	91.72	11.3
β_1 KM_3	92.30	22.0
β_2^{II} KN_2	94.84	2.72
β_2^I KN_3	94.99	5.41
L - S e r i e s		
β_3 L_1M_3	14.0670	33.55
β_1 L_2M_4	13.8760	131.50
γ_1 L_2N_4	16.2510	27.95
α_2 L_3M_4	11.3048	11.40
α_1 L_3M_5	11.4268	100.0 (5.21)*

*Relative intensity of the L_{α_1} line with respect to $K_{\alpha_1} = 100\%$.

5.11.3.2 X-Ray Atomic Energy Levels

Most of available atomic electron binding energy (E_b) values for ground state astatine have been estimated by interpolation in Z between the experimental binding energies of neighboring elements [127,128,130 to 133]. The X-ray atomic electron binding energy levels, given in Table 14, are taken from the compilation of Sevier [132]. Electron binding energies for neutral astatine atoms have also been determined by theoretical ab initio calculations [134 to 136]. The theoretical data of Huang et al. [135] are also included in Table 14. The E_b values for free astatine atom, deduced from the X-ray data, are given in the last column of Table 14 [133]. It can be seen from these data that the theoretically calculated electron binding energy values are closer to those determined for the free astatine atom.

Table 14. Atomic Electron Binding Energies for Astatine

Level	$-E_b$ in eV		
	To Fermi Level [132]	Theor Calc. [135]	In Free Atom [133]
K $(1s_{1/2})$	95 724.0	95 721.9	95 729
L ₁ $(2s_{1/2})$	17 481.5	17 496.0	17 490
L ₂ $(2p_{1/2})$	16 777.3	16 781.4	16 782
L ₃ $(2p_{3/2})$	14 208.0	14 213.4	14 212
M ₁ $(3s_{1/2})$	4 311.7	4 335.9	4 320
M ₂ $(3p_{1/2})$	3 995.8	4 009.2	4 005
M ₃ $(3p_{3/2})$	3 410.5	3 423.1	3 420
M ₄ $(3d_{3/2})$	2 901.8	2 909.6	2 910
M ₅ $(3d_{5/2})$	2 780.7	2 788.7	2 788
N ₁ $(4s_{1/2})$	1 038.2	1 054.9	1 044
N ₂ $(4p_{1/2})$	897.7	912.7	904
N ₃ $(4p_{3/2})$	753.7	765.2	761
N ₄ $(4d_{3/2})$	527.6	538.1	535
N ₅ $(4d_{5/2})$	500.1	510.6	508
N ₆ $(4f_{5/2})$	207.0	212.6	217
N ₇ $(4f_{7/2})$	200.8	206.3	211
O ₁ $(5s_{1/2})$	193.4	206.6	196
O ₂ $(5p_{1/2})$	145.6	154.3	153
O ₃ $(5p_{3/2})$	113.6	124.4	123
O ₄ $(5d_{3/2})$	40.9	47.9	48
O ₅ $(5d_{5/2})$	37.4	43.9	44
P ₁ $(6s_{1/2})$	15.0	24.5	19
P ₂ $(6p_{1/2})$	5.7	11.9	11
P ₃ $(6p_{3/2})$	2.8	8.6	9.3

5.11.3.3 K- and L-Shell Fluorescence Yields

The K-shell fluorescence yield (ω_K) has been estimated as 0.971 [137] and 0.969 [138]. The high value of ω_K indicates the high probability that a vacancy in the K-shell of astatine is filled via radiative transition. Theoretical calculations on the L-shell fluorescence yields have given the following results: $\omega_{L1} = 0.129$ [139], $\omega_{L2} = 0.422$, and $\omega_{L3} = 0.380$ [140]. Similar values can be found in Krause's compilation: $\omega_{L1} = 0.128$, $\omega_{L2} = 0.415$, and $\omega_{L3} = 0.399$ [138].

5.11.3.4 Natural Widths of Atomic K and L Levels and K_{α} X-Ray Lines

Semi-empirical values of natural widths for K, L_1 , L_2 , and L_3 levels, have been estimated for atomic astatine from its corresponding theoretical radiative rate and estimated fluorescence yield. $K_{\alpha 1}$ and $K_{\alpha 2}$ X-ray line widths were calculated as the sum of the widths of the levels involved in the transition [141]. The semi-empirical values of the natural widths for astatine atom are given below.

Natural Widths in eV					
K	L_1	L_2	L_3	$K_{\alpha 1}$	$K_{\alpha 2}$
69.8	12.8	7.01	6.29	76.1	76.8

5.11.3.5 X-Ray Screening Constants

X-Ray screening constants (σ_1 and σ_2), accounting for the screening of nuclear charge due to other electrons, can be calculated by Sommerfeld's classic relativistic energy formula [142]. In order to calculate the screening parameters in the X-ray spectra of astatine, the energy levels given by Bearden and Burr [130] were used. The value of σ_1 for the K level was estimated as 6.494 [143]; values of σ_2 for the $S_{1/2}$ terms of L_1 , M_1 , and N_1 levels are given as 2.5, 7.0, and 13.0, respectively [144]. The calculated values of σ_1 and σ_2 for various spin doublets are summarized in Table 15 [145 to 148].

Table 15. X-Ray Screening Constants for Various Spin Doublets of Astatine

Screening Constant	L_2L_3	M_2M_3	M_4M_5	N_2N_3	Ref.
σ_1	21.549	39.20	42.52	57.0	[145]
σ_2	3.580	8.64	13.60	16.7	[146, 147]
	3.550	8.00	13.60	17.0	[148]

5.11.4 Spectroscopic Constants of At_2

The *ground state vibrational constant* (ω_e) for the At_2 molecule was estimated using empirical relationships, combining the ω_e values with different atomic and molecular properties of astatine, such as atomic number (Z) [149], ionization energy and the principal quantum number of valence electrons (I, n) [150], electronegativity and the reduced mass (X, μ) [151,152]. Theoretical calculations were also utilized [115,153]. The ω_e values for the astatine molecule are given in Table 16. Lippincott's estimation of 99.0 cm^{-1} [115] seems to be too low compared with the other predicted ω_e values for At_2 . From the sequence of ground state vibrational frequency values for other halogens [154], the estimated ω_e data for At_2 reported in [149 to 153] seem reasonable.

Table 16. Ground State Vibrational Constant Values for Astatine Molecule

Method of Calculation	ω_e in cm^{-1}	Ref.
$\lg \omega_e = f(\lg 2Z)$	139.4	[149]
$\lg \omega_e = f(\lg n^2 I)$	172.9	[150]
$\omega_e = f(X/\mu^p)$	139.0	[151]
$\lg \omega_e = f(\lg X/\mu^2)$	132.9	[152]
Theoretical	141.0	[153]
	99.0	[154]

A theoretical calculation of the ground state *anharmonic vibrational constant* ($\omega_e x_e$) for the astatine molecule gave a value of 0.29 cm^{-1} [115].

From the ω_e values estimated by Clark [149] and by Tandon et al. [152], the *force constant* (k_e) for At_2 has been calculated as 1.213 N/cm (1.213 mdyn/\AA)* and 1.195 N/cm (1.195 mdyn/\AA)*, respectively [112].

*Originally quoted values are given in parentheses.

The *interatomic distance* (r_e) for At_2 has been calculated from the linear plot $\ln k_e$ vs. r_e for halogen molecules. Using the two estimated k_e values for At_2 (see above), the interatomic distance was found to be 0.2967 nm and 0.2981 nm [112]. Theoretical calculations resulted in a value of 0.352 nm [115].

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*Yu.V. Norseyeve, Yu.V. Norseev, J.W. Norseev, J.V. Norszejev are the different transliterations of the same name.

**V.A. Khalkin, W.A. Chalkin, V.A. Halkin are the different transliterations of the same name.

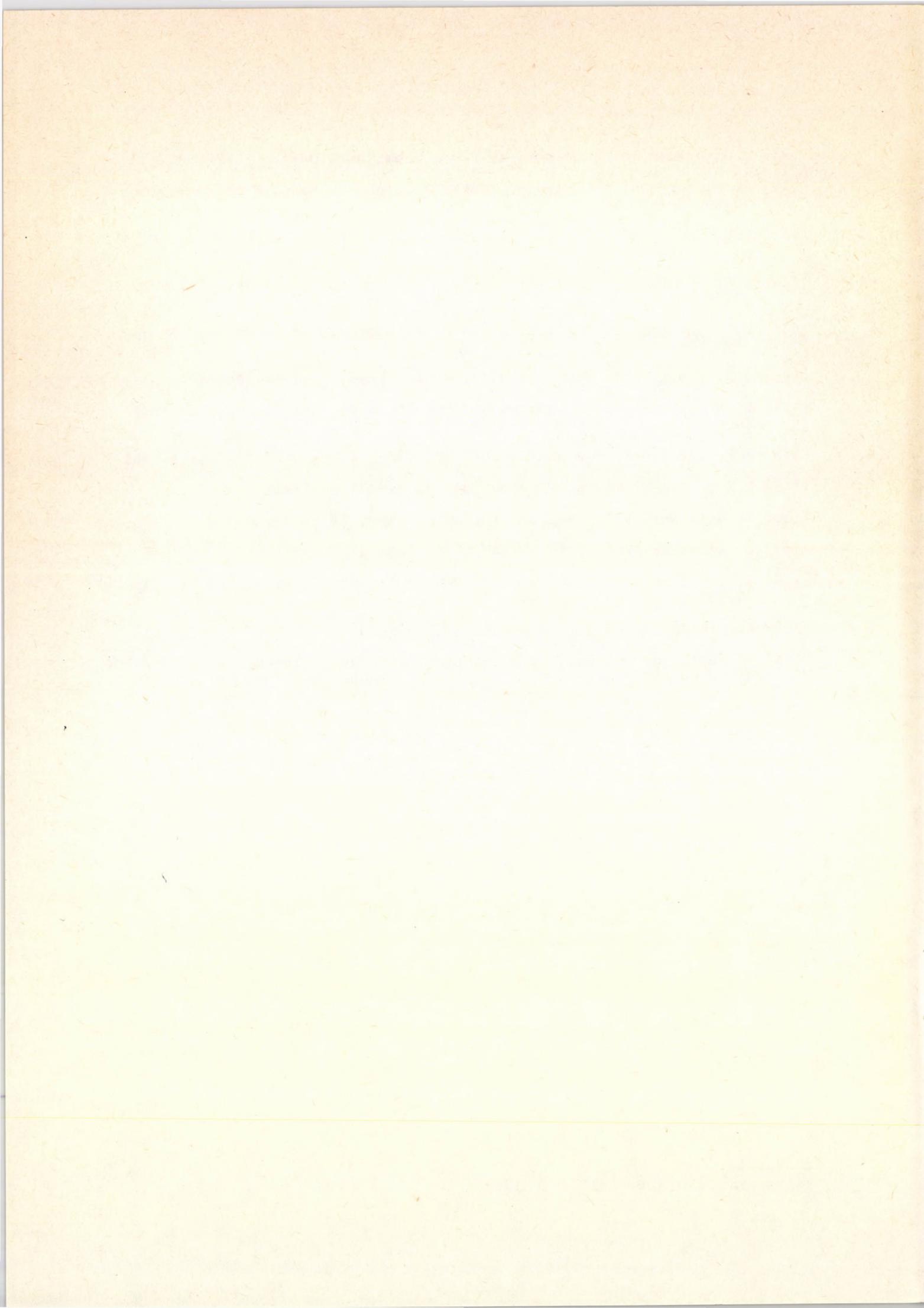
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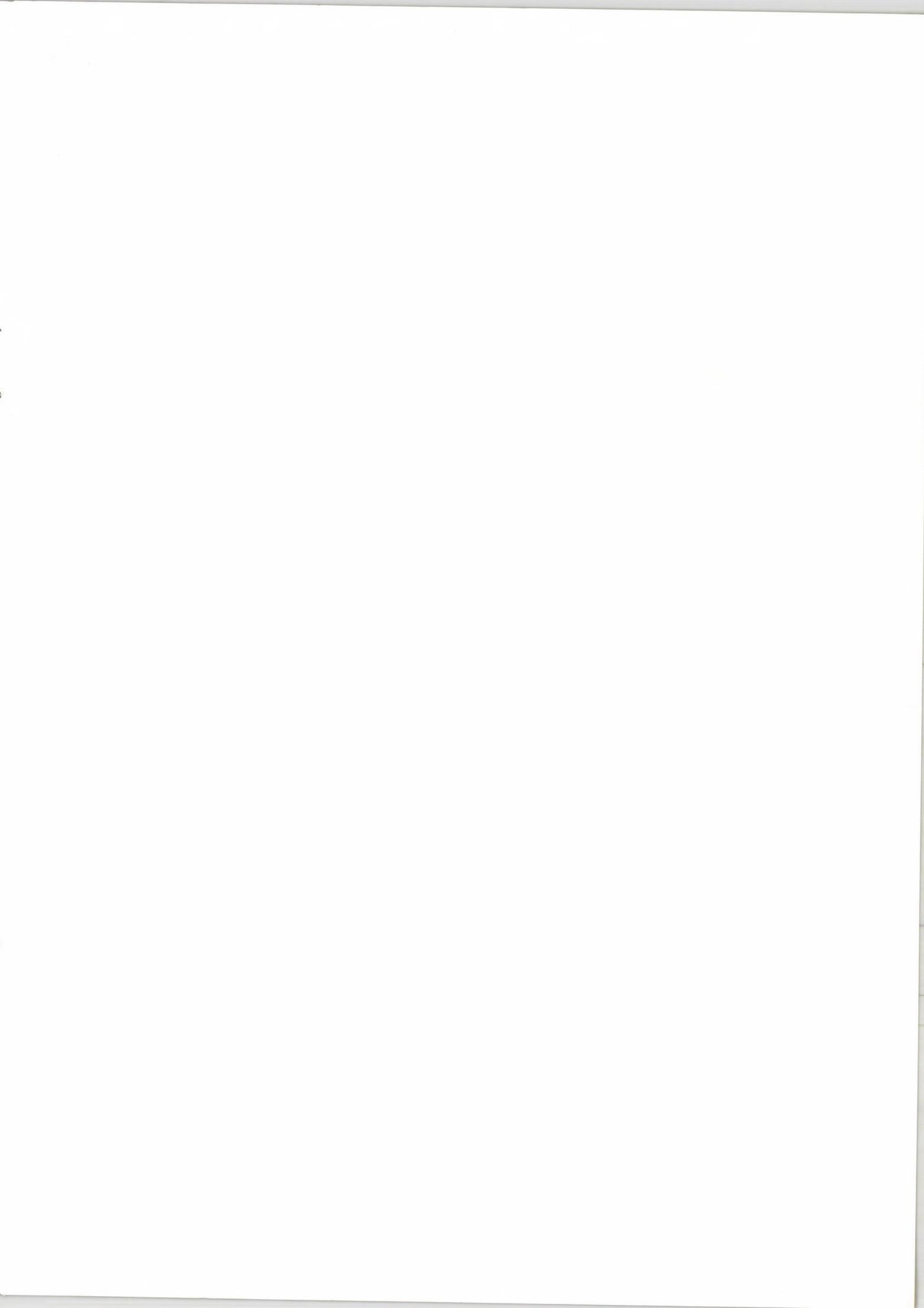
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