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## Vibrationally Excited Hydrogen Halides:

A Bibliography on  
Chemical Kinetics of Chemiexcitation  
and Energy Transfer Processes  
(1958 through 1973)

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# **Vibrationally Excited Hydrogen Halides: A Bibliography on Chemical Kinetics of Chemiexcitation and Energy Transfer Processes (1958 through 1973)**

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National Bureau of Standards

MAY 6 1974

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David R. Lide, Jr., Chief  
Office of Standard Reference Data



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# VIBRATIONALLY EXCITED HYDROGEN HALIDES:

## A Bibliography on Chemical Kinetics of Chemi-excitation and Energy Transfer Processes\*

Francis Westley

A bibliography, a reaction oriented list of references, is provided for published papers and reports containing rate data for reactions of halogen atoms with hydrogen-containing compounds, or of H (D, or T) atoms with halogen-containing compounds to form vibrationally chemiexcited hydrogen halides. The reactions for vibroexcitation of hydrogen halides through unimolecular or photochemical elimination, as well as the processes for vibrational energy transfer between hydrogen halides and various second bodies are also included. In addition, four lists of theoretical papers and a list of critical reviews and bibliographies are provided. Over 300 papers covering 50 types of reactions are listed. The period covered extends from 1958 through 1973.

Key words: Bibliography; chemical kinetics; chemiexcitation; gas phase; halogens; hydrogen; hydrogen halides; laser; quenching; vibrational energy transfer.

### Introduction

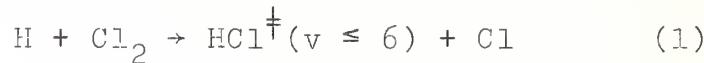
The bibliography lists papers and reports on the gas phase reaction kinetics of two types of chemical processes: a) formation of vibrationally excited hydrogen halides through abstraction or elimination and b) vibrational energy transfer - including quenching - between hydrogen halides and various second bodies.

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\* This publication is an activity of the Chemical Kinetics Information Center, National Bureau of Standards. The work was supported by the Office of Standard Reference Data, National Bureau of Standards and the Air Force Office of Scientific Research as part of a program to provide information and data on rates of chemical reactions.

The articles have been selected from the files of the Chemical Kinetics Information Center. The criterion for inclusion of an article is that it must contain some new information on the reaction. That is, simple quotations of the results of others and ad hoc guesses have been excluded. There are gray areas, such as the statement of a rate calculated from that of the reverse reaction and the equilibrium constant, or information such as: suggestion of a new mechanism, or a theoretical calculation, or a new theoretical approach derived from kinetic experiments. If the information seemed to be important the reference was included.

The two above mentioned types of reactions (formation of vibrationally excited hydrogen halides and transfer of vibrational energy between hydrogen halides and other bodies) are essential in a fairly new branch of quantum electronics: the chemical laser. Light amplification by stimulated emission of radiation (in short: laser) is a fairly recent development in science dealing with the generation of coherent radiation in the infrared and visible regions of the spectrum. The chemical lasers are based on the new principle of obtaining energy - in the form of coherent radiation - from chemical reactions: the principle of "chemical pumping". In other words, chemical interaction between two gaseous molecules results in the pumping of electronic, vibrational, or rotational energy into the newly formed bond of one to the reaction products. The new bond "stores" for a short time an amount of energy available for other uses. Such a reaction, which is only the first elementary step in the more complex lasing process, is called in short "chemiexcitation". The first observation of an infrared emission from the reaction of atomic hydrogen with molecular chlorine, was reported in 1958 by Cashion and Polanyi<sup>1,2</sup>. They attributed this emission to the vibrationally excited hydrogen chloride, which was one of the products of the reaction:



In 1961, Polanyi suggested the construction of a HCl laser, dependent on vibrational excitation, which would operate in the infrared region<sup>8</sup>. Polanyi and coworkers have continued their pioneering work in the field of chemical lasers, by following a double path: experimental [infrared spectroscopy<sup>3,4,5</sup>], energy distribution among reaction products<sup>6,13,14,17,18,29,21,22,23)</sup>] and theoretical [energy distribution<sup>7,9,10,12,15,19,23)</sup>, potential energy surface<sup>11,12,23)</sup>, trajectories<sup>12,15,23)</sup>, chemical kinetics<sup>16)</sup>]

However, the first description of an operational HCl pulsed chemical laser was published in 1965 by Kasper and Pimentel<sup>24</sup>. In the following years the research on chemical lasers has been continually expanding. A list of the universities and industrial research laboratories, as well as of their scientists carrying out research in chemical lasers can be found in the introduction of a bibliography published in 1972 by the U.S. Atomic Energy Commission [Chemical Lasers: An Overview of the Literature, (1960 - 1971)<sup>25</sup>].

Since 1965, many chemiexcited molecules have been found suitable in the operation of chemical lasers. However, the hydrogen halides are the most used molecules for that purpose. To date, the highest energy level of a chemiexcited hydrogen halide molecule is vibrational. The search of the literature failed to show the existence of a laser based on an electronically excited hydrogen halide molecule. For these reasons, this bibliography is confined only to two types of reactions involving hydrogen halides: a) vibrational chemiexcitation and b) vibrational energy transfer. No attempt was made to cover the literature dealing with the operation of hydrogen halide lasers. The reader interested in operation of chemical lasers should consult the "Comprehensive Literature Survey of Chemical Lasers" by Arnold and Rojeska<sup>26</sup> or the above mentioned bibliography of Dobratz<sup>25</sup>, as well as other reviews and bibliographies listed in part V of this work.

This bibliography is not the result of the effort of a single person, but of the whole staff of Chemical Kinetics Information Center. My thanks to all of them.

In particular, I wish to thank Dr. David Garvin, Director of the Center, and Dr. Robert Hampson for their more than helpful suggestions and constant guidance; Mr. James G. Koch, Supervisor, for tracking down and obtaining papers and reports, otherwise very difficult to obtain; Mrs. Ann C. Robertson, Mrs. Geraldine Zumwalt and Miss Darlene Connelly, for typing a difficult manuscript with particular care.

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15. Anlauf, K. G., Polanyi, J. C., Wong, W. H., and Woodall, K. B., "Distribution of Reaction Products. III.  $Cl + HI$ ,  $Cl + DI$ ," *J. Chem. Phys.* 49, 5189 (1968)
16. Anlauf, K. G., Maylotte, D. H., Polanyi, J. C., and Bernstein, R. B., "Rates of the Endothermic Reactions  $HCl + X(X \equiv I, Cl)$  as a Function of Reagent Vibration, Rotation, and Translation," *J. Chem. Phys.* 51, 5716 (1969)
17. Polanyi, J. C., and Tardy, D. C., "Energy Distribution in the Exothermic Reaction  $F + H_2$  and Endothermic Reaction  $HF + H$ ," *J. Chem. Phys.* 51, 5717 (1969)
18. Anlauf, K. G., Charters, P. E., Horne, D. S., MacDonald, R. G., Maylotte, D. H., Polanyi, J. C., Skrlac, W. J., Tardy, D. C., and Woodall, K. B., "Translational Energy-Distribution in the Products of Some Exothermic Reactions," *J. Chem. Phys.* 53, 4091 (1970)

19. Polanyi, J. C., and Woodall, K. B., "Mechanism of Rotational Relaxation," *J. Chem. Phys.* 56, 1563 (1972)
20. Maylotte, J. C., Polanyi, J. C., and Woodall, K. B., "Energy Distribution among Reaction Products. IV.  $X + HY$  ( $X \equiv Cl, Br, Y \equiv Br, I$ ),  $Cl + DI$ ," *J. Chem. Phys.* 57, 1547 (1972)
21. Polanyi, J. C., and Woodall, K. B., "Energy Distribution among Reaction Products. VI.  $F + H_2, D_2$ ," *J. Chem. Phys.* 57, 1574 (1972)
22. Polanyi, J. C., and Sloan, J. J., "Energy Distribution among Reaction Products. VII.  $H + F_2$ ," *J. Chem. Phys.* 57, 4988 (1972)
23. Parr, C. A., Polanyi, J. C., and Wong, W. H., "Distribution of Reaction Products (Theory). VIII.  $Cl + HI, Cl + DI$ ," *J. Chem. Phys.* 58, 5 (1973)
24. Kasper, J. V. V., and Pimentel, G. C., "HCl Chemical Laser," *Phys. Rev. Letters* 14, 352 (1965)
25. Dobratz, B. M., "Chemical Lasers: An Overview of the Literature, 1960 - 1971," U.S. Atomic Energy Commission, UCRL 51285 (Sept. 1972) (National Techn. Information Service)
26. Arnold, S. J., and Rojeska, H., "Chemical Lasers: A Comprehensive Literature Survey," *Appl. Opt.* 12, 169 (1973)

## Guidelines for the user

Arrangement of the report. This bibliography is in six parts:

Part I. Hydrogen fluoride ( $\text{HF}^{\ddagger}$ , or  $\text{DF}^{\ddagger}$ )

Part II. Hydrogen chloride ( $\text{HCl}^{\ddagger}$ , or  $\text{DCl}^{\ddagger}$ )

Part III. Hydrogen bromide ( $\text{HBr}^{\ddagger}$ , or  $\text{DBr}^{\ddagger}$ )

Part IV. Hydrogen iodide ( $\text{HI}^{\ddagger}$ , or  $\text{DI}^{\ddagger}$ )

Part V. Reviews and Bibliographies (Critical reviews, or surveys and general bibliographies dealing with the reactions listed in parts I to IV).

Part VI. The combined bibliography for Parts I to V arranged alphabetically by authors. The complete reference citation for each article mentioned is given here. Occasionally explanatory notes are appended. These establish the "bibliography chain" for closely related papers by the same authors.

IIIIV .(VIBRATION)

Parts I to IV are arranged in the order of their importance: Hydrogen fluoride (Part I) is the most intensively studied chemical laser, while hydrogen iodide (Part IV) is the least studied.

Ordering of chemical reactions. The purpose of this work is to provide the chemical kineticist with a useful list of articles and papers dealing with the vibrationally excited hydrogen halides. For that reason, the arrangement of the bibliography is reaction oriented: parts I to IV are each divided into three large sections:

Section A. Formation of  $\text{HX}^{\ddagger}$  ( $\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$ )

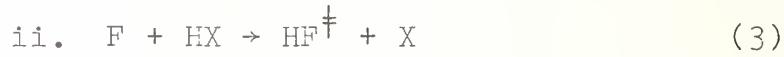
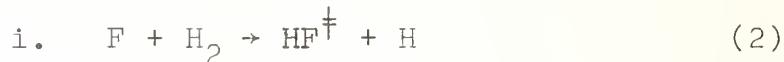
Section B.  $\text{HX}^{\ddagger}$  Energy Transfer and Quenching

Section C.  $\text{HX}^{\ddagger}$  Theoretical Papers

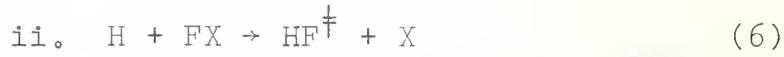
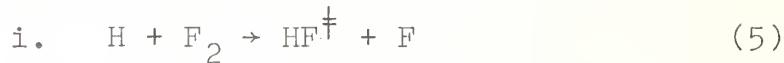
The titles of Sections A and B define very broad categories of reactions. Section C includes only theoretical papers, very closely related to the kinetics of vibrationally excited hydrogen halides. Section A does not include formation of  $\text{HX}^{\ddagger}$  by energy transfer. This type of reaction may be found in Section B, under 1.a. Each of the Sections A and B is divided into smaller categories of reactions and so on, as indicated in the table of contents.

Display of Chemical Reactions and Formulae. With the exception of subgroups A.1.a and A.1.b, all the other subgroups define a type of chemical reaction. Subgroups A.1.a and A.1.b are each further divided into three types of reactions. For instance, in part I (Hydrogen fluoride) these types are:

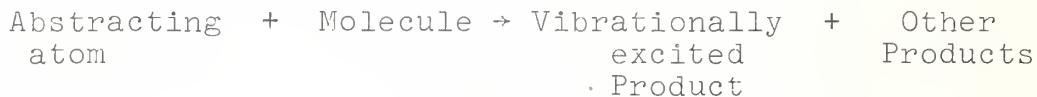
A.1.a. Abstraction of H atom by F atom.



A.1.b. Abstraction of F atom by H atom.

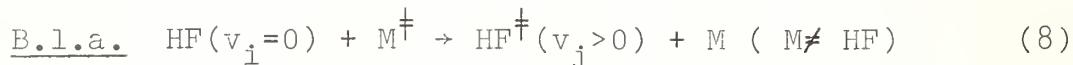


Throughout the work these different types of reactions are displayed according to a scheme trying to emphasize the direction and nature of the chemical process, rather than to follow a mere alphabetical order. So, the above listed reactions (2) to (7) are all written according to the invariable pattern:

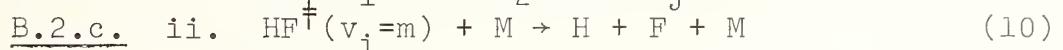
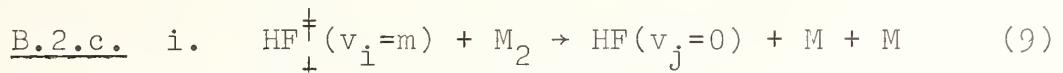


In reactions (4) and (7), the terms RH and RF denote in general a hydrogen containing - and, respectively, a halogen containing - organic molecule. However, in some instances, a reference listed under the headings A.1.a.iii. or A.1.b.iii. (Reactions (4) and (7)), might deal with a hydrogen - or halogen - containing inorganic molecule.

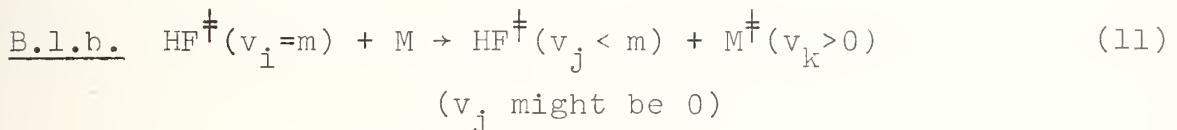
The general "third body", whether excited or in ground state, is always last:



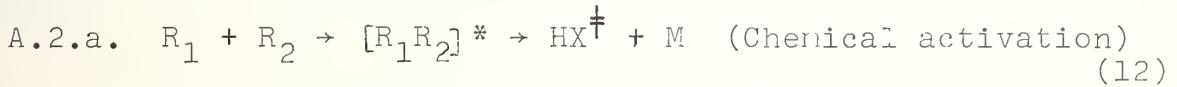
In general, the first term at the right side of a reaction indicates a vibrationally excited product. The only exception is the reaction type B.2.c (Dissociative quenching).



Excited states of reactants and products. This bibliography deals exclusively with vibrationally excited hydrogen halides. The sign used to indicate the vibronic state of a molecules is the double dagger superscript. If the double dagger appears inside a bracket, it indicates that the molecule might be in its ground state (zero vibrational level):



Only in one instance an asterisk is used to indicate the formation of an intermediate activated complex, which subsequently is dissociated into a vibrationally excited hydrogen halide molecule and another product:



Reactions of the type B.1.c. are expressed by a generalized chemical equation including all the HX - HX vibrational energy transfer processes. The multiplicity of vibrational levels (some authors consider 8 vibrational levels in the same paper) would have made it very difficult to arrange this bibliography according to all the possible HX - HX vibronic interactions. Although, in this type of process, four different vibronic levels coexist, the double dagger superscript is entirely omitted and the different vibronic levels are indicated in a bracket following each HX molecule. The reason for omitting the dagger symbol is that only one of the four vibronic levels (v<sub>i</sub>, v<sub>j</sub>, v<sub>k</sub>, v<sub>l</sub>) may be zero, provided that the condition i + j = k + l is satisfied. (If two, or three of these vibronic levels are zero, then the process becomes a simple quenching, or excitation one.). For the case of the HF - HF vibrational energy transfer, the B.1.c. process is indicated as follows:



(only one of four levels v<sub>i</sub>, v<sub>j</sub>, v<sub>k</sub>, v<sub>l</sub> may be zero)

## Reference Citations.

The references under each reaction list the author(s) and the sources, in the following form:

| Author(s)       | Source-Year-Volume-Page | Number of Author(s) |
|-----------------|-------------------------|---------------------|
| Airey, J. R.    | IJCKBO-1970-2-65        | 1                   |
| Airey and Fried | CHPLBC-1971-8-23        | 2                   |
| Airey, et al.   | JCPA6-1964-41-3255      | 3 or more           |

Variations from this format (which we will call "short reference") are usually in the direction of more explicit specification. These variations are never made in the first two fields, source and year. They are fixed and always present.

The sources are indicated by their ASTM CODEN abbreviations<sup>\*</sup>). A guide to these codes follows. As listed in this guide, the codes include an additional sixth cipher,<sup>\*\*</sup>) which is a "check character"<sup>\*\*</sup>). A code prefixed with an asterisk is a code not in the ASTM CODEN set. These are codes we have assigned for reports from industrial laboratories, research institutes and universities. When the CODEN system adopts appropriate codes they will be replaced. The present, temporary codes usually end with Z or U.

<sup>\*</sup>) Blumenthal, J. G., Karaman, M., Editors, "CODEN FOR PERIODICAL TITLES" (Including Non-Periodical Titles and Deleted Coden), Vol. I and II, ASTM Data Series DS 23B, Third Edition, (1970); Padusis, M., Editor, First Supplement to Third Edition, DS 23B-S1 (05-023021-42, 1972). (American Society for Testing and Materials, 1916 Race St., Philadelphia, Pa. 19103)

<sup>\*\*</sup>) The final sixth character in the journal code is a "check character". This is not shown in the listings in ASTM DS 23B and DS 23B-S1, but the calculation is explained in the introductions to them. See also "Subroutine for the Calculation of CODEN Check Characters, D. Garvin, National Bureau of Standards, Tech. Note 738 (Sept. 1972)

JOURNAL AND REPORT CODES

|         |  |
|---------|--|
| ACHRAY  | ACCOUNTS OF CHEMICAL RESEARCH (Washington)   |
| ACIEAY  | ANGEWANDTE CHEMIE (International Edition in English)   |
| ACSRAL  | AMERICAN CHEMICAL SOCIETY, ABSTRACT OF PAPERS  |
| ADCPAA  | ADVANCES IN CHEMICAL PHYSICS (New York)  |
| APOPAI  | APPLIED OPTICS (Washington)  |
| APOSAR  | APPLIED OPTICS, SUPPLEMENT (Washington)  |
| APPLAB  | APPLIED PHYSICS LETTERS (New York)   |
| ARPLAP  | ANNUAL REVIEW OF PHYSICAL CHEMISTRY  |
| *ASTSZU | THE AEROSPACE CORPORATION  |
| BBPCAX  | BERICHTE DER BUNSENGESELLSCHAFT FUER PHYSIKALISCHE<br>CHEMIE (Germany)   |
| BOOKA7  | BOOK   |
| CBFMAO  | COMBUSTION AND FLAME   |
| CCHKAZ  | COMPREHENSIVE CHEMICAL KINETICS (Amsterdam)  |
| CHDBAN  | COMPTEES RENDUS HEBDOMADAIRE DES SEANCES DE<br>L'ACADEMIE DES SCIENCES, SERIE B. SCIENCES<br>PHYSIQUES (Paris) |
| CHMBAY  | CHEMISTRY IN BRITAIN (London)  |
| CHPLBC  | CHEMICAL PHYSICS LETTERS (Amsterdam)   |
| CITEAH  | CHEMIE-INGENIEUR-TECHNIK (Germany)   |
| CJCHAG  | CANADIAN JOURNAL OF CHEMISTRY  |
| CSSPAD  | CHEMICAL SOCIETY, SPECIAL PUBLICATION (London)   |
| DABBBA  | DISSERTATION ABSTRACTS INTERNATIONAL, B.<br>THE SCIENCES AND ENGINEERING                                       |
| DABSA9  | DISSERTATION ABSTRACTS PART B. SCIENCES AND<br>ENGINEERING   |
| DAKEAT  | DANSK KEMI (Copenhagen)  |
| DFSOAW  | DISCUSSIONS OF FARADAY SOCIETY   |
| DIASA9  | DISSERTATION ABSTRACTS   |
| DKPCAG  | DOKLADY PHYSICAL CHEMISTRY, PROCEEDINGS OF THE<br>ACADEMY OF SCIENCES OF THE USSR (New York)                   |
| HIECAP  | HIGH ENERGY CHEMISTRY (New York)   |
| IEJQA7  | IEEE JOURNAL OF QUANTUM ELECTRONICS (New York)   |
| IJCKBO  | INTERNATIONAL JOURNAL OF CHEMICAL KINETICS<br>(New York)   |

|        |  |
|--------|--|
| JAPIAU | JOURNAL OF APPLIED PHYSICS (New York)  |
| JASMAN | JOURNAL OF THE ACOUSTICAL SOCIETY OF AMERICA   |
| JCFTAR | JOURNAL OF CHEMICAL SOCIETY, FARADAY TRANSACTIONS I<br>(London)                              |
| JCFTBS | JOURNAL OF CHEMICAL SOCIETY, FARADAY TRANSACTIONS II<br>(London)                             |
| JCPQAY | JOURNAL DE CHIMIE PHYSIQUE   |
| JCPSA6 | JOURNAL OF CHEMICAL PHYSICS  |
| JCSOA9 | JOURNAL OF THE CHEMICAL SOCIETY (London)   |
| JPCHAX | JOURNAL OF PHYSICAL CHEMISTRY  |
| JQSRAE | JOURNAL OF QUANTITATIVE SPECTROSCOPY AND RADIATIVE TRANSFER                                  |
| JTPLA2 | JETP LETTERS, SOVIET PHYSICS (New York)  |
| KICAA8 | KINETICS AND CATALYSIS   |
| LSRVAN | LASER FOCUS  |
| MOPHAM | MOLECULAR PHYSICS (London)   |
| NATUAS | NATURE (London)  |
| PACHAS | PURE AND APPLIED CHEMISTRY (London)  |
| PRKNAZ | PROGRESS IN REACTION KINETICS  |
| PRLAAZ | PROCEEDINGS OF ROYAL SOCIETY, SERIES A.<br>MATHEMATICAL AND PHYSICAL SCIENCES (London)       |
| PRLTAO | PHYSICAL REVIEW LETTERS (New York)   |
| PYLAAG | PHYSICS LETTERS, SECTION A (Amsterdam)   |
| QRCSAL | QUARTERLY REVIEW OF THE CHEMICAL SOCIETY (London)  |
| RJPCAR | RUSSIAN JOURNAL OF PHYSICAL CHEMISTRY  |
| SCAMAC | SCIENTIFIC AMERICAN (New York)   |
| SCIEAS | SCIENCE (Washington)   |
| SPHJAR | SOVIET PHYSICS JETP (New York)   |
| SPUSBI | SOVIET PHYSICS - USPEKHI (New York)  |
| SYMCAQ | SYMPOSIUM ON COMBUSTION  |
| TFSOA4 | TRANSACTIONS OF THE FARADAY SOCIETY  |
| UCRLAE | UNIVERSITY OF CALIFORNIA, LAWRENCE RADIATION LABORATORY, REPORTS                             |
| XADRCH | UNITED STATES DEPARTMENT OF COMMERCE, NATIONAL TECHNICAL INFORMATION SERVICE                 |
| XCCIAV | UNITED STATES DEPARTMENT OF COMMERCE, CLEARINGHOUSE FOR SCIENTIFIC AND TECHNICAL INFORMATION |

XERLAR U.S. ATOMIC ENERGY COMMISSION, UNIVERSITY OF  
CALIFORNIA, RADIATION LABORATORY

ZEPCAC ZEITSCHRIFT FUER PHYSIKALISCHE CHEMIE, STOECHIO-  
METRIE UND VERWANDSCHAFTSLIHRE

ZPCBAL ZEITSCHRIFT FUER PHYSIKALISCHE CHEMIE, ABTEILUNG B:  
CHEMIE DER ELEMENTARPROZESSE, AUFBAU DER MATERIE

26BMAD MTP (MEDICAL AND TECHNICAL PUBLISHING COMPANY)  
INTERNATIONAL REVIEW OF SCIENCE: PHYSICAL CHEMISTRY,  
SERIES ONE 1972-1973

## Abbreviations

The abbreviations listed below, are used in parts I through IV of this bibliography.

|                |                              |
|----------------|------------------------------|
| (calc.)        | = (calculation)              |
| (cr. sect.)    | = (cross section)            |
| (d.r.)         | = (detailed rates)           |
| (mech.)        | = (mechanism)                |
| (model.)       | = (modelling)                |
| (pop. distr.)  | = (population distribution)  |
| (pot. surf.)   | = (potential energy surface) |
| (r.p.)         | = (related paper)            |
| (rev.)         | = (review)                   |
| (traj.)        | = (trajectories)             |
| (trans. prob.) | = (transition probability)   |

They are appended inside brackets at the end of the short references. In general, a short reference without appended abbreviations indicates a work including rate constants while a reference followed by appended abbreviations may or may not include rate constants.

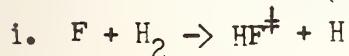
The abbreviation r.p. (related paper) indicates a paper which cannot fit in any of the above listed categories. For instance, a work dealing with laser operation will be followed by (r.p.) if it is considered of interest. However, a number of papers with rate constants are included in the r.p. category. For instance, under the heading:  $\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$  a number of papers giving rate constants for the overall reaction  $\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$  are included. In this reaction, the product HCl indicates all molecules of hydrogen chloride whether in the ground state or in an excited state. Such a paper is therefore a very closely related paper.

# Part I. Hydrogen fluoride (HF, DF)

## A. Formation of $\text{HF}^{\ddagger}$ ( $\text{DF}^{\ddagger}$ )

### 1. Bimolecular Reactions (Abstraction Lasers)

#### a. Abstraction of H(D) Atom by F Atom



|                         |  |
|-------------------------|--|
| Airey, J. R.            | IJCKBO-1970-2-65                               |
| Anlauf, et al.          | JCPSA6-1970-53-4091 (calc., pop. distr.)       |
| Basov, et al.           | JTPLA2-1969-9-375 (r. p.)                      |
| Beattie, et al.         | IEJQA7-1973-9-202 (r.p.)                       |
| Ben-Shaul, et al.       | JCPSA6-1972-57-5427 (calc., pop. distr.)       |
| Ben-Shaul, et al.       | CHPLBC-1972-15-160 (pop. distr.)               |
| Berry, M. J.            | ACSRAL-1973-166-Phys. 98                       |
| Brokaw, R. S.           | JPCHAX-1965-69-2808 (r. p.)                    |
| Burmasov, et al.        | JTPLA2-1969-10-28 (r. p.)                      |
| Chang and Setser        | JCPSA6-1973-58-2298 (pop. distr.)              |
| Chester and Hess        | IEJQA7-1972-8-1 (rev.)                         |
| Clyne, et al.           | CJCHAG-1973-51-3596 (r. p.)                    |
| Cohen, N.               | XADRCA-1972-AD 763715                          |
| Cool, et al.            | APPLAB-1969-15-318 (r. p.)                     |
| Cool, et al.            | JAPIAU-1970-41-4038                            |
| Coombe and Pimentel     | IEJQA7-1973-9-192                              |
| Coombe and Pimentel     | JCPSA6-1973-59-251                             |
| Coombe and Pimentel     | JCPSA6-1973-59-1535                            |
| Deutsch, T. F.          | APPLAB-1967-10-234 (r. p.)                     |
| Deutsch, T. F.          | APPLAB-1967-11-18 (r. p.)                      |
| Dodonov, et al.         | DKPCAG-1971-198-440                            |
| Dolgov-Savel'ev, et al. | SPHJAR-1970-31-643                             |
| Duewer and Setser       | JCPSA6-1973-58-2310 (pop. distr.)              |
| Dolgov-Savel'ev, et al. | SPHJAR-1972-34-34                              |
| Emanuel, et al.         | XADRCA-1972-AD 746685 (rev.)                   |
| Fettis and Knox         | PRKNNAZ-1964-2-2 (r. p.)                       |
| Green and Lin           | JCPSA6-1971-74-3222 (calc.)                    |
| Gregg, et al.           | CHPLBC-1971-8-609 (r. p.)                      |
| Gross, R. W. F.         | JCPSA6-1969-50-1889 (r. p.)                    |
| Gross, et al.           | JCPSA6-1968-48-3821 (r. p.)                    |
| Gross, et al.           | JCPSA6-1969-51-1250 (r. p.)                    |
| Gross, et al.           | IEJQA7-1970-6-168 (r. p.)                      |
| Hess, L. D.             | IEJQA7-1973-9-201 (r. p.)                      |
| Hess, L. D.             | JAPIAU-1972-43-1157 (r. p.)                    |
| Hess, L. D.             | JCPSA6-1971-55-2466                            |
| Homann, et al.          | BBPCAX-1970-74-585 (r. p.)                     |
| Jaffe, et al.           | JCPSA6-1973-59-1128 (calc., pot. surf., traj.) |
| Jensen and Rice         | CHPLBC-1970-7-627 (r. p.)                      |
| Jensen and Rice         | CHPLBC-1971-8-214 (r. p.)                      |
| Jonathan, et al.        | MOPHAM-1971-20-93                              |
| Jonathan, et al.        | APOPNAI-1971-10-1821                           |
| Kapralova and Chaikin   | CBFMAO-1969-13-557 (r. p.)                     |
| Kapralova, et al.       | KICAA8-1970-11-669 (r. p.)                     |

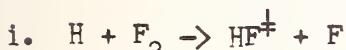
|                       |  |
|-----------------------|--|
| Kerber, et al.        | IEJQA7-1973-9-94 (rev.)  |
| Kerber and Whittier   | *ASTSzx-1970-TOR-0059(6753-10)-1                                 |
| Kompa, K. L.          | ACIEAY-1970-9-773 (rev.)   |
| Kompa, K. L.          | CITEAH-1970-42-573 (rev.)  |
| Kompa, et al.         | CHPLBC-1969-3-210 (r. p.)  |
| Kompa, et al.         | JCPSA6-1968-49-4257  |
| Kompa and Pimentel    | JCPSA6-1967-47-857   |
| Kompa and Wanner      | CHPLBC-1972-12-560   |
| Kompa, et al.         | IEJQA7-1970-6-185 (r. p.)  |
| Krogh and Pimentel    | JCPSA6-1972-56-969   |
| Kwok, et al.          | APPLAB-1970-16-386 (r. p.)                                       |
| Levine, et al.        | CHPLBC-1973-19-1 (pop. distr.)                                   |
| Levy and Copeland     | JPCHAX-1963-67-2156 (r. p.)                                      |
| Levy and Copeland     | JPCHAX-1965-69-408 (r. p.)                                       |
| Levy and Copeland     | JPCHAX-1968-72-3168 (r. p.)                                      |
| Meinzer, R. A.        | IJCKBO-1970-2-335 (r. p.)  |
| Mercer and Pritchard  | JPCHAX-1959-63-1468 (r. p.)                                      |
| Mirels and Spencer    | IEJQA7-1971-7-501 (r. p.)  |
| Pan, et al.           | CHPLBC-1971-10-577 (r. p.)                                       |
| Parker and Pimentel   | JCPSA6-1969-51-91  |
| Pearson, et al.       | IEJQA7-1973-9-723 (r. p.)  |
| Persky, A.            | JCPSA6-1973-59-3612 (r. p.)                                      |
| Pimentel, G. C.       | DAKEAT-1969-50-1 (rev.)  |
| Pimentel, G. C.       | IEJQA7-1970-6-174 (rev.)   |
| Pimentel, G. C.       | PACHAS-1969-18-275 (rev.)  |
| Pummer and Kompa      | APPLAB-1972-20-356 (r. p.)                                       |
| Schafer, et al.       | JCPSA6-1970-53-3385  |
| Semenov and Shilov    | KICAA8-1964-6-1 (mech.)  |
| Spencer, et al.       | IJCKBO-1969-1-493 (r. p.)  |
| Spinnler and Kittle   | IEJQA7-1970-6-169 (r. p.)  |
| Suchard, S. N.        | JCPSA6-1973-58-1269  |
| Suchard, et al.       | APPLAB-1971-19-411 (r. p.)                                       |
| Suchard, et al.       | JCPSA6-1972-57-5065  |
| Suchard, et al.       | XADRCA-1973-AD 763716  |
| Vedeneev, et al.      | RJPCAR-1969-43-713   |
| Vedeneev, et al.      | KICAA8-1969-10-949 (r. p.)                                       |
| Wilkins, R. L.        | JCPSA6-1972-57-912 (calc.,d.r.,pop. distr.,<br>pot. surf.,traj.) |
| Wilkins, R. L.        | XADRCA-1971-AD 725031 (calc.)                                    |
| Wilson and Stephenson | APPLAB-1972-20-64 (r. p.)  |
| Wilson, et al.        | IEJQA7-1973-9-202 (r. p.)  |



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| Airey and McKay     | APPLAB-1969-15-401 (r. p.) |
| Berry, M. J.        | DABBBA-1971-31-7210        |
| Cool, et al.        | JAPIAU-1970-41-4038        |
| Coombe and Pimentel | IEJQA7-1973-9-192          |
| Cool, et al.        | APPLAB-1969-15-318 (r. p.) |
| Green and Lin       | IEJQA7-1971-7-98 (r. p.)   |
| Jensen and Rice     | CHPLBC-1970-7-627 (r. p.)  |
| Jonathan, et al.    | MOPHAM-1971-22-561         |

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| Jonathan, et al.                              | CHPLBC-1970-7-257  |
| Jonathan, et al.                              | APOPAI-1971-10-1821 (calc.)                                    |
| Kirsch and Polanyi                            | JCPA6-1972-57-4498 (calc.)                                     |
| Kompa and Wanner                              | CHPLBC-1972-12-560   |
| <br>iii. $F + RH \rightarrow HF^\ddagger + R$ |  |
| Perry, M. J.                                  | IEJQA7-1973-9-199 (r. p.)                                      |
| Brus and Lin                                  | JPCHAX-1971-75-2546  |
| Chang and Setser                              | JCPA6-1973-58-2298 (pop. distr.)                               |
| Chang, et al.                                 | JPCHAX-1971-75-2070  |
| Chang, et al.                                 | CHPLBC-1971-9-587  |
| Clyne, et al.                                 | CJCHAG-1973-51-3596 (r. p.)                                    |
| Creighton, et al.                             | IEJQA7-1973-9-200  |
| Duewer and Setser                             | JCPA6-1973-58-2310 (pop. distr.)                               |
| Fettis, et al.                                | JCSOA9-1960-1064 (r. p.)                                       |
| Green and Lin                                 | JCPA6-1971-54-3222   |
| Gregg, et al.                                 | CHPLBC-1971-8-609  |
| Jacobson and Kimbell                          | CHPLBC-1971-8-309 (r. p.)                                      |
| Jacobson and Kimbell                          | JAPIAU-1971-42-3402 (r. p.)                                    |
| Johnson, et al.                               | JPCHAX-1973-77-2499 (calc., pop. distr.,<br>pot. surf., traj.) |
| Jonathan, et al.                              | MOPHAM-1971-20-93  |
| Jonathan, et al.                              | APOPAI-1971-10-1821  |
| Kaprалова, et al.                             | KICAA8-1970-11-669 (r. p.)                                     |
| Kim and Setser                                | ACSRAL-1973-166-Phys. 99                                       |
| Kim and Setser                                | JPCHAX-1973-77-2493 (pop. distr.)                              |
| Kompa, et al.                                 | CHPLBC-1969-3-210 (r. p.)                                      |
| Kompa and Wanner                              | CHPLBC-1972-12-560   |
| Krogh and Pimentel                            | JCPA6-1972-56-969  |
| Lin and Green                                 | JCPA6-1970-53-3383   |
| Mercer and Pritchard                          | JPCHAX-1959-63-1468 (r. p.)                                    |
| Molina and Pimentel                           | IEJQA7-1973-9-64   |
| Padrick and Pimentel                          | APPLAB-1972-20-167   |
| Parker and Pimentel                           | IEJQA7-1970-6-175  |
| Parker and Pimentel                           | JCPA6-1968-48-5273 (r. p.)                                     |
| Parker and Pimentel                           | JCPA6-1971-55-857  |
| Pimentel, G. C.                               | DAKEAT-1969-50-1 (rev.)  |
| Pimentel, G. C.                               | IEJQA7-1970-6-174 (rev.)                                       |
| Suchard and Pimentel                          | APPLAB-1971-18-530   |
| Vedeneev, et al.                              | KICAA8-1963-4-278 (r. p.)                                      |

b. Abstraction of F Atom by H(D) Atom



|                  |                            |
|------------------|----------------------------|
| Airey, J. R.     | IJCKBO-1970-2-65           |
| Albright, et al. | JCPA6-1969-50-3632         |
| Basov, et al.    | JTPLA2-1969-9-375 (r. p.)  |
| Burmasov, et al. | JTPLA2-1969-10-28 (r. p.)  |
| Cohen, N.        | XADRCA-1972-AD 763715      |
| Cool, et al.     | APPLAB-1969-15-318 (r. p.) |
| Cool, et al.     | JAPIAU-1970-41-4038        |
| Dodonov, et al.  | KICAA8-1970-11-677         |

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| Emanuel, et al.               | XADRCA-1972-AD 746685 (rev.)                       |
| Hess, L. D.                   | JCPA6-1971-55-2466                                 |
| Jonathan, et al.              | JCPA6-1970-53-4396 (r. p.)                         |
| Jonathan, et al.              | APOPAI-1971-10-1821 (calc.)                        |
| Jonathan, et al.              | MOPHAM-1972-24-1143 (calc., pot. surf., traj.)     |
| Kabralova and Chaikin         | CBFMAO-1969-13-557 (mech.)                         |
| Kerber, et al.                | IIEJQA7-1973-9-94 (rev.)                           |
| Kerber and Whittier           | *ASTSZx-1970-TOR-0059(6753-10)-1                   |
| Kompa, K. L.                  | CITEAH-1970-42-573 (rev.)                          |
| Levy and Copeland             | JPCHAX-1963-67-2156 (mech.)                        |
| Levy and Copeland             | JPCHAX-1965-69-408 (r. p.)                         |
| Levy and Copeland             | JPCHAX-1968-72-3168 (r. p.)                        |
| Mayer, et al.                 | SYMCAQ-1967-11-837 (r. p.)                         |
| O'Neil, et al.                | JCPA6-1973-58-1126 (calc., pot. surf.)             |
| Polanyi and Sloan             | JCPA6-1972-57-4988 (calc., d.r.)                   |
| Semenov and Shilov            | KICAA8-1964-6-1 (mech.)                            |
| Slootmaekers and Van Tiggelen | BSCBAG-1958-67-135 (r. p.)                         |
| Suchard, et al.               | APPLAB-1971-19-411 (r. p.)                         |
| Suchard, et al.               | JCPA6-1972-57-5065                                 |
| Suchard, et al.               | XADRCA-1973-AD 763716                              |
| Tal'roze, et al.              | KICAA8-1970-11-233                                 |
| Vedeneev, et al.              | KICAA8-1963-4-278 (r. p.)                          |
| Vedeneev, et al.              | RJPCAR-1969-43-713                                 |
| Wilkins, R. L.                | JCPA6-1973-58-2326 (calc., d.r., pot.surf., traj.) |
| Wilkins, R. L.                | XADRCA-1971-AD 725031 (calc.)                      |
| Wilson and Stephenson         | APPLAB-1972-20-64 (r. p.)                          |



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|--------------------|----------------------------|
| Krogh and Pimentel | JCPA6-1972-56-969          |
| Mayer, et al.      | SYMCAQ-1967-11-837 (r. p.) |
| Pimentel, G. C.    | JCPA6-1973-58-1270 (r. p.) |



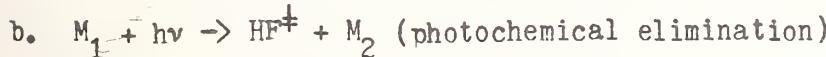
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| Cross, J. B.       | JCPA6-1973-59-966 (r. p.)  |
| Gensel, et al.     | CHPLBC-1970-5-179 (r. p.)  |
| Herbelin and Cohen | CHPLBC-1973-20-605 (r. p.) |
| Krogh and Pimentel | JCPA6-1972-56-969          |
| Perona, M. J.      | JCPA6-1971-54-4024         |
| Pimentel, G. C.    | JCPA6-1973-58-1270 (r. p.) |
| Rabideau, S. W.    | JCPA6-1973-59-1533         |

## 2. Unimolecular Reactions (elimination lasers)

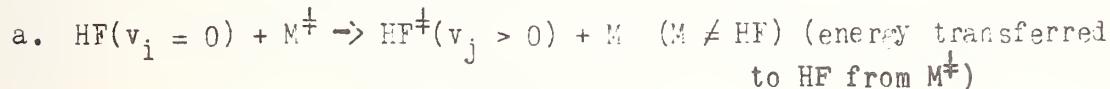


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|--------------------|---------------------|
| Berry, M. J.       | DABBBA-1971-31-7210 |
| Berry and Pimentel | IIEJQA7-1970-6-176  |
| Berry and Pimentel | JCPSAE-1968-49-5190 |

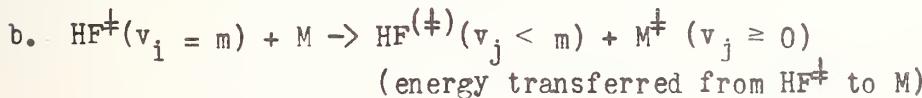
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|-------------------------------|-----------------------------|
| Brus and Lin                  | JPCHAX-1971-75-2546         |
| Clough, et al.                | CJCHAG-1970-48-2919         |
| Cuellar-Ferreira and Pimentel | IEJQA7-1973-9-201           |
| Gordon and Lin                | ACSRAL-1973-166-Phys. 137   |
| Lin, M. C.                    | IEJQA7-1973-9-200 (r. p.)   |
| Lin, M. C.                    | JPCHAX-1971-75-3642         |
| Padrick and Pimentel          | APPLAB-1972-20-167          |
| Padrick and Pimentel          | JCPA6-1971-54-720           |
| Pimentel, G. C.               | IEJQA7-1970-6-174 (rev.)    |
| Roeber and Pimentel           | IEJQA7-1973-9-201 (r. p.)   |
| Ross and Shaw                 | JPCHAX-1971-75-1170 (r. p.) |



|                    |                            |
|--------------------|----------------------------|
| Berry, M. J.       | DABBBA-1971-31-7210        |
| Berry and Pimentel | IEJQA7-1970-6-176          |
| Berry and Pimentel | JCPA6-1969-51-2274 (r. p.) |
| Klimek and Berry   | ACSRAL-1973-166-Phys. 103  |
| Klimek and Berry   | CHPLBC-1973-20-141         |
| Kompa, K. L.       | ACIEAY-1970-9-773 (rev.)   |
| Pimentel, G. C.    | IEJQA7-1970-6-174 (rev.)   |



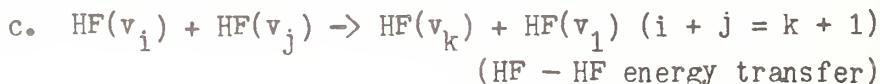
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|-------------------|-----------------------|
| Hancock and Green | JCPA6-1972-56-2474    |
| Heydtmann, et al. | APOPAI-1971-10-1755   |
| Suchard, et al.   | XADRCA-1973-AD 763716 |



|                       |                            |
|-----------------------|----------------------------|
| Ahl and Cool          | JCPA6-1973-58-5540         |
| Basov, et al.         | APOPAI-1971-10-1814        |
| Basov, et al.         | JTPLA2-1969-9-375 (r. p.)  |
| Basov, et al.         | IEJQA7-1970-6-183 (r. p.)  |
| Berend and Thommarson | IEJQA7-1973-9-195          |
| Berend and Thommarson | XADRCA-1973-AD 763817      |
| Blauer, et al.        | SYMCAQ-1971-13-109         |
| Blauer, et al.        | JCPA6-1972-57-3277         |
| Bott and Cohen        | JCPA6-1973-58-4539         |
| Bott and Cohen        | JCPA6-1973-59-447          |
| Chester, A. N.        | JCPA6-1970-53-3595 (r. p.) |
| Cohen, N.             | XADRCA-1972-AD 763715      |
| Cohen, et al.         | IEJQA7-1970-6-168 (r. p.)  |
| Cool, et al.          | APPLAB-1969-15-318 (r. p.) |
| Cool, et al.          | JAPIAU-1970-41-4038        |

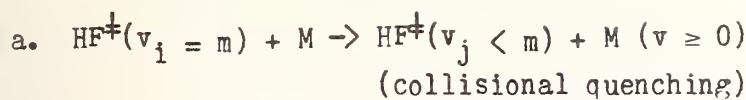
Dillon and Stephenson  
 Falk, T. J.  
 Green and Hancock  
 Gross, R. W. F.  
 Hancock and Green  
 Hancock and Green  
 Herbelin and Cohen  
 Hinchen, J. J.  
 Kapralova, et al.  
 Kapralova, et al.  
 Kerber, et al.  
 Kerber, et al.  
 Kerber and Whittier  
 Sentman, L. H.  
 Sentman and Solomon  
 Stephens and Cool  
 Suchard, et al.  
 Vasil'ev, et al.  
 Vedeneev, et al.  
 Vedeneev, et al.

JCPSA6-1973-58-2056 (calc., cr. sect.)  
 XCCIAV-1972-AD 745450  
 IEJQA7-1973-9-50  
 JCPSA6-1969-50-1889 (r. p.)  
 JCPSA6-1972-56-2474  
 JCPSA6-1972-57-4515  
 CHPLBC-1973-20-605 (r. p.)  
 JCPSA6-1973-59-233  
 DKPCAG-1971-197-281 (calc.)  
 DKPCAG-1971-198-452 (r. p.)  
 IEJQA7-1973-9-94 (rev.)  
 IEJQA7-1973-9-190 (r. p.)  
 \*ASTSZx-1970-TOR-0059(6753-10)-1 (calc.)  
 CHPLBC-1973-18-493 (calc.)  
 JCPSA6-1973-59-89 (calc.)  
 JCPSA6-1972-56-5863  
 JCPSA6-1972-57-5065  
 SPHJAR-1972-34-51  
 RJPCAR-1969-43-713  
 KICAA8-1970-11-26 (rev.)

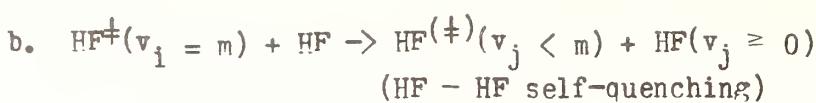


Ahl and Cool  
 Berend and Thommarson  
 Bott, J. F.  
 Bott, J. F.  
 Pott and Cohen  
 Cohen, N.  
 Emanuel, et al.  
 Green and Hancock  
 Hinchen, J. J.  
 Kerber, et al.  
 Kerber and Whittier  
 Kerber, et al.  
 Kompa, et al.  
 Osgood, et al.  
 Osgood, et al.  
 Sentman, L. H.  
 Suchard, et al.  
 Suchard, et al.

JCPSA6-1973-58-5540  
 XADRCA-1973-AD 763817  
 IEJQA7-1973-9-189  
 JCPSA6-1972-57-96  
 JCPSA6-1973-59-447  
 XADRCA-1972-AD 763715  
 XADRCA-1972-AD 746685 (rev.)  
 IEJQA7-1973-9-50  
 JCPSA6-1973-59-233  
 IEJQA7-1973-9-190  
 \*ASTSZx-1970-TOR-0059(6753-10)-1  
 IEJQA7-1973-9-94 (rev.)  
 JCPSA6-1968-49-4257  
 IEJQA7-1973-9-190  
 APPLAB-1972-20-469  
 CHPLBC-1973-18-493 (calc.)  
 JCPSA6-1972-57-5065  
 XADRCA-1973-AD 763716

2. HF<sup>‡</sup>(DF<sup>‡</sup>) Quenching

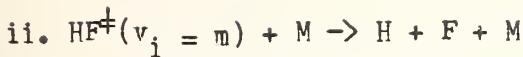
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|-----------------------|--|
| Ahl and Cool          | JCPA6-1973-58-5540   |
| Airey, J. R.          | IJCKBO-1970-2-65   |
| Airey and Fried       | CHPLBC-1971-8-23   |
| Airey and Smith       | JCPA6-1972-57-1669   |
| Anlauf, et al.        | JCPA6-1973-58-5354   |
| Berend and Thommarson | IEJQA7-1973-9-195  |
| Berend and Thommarson | JCPA6-1973-58-3454 (calc.,traj.)                           |
| Blair, et al.         | JCPA6-1973-59-1582   |
| Blauer and Solomon    | IJCKBO-1973-5-553  |
| Blauer and Solomon    | SYMCAQ-1973-14-189   |
| Blauer, et al.        | IJCKBO-1972-4-293  |
| Blauer, et al.        | XCCIAV-1972-AD 738296                                      |
| Bott and Cohen        | JCPA6-1971-55-3698   |
| Bott and Cohen        | JCPA6-1971-55-51 4   |
| Bott and Cohen        | JCPA6-1973-58-934  |
| Bott and Cohen        | JCPA6-1973-58-4539   |
| Brokaw, R. S.         | JPCHAX-1965-69-2488  |
| Cohen, N.             | XADRCA-1972-AD 763715                                      |
| Emanuel, et al.       | XADRCA-1972-AD 746685 (rev.)                               |
| Fried, et al.         | IEJQA7-1973-9-59   |
| Green and Hancock     | IEJQA7-1973-9-50   |
| Hancock and Green     | JCPA6-1972-56-2474   |
| Hancock and Green     | JCPA6-1972-57-4515   |
| Hess, L. D.           | IEJQA7-1973-9-201 (r. p.)                                  |
| Hinchen, J. J.        | IEJQA7-1973-9-196  |
| Hinchen, J. J.        | JCPA6-1973-59-233  |
| Just and Rimpel       | IEJQA7-1973-9-196  |
| Kaprалова and Chaikin | CBFMAO-1969-13-557   |
| Kaprалова, et al.     | KICAA8-1969-10-23  |
| Kaprалова, et al.     | CHPLBC-1968-2-581 (calc.,trans. prob.)                     |
| Kaprалова, et al.     | KICAA8-1964-6-884  |
| Kerber, et al.        | IEJQA7-1973-9-190 (r. p.)                                  |
| Kerber and Whittier   | *ASTSx-1970-TOR-0059(6753-10)-1                            |
| Kerber, et al.        | IEJQA7-1973-9-94 (rev.)                                    |
| Kompa, et al.         | JCPA6-1968-49-4257   |
| Kwok, M. A.           | IEJQA7-1973-9-196  |
| Molina and Pimentel   | IEJQA7-1973-9-64   |
| Parker, J. V.         | IEJQA7-1973-9-189  |
| Sentman, L. H.        | CHPLBC-1973-18-493 (calc.)                                 |
| Shin, H. K.           | CHPLBC-1972-14-64 (calc.)                                  |
| Suchard, et al.       | JCPA6-1972-57-5065   |
| Suchard, et al.       | XADRCA-1973-AD 763715                                      |
| Thompson, D. L.       | JCPA6-1972-57-4164 (calc.,pot surf.,traj.)                 |
| Thompson, D. L.       | JCPA6-1972-57-4170 (calc.,traj.)                           |
| Wilkins, R. L.        | JCPA6-1973-58-3038 (calc.,pop. distr.,<br>pot.surf.,traj.) |
| Wilkins, R. L.        | JCPA6-1973-59-698  |



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|-----------------------|----------------------------|
| Ahl and Cool          | JCPA6-1973-58-5540         |
| Airey and Fried       | CHPLBC-1971-8-23           |
| Airey and Smith       | JCPA6-1972-57-1669         |
| Berend and Thommarson | IEJQA7-1973-9-195          |
| Berend and Thommarson | JCPA6-1973-58-3203         |
| Blair, et al.         | JCPA6-1973-59-1582         |
| Blauer, et al.        | SYMCAQ-1971-13-109         |
| Bott, J.              | IEJQA7-1973-9-189          |
| Bott and Cohen        | JCPA6-1971-55-3698         |
| Bott and Cohen        | JCPA6-1973-58-934          |
| Bott and Cohen        | JCPA6-1973-58-4539         |
| Emanuel, et al.       | XADRCA-1972-AD 746685      |
| Falk, T. J.           | XCCIAV-1972-AD 745450      |
| Fried, et al.         | IEJQA7-1973-9-59           |
| Green and Hancock     | IEJQA7-1973-9-50           |
| Hancock and Green     | JCPA6-1972-56-2474         |
| Hancock and Green     | JCPA6-1972-57-4515         |
| Hinchen, J. J.        | IEJQA7-1973-9-196          |
| Hinchen, J. J.        | JCPA6-1973-59-233          |
| Just and Rimpel       | IEJQA7-1973-9-196          |
| Komua, et al.         | JCPA6-1968-49-4257         |
| MacLean and Tregay    | XADRCA-1971-AD 732927      |
| Molina and Pimentel   | IEJQA7-1973-9-64           |
| Sentman, L. H.        | CHPLBC-1973-18-493 (calc.) |
| Shin, H. K.           | CHPLBC-1971-10-81 (calc.)  |
| Shin, H. K.           | JCPA6-1973-59-879 (calc.)  |
| Solomon, et al.       | IJCKBO-1971-3-215          |
| Stephens and Cool     | JCPA6-1972-56-5863         |
| Suchard, et al.       | JCPA6-1972-57-5065         |
| Tal'roze, et al.      | KICAA8-1970-11-233         |
| Thompson, D. L.       | JCPA6-1972-57-2589         |
| Vasil'ev, et al.      | DKPCAG-1970-191-296        |



|   |                             |
|---|-----------------------------|
| i. $\text{HF}^{\ddagger}(v_i = m) + M_2 \rightarrow \text{HF}(v_j = 0) + M + M$ |                             |
| Airey, J. R.  | IJCKBO-1970-2-65            |
| Basov, et al.   | JTPLA2-1969-9-375 (r. p.)   |
| Brokaw, R. S.   | JCPA6-1965-69-2488          |
| Kapralova and Chaikin   | CBFMAO-1969-13-557          |
| Kapralova and Chaikin   | KICAA8-1969-10-195 (r. p.)  |
| Kapralova, et al.   | DKPCAG-1971-198-452 (r. p.) |
| Kapralova, et al.   | KICAA8-1969-10-23           |
| Kapralova, et al.   | KICAA8-1963-4-567 (r. p.)   |
| Kapralova, et al.   | KICAA8-1964-6-884           |
| Kompa, K. L.  | ACIEAY-1970-9-773 (rev.)    |
| Tal'roze, et al.  | KICAA8-1970-11-233          |
| Vasil'ev, et al.  | DKPCAG-1970-191-296         |



MacLean and Tregay

SYMCAQ-1973-14-157

C.  $\text{HF}^\ddagger$  ( $\text{DF}^\ddagger$ ) Theoretical papers

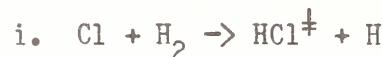
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| Anlauf, et al.        | JCPSA6-1970-53-4091 (pop. distr.)                                   |
| Ben-Shaul, et al.     | JCPSA6-1972-57-5427 (calc., pop. distr.)                            |
| Ben-Shaul, et al.     | CHPLBC-1972-15-160 (pop. distr.)                                    |
| Berend and Thommarson | JCPSA6-1973-58-3454 (calc., traj.)                                  |
| Blais and Truhlar     | JCPSA6-1973-58-1090 (pot. surf., traj.)                             |
| Dillon and Stephenson | JCPSA6-1973-58-2056 (calc., cr. sect.)                              |
| Emanuel and Whittier  | APOPAI-1972-11-2047 (calc.)   |
| Jaffe and Anderson    | JCPSA6-1971-54-2224 (pot. surf., traj.)                             |
| Jaffe, et al.         | JCPSA6-1973-59-1128 (pot. surf., traj.)                             |
| Jonathan, et al.      | MOPHAM-1972-24-1143 (pop. distr.,<br>pot. surf., traj.)             |
| Kapralova, et al.     | CHPLBC-1968-2-581 (trans. prob.)                                    |
| Kerber, et al.        | APOPAI-1972-11-1112 (pop distr., model.)                            |
| Levine, et al.        | CHPLBC-1973-19-1 (pop. distr.)                                      |
| Muckerman, J. T.      | JCPSA6-1971-54-1155 (traj.)   |
| Muckerman, J. T.      | JCPSA6-1972-56-2997 (pot. surf., traj.)                             |
| Muckerman, J. T.      | JCPSA6-1972-57-3388 (pop. distr., traj.)                            |
| Muckerman and Newton  | JCPSA6-1972-56-3191 (pot. surf.)                                    |
| O'Neil, et al.        | JCPSA6-1973-58-1126 (calc., pot. surf.)                             |
| Polanyi and Sloan     | JCPSA6-1972-57-4988 (d. r.)   |
| Polanyi and Tardy     | JCPSA6-1969-51-5717 (pop. distr.)                                   |
| Polanyi and Woodall   | JCPSA6-1972-57-1574 (d. r.)   |
| Schatz, et al.        | JCPSA6-1973-58-4023 (pop. distr.)                                   |
| Thompson, D. L.       | JCPSA6-1972-57-4164 (calc., pot. surf.<br>traj.)                    |
| Thompson, D. L.       | JCPSA6-1972-57-4170 (calc., traj.)                                  |
| Thruhlar, D. G.       | JCPSA6-1972-56-3189 (pot. surf.)                                    |
| Wilkins, R. L.        | JCPSA6-1972-57-912 (calc., pop. distr.,<br>pot. surf., traj.)       |
| Wilkins, R. L.        | JCPSA6-1973-58-3038 (calc., pop. distr.<br>pot. surf., traj.)       |
| Wilkins, R. L.        | JCPSA6-1973-58-2326 (calc., pop. distr.,<br>pot. surf., traj.)      |
| Wilkins, R. L.        | JCPSA6-1973-59-698 (calc., d.r., pop. distr.,<br>pot. surf., traj.) |

Part II. Hydrogen chloride (HCl, DC1)

A. Formation of HCl<sup>‡</sup> (DC1<sup>‡</sup>)

1. Bimolecular reactions (abstraction lasers)

a. Abstraction of H(D) atom by Cl atom



|                        |                             |
|------------------------|-----------------------------|
| Ashmore, P. G.         | TFSOA4-1953-49-251 (r. p.)  |
| Ashmore and Channugam  | TFSOA4-1953-49-254 (r. p.)  |
| Benson, et al.         | IJCCKBO-1969-1-29 (r. p.)   |
| Clyne and Walker       | JCFTAR-1973-69-1547 (r. p.) |
| Corneil, P. H.         | DABSA9-1968-28-4524         |
| Corneil and Kasper     | IEJQA7-1970-6-170           |
| Corneil and Pimentel   | JCPA6-1968-49-1379          |
| Davis, et al.          | IJCCKBO-1970-2-101 (r. p.)  |
| Deutsch, T. F.         | APPLAB-1967-10-234 (r. p.)  |
| Deutsch, T. F.         | APPLAB-1967-11-13 (r. p.)   |
| Deutsch, T. F.         | IEJQA7-1967-3-419 (r. p.)   |
| Fettis and Knox        | PRKNAZ-1964-2-2 (r. p.)     |
| Galante and Gislason   | CHPLBC-1973-18-231 (r. p.)  |
| Henry, et al.          | CHDBAN-1968-267-616         |
| Johnson, et al.        | JCPA6-1970-52-6372          |
| Klein, et al.          | JCPA6-1964-41-1799          |
| Kompa, K. L.           | CITEAH-1970-42-573 (rev.)   |
| Norrish, R. G. W.      | PRLAAZ-1967-301-1 (r. p.)   |
| Pimentel, G. C.        | SCAMAC-1966-214-32 (r. p.)  |
| Raff, et al.           | JCPA6-1970-53-1606          |
| Shizgal and Karplus    | JCPA6-1971-54-4357 (r. p.)  |
| Snider, N. S.          | JCPA6-1970-53-4116 (r. p.)  |
| Stedman, et al.        | CHPLBC-1970-7-173           |
| Truhlar, D. G.         | JCPA6-1972-56-3189 (r. p.)  |
| Westenberg, A. A.      | JCPA6-1970-53-4117 (r. p.)  |
| Westenberg and de Haas | JCPA6-1968-48-4405 (r. p.)  |
| Wood, G. O.            | JCPA6-1972-56-1723 (r. p.)  |
| Wood and Chang         | APPLAB-1972-20-77 (r. p.)   |
| Yaakov, et al.         | JCPA6-1973-59-2415 (r. p.)  |



|                   |                                  |
|-------------------|----------------------------------|
| Airey, J. R.      | IEJQA7-1967-3-203 (r. p.)        |
| Airey, J. R.      | IEJQA7-1970-6-175                |
| Airey, J. R.      | JCPA6-1970-52-156                |
| Anlauf, et al.    | JCPA6-1970-53-4091               |
| Anlauf, et al.    | DFSOAW-1967-44-183 (pop. distr.) |
| Anlauf, et al.    | PYLAAG-1967-24-208 (pop. distr.) |
| Anlauf, et al.    | JCPA6-1968-49-5189 (calc.)       |
| Ben-Shaul, et al. | CHPLBC-1972-15-160 (pop. distr.) |
| Ben-Shaul, et al. | JCPA6-1972-57-5427 (calc.)       |
| Blauer, et al.    | XADRCA-1972-AD 738296            |
| Chester, A. N.    | JCPA6-1970-53-3595               |
| Cool, et al.      | APPLAB-1969-15-318 (r. p.)       |

Cool, et al.  
 Cool, et al.  
 Cowley, et al.  
 Glaze, et al.  
 Kompa, K. L.  
 Levine, et al.  
 Maylotte, et al.  
 Moore, C. B.  
 Moore and Zittel  
 Naegeli and Ultee  
 Pimentel, G. C.  
 Polanyi, J. C.  
 Polanyi and Woodall

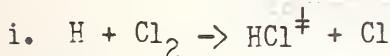
IJCKBO-1969-1-495 (r. p.)  
 JAPIAU-1970-41-4038 (r. p.)  
 CHPLBC-1971-12-144  
 APPLAB-1971-18-173 (r. p.)  
 ACIEAY-1970-9-773 (rev.)  
 CHPLBC-1973-19-1 (pop. distr.)  
 JCPSA6-1972-57-1547  
 IEJQA7-1968-4-52 (r. p.)  
 SCIEAS-1973-182-541 (rev.)  
 CHPLBC-1970-6-121 (r. p.)  
 PACHAS-1969-18-275 (rev.)  
 APOSAR-1965-2-109 (theory)  
 JCPSA6-1972-56-1563 (calc.)



Clyne and Walker  
 Davis, et al.  
 Fettis and Knox  
 Knox and Nelson

JCFTAR-1973-69-1547 (r. p.)  
 IJCKBO-1970-2-101 (r. p.)  
 PRKNAZ-1964-2-2 (r. p.)  
 TFSOA4-1959-55-937

b. Abstraction of Cl Atom by H(D) Atom



Airey, J. R.  
 Airey, et al.  
 Airey, et al.  
 Albright, et al.  
 Anlauf, K. G.  
 Anlauf, et al.  
 Anlauf, et al.  
 Anlauf, et al.  
 Anlauf, et al.  
 Ashmore, P. G.  
 Basov, et al.  
 Ben-Shaul, et al.  
 Bowen and Overholser  
 Cabre and Henry  
 Cabre and Henry  
 Charters, et al.  
 Cashion and Polanyi  
 Charters and Polanyi  
 Chester, A. N.  
 Cool, et al.  
 Cool, et al.  
 Corneil and Kasper  
 Dodonov, et al.

IJCKBO-1970-2-65  
 CJCHAG-1964-42-2193  
 JCPSA6-1964-41-3255  
 JCPSA6-1969-50-3632  
 DABBBA-1970-31-1195 (calc., pop. distr.)  
 JCPSA6-1970-53-4091 (calc., pop. distr.)  
 JCPSA6-1972-57-1561 (d. r.)  
 DFSOAW-1967-44-183 (pop. distr.)  
 PYLAAG-1967-24-208 (pop. distr.)  
 TFSOA4-1953-49-251 (mech.)  
 JTPLA2-1969-9-147 (rev.)  
 JCPSA6-1972-57-5427 (calc., pop. distr.)  
 ASACAW-1969-14-475 (pop. distr.)  
 JCPQAY-1967-64-119 (pop. distr.)  
 CHDBAN-1969-269-46 (pop. distr.)  
 NATUAS-1962-193-367 (r. p.)  
 JCPSA6-1958-29-455 (r. p.)  
 JCPSA6-1959-30-1097 (pop. distr.)  
 JCPSA6-1961-35-600  
 PRLAAZ-1960-258-529 (pop. distr.)  
 PRLAAZ-1960-258-564 (r. p.)  
 DFSOAW-1962-33-107 (pop. distr.)  
 JCPSA6-1970-53-3595 (calc., pop. distr.)  
 APPLAB-1969-15-318 (r. p.)  
 JAPIAU-1970-41-4038 (r. p.)  
 IEJQA7-1970-6-170  
 KICAA8-1970-11-677

|                               |   |
|-------------------------------|---|
| Fass, et al.                  | JPCCHAX-1972-76-2801 (r. p.)                    |
| Henry, et al.                 | CHDBAN-1968-267-616                             |
| Kasper, J. V. V.              | DIASAA-1966-26-5062 (r. p.)                     |
| Kasper and Pimentel           | PRLTAO-1965-14-352                              |
| Klein and Wolfsberg           | JCPSA6-1961-34-1494 (r. p.)                     |
| Kompa, K. L.                  | CITEAH-1970-42-573 (rev.)                       |
| Levine, et al.                | CHPLBC-1973-19-1 (pop. dist.)                   |
| Mayer, et al.                 | SYMCAQ-1967-11-837 (r. p.)                      |
| Ménard-Bourcin, et al.        | CHDBAN-1972-274-241 (pop. distr.)               |
| Miller and Light              | JCPSA6-1971-54-1643 (calc., pot. surf.)         |
| Moore, C. B.                  | IEJQA7-1968-4-52 (r. p.)                        |
| Norrish, R. G. W.             | PRLAAZ-1967-301-1 (r. p.)                       |
| Pacey and Polanyi             | APOPAI-1971-10-1725                             |
| Perona, et al.                | JCPSA6-1970-52-6384                             |
| Pimentel, G. C.               | DAKEAT-1969-50-1 (rev.)                         |
| Pimentel, G. C.               | IEJQA7-1970-6-174 (rev.)                        |
| Pimentel, G. C.               | PACHAS-1969-18-275 (rev.)                       |
| Pimentel, G. C.               | SCAMAC-1966-214-32 (r. p.)                      |
| Polanyi, J. C.                | APOSAR-1965-2-109 (calc., pop. distr.)          |
| Polanyi, J. C.                | CHMBAY-1966-2-151 (rev.)                        |
| Polanyi, J. C.                | DFSOAW-1962-33-279 (r. p.)                      |
| Polanyi, J. C.                | IEJQA7-1970-6-168 (r. p.)                       |
| Polanyi, J. C.                | JCPSA6-1959-31-1338 (rev.)                      |
| Polanyi, J. C.                | JCPSA6-1961-34-347 (calc., pop. distr.)         |
| Polanyi, J. C.                | JQSRAE-1963-3-471 (rev.)                        |
| Polanyi and Rosner            | JCPSA6-1963-38-1028 (r. p.)                     |
| Polanyi and Woodall           | JCPSA6-1972-56-1563 (cal ., pop. distr.)        |
| Rice and Jensen               | IEJQA7-1973-9-199                               |
| Russell and Light             | JCPSA6-1969-51-1720 (calc., pop. distr., traj.) |
| Semenov and Shilov            | KICAA8-1964-6-1 (r. p.)                         |
| Slootmaekers and Van Tiggelen | BSCBAG-1958-67-135 (r. p.)                      |
| Spinnler and Kittle           | IEJQA7-1970-6-169 (r. p.)                       |
| Stedman, et al.               | CHPLBC-1970-7-173                               |
| Wilkins, R. L.                | JCPSA6-1965-42-806 (r. p.)                      |
| Waerner and Wolfrum           | ACIEAY-1971-10-604 (rev.)                       |

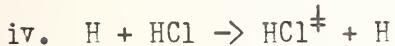


|                    |  |
|--------------------|--|
| Anlauf, et al.     | JCPSA6-1970-53-4091 (calc.pop. distr.) |
| Krogh and Pimentel | JCPSA6-1972-56-969                     |
| Mayer, et al.      | SYMCAQ-1967-11-837 (r. p.)             |



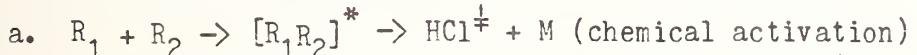
|                       |                                   |
|-----------------------|-----------------------------------|
| Anlauf, K. G.         | DABBBA-1970-31-1195 (pop. distr.) |
| Charters, et al.      | NATUAS-1962-193-367 (r. p.)       |
| Cabre and Henry       | CHDBAN-1969-269-46 (pop. distr.)  |
| Cashion and Polanyi   | JCPSA6-1961-35-600                |
| Freeman and Phillips  | JPCCHAX-1968-72-3031 (r. p.)      |
| Henry, et al.         | CHDBAN-1968-267-616               |
| Heydtmann and Polanyi | APOPAI-1971-10-1738 (pop. distr.) |

|                        |                                   |
|------------------------|-----------------------------------|
| Johnson, R. L.         | DABBBA-1969-30-2632 (pop. distr.) |
| Johnson, et al.        | JCPA6-1970-52-6372 (pop. distr.)  |
| Johnson and Setser     | CHPLBC-1969-3-207 (pop. distr.)   |
| Lin, M. C.             | CHPLBC-1970-7-209 (mech.)         |
| Ménard-Bourcin, et al. | CHDBAN-1972-274-241 (pop. distr.) |
| Perona, et al.         | JCPA6-1970-52-6384                |
| Perona, et al.         | JPCHAX-1969-73-2091               |
| Rabideau, S. W.        | JCPA6-1973-59-1533                |
| Rice and Jensen        | IEJQA7-1973-9-199                 |

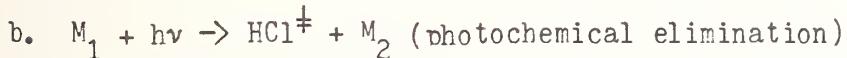


|                     |                                   |
|---------------------|-----------------------------------|
| Cashion and Polanyi | PRLAAZ-1960-258-529 (pop. distr.) |
| Wood, G. O.         | JCPA6-1972-56-1723 (r. p.)        |

## 2. Unimolecular Reactions (elimination lasers)



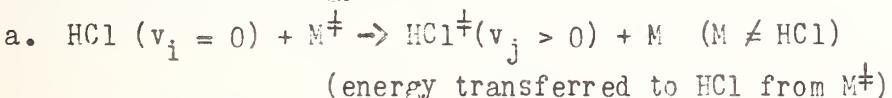
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| Berry and Pimentel | IEJQA7-1970-6-176                 |
| Chang, et al.      | JPCHAX-1971-75-2070 (pop. distr.) |
| Lin, M. C.         | IEJQA7-1973-9-200 (r. p.)         |



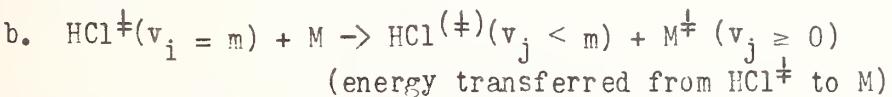
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|---------------------|---------------------|
| Berry, M. J.        | DABBBA-1971-31-7210 |
| Berry and Pimentel  | IEJQA7-1970-6-176   |
| Berry and Pimentel  | JCPA6-1969-51-2274  |
| Berry and Pimentel  | JCPA6-1970-53-3453  |
| Molina and Pimentel | IEJQA7-1973-9-64    |
| Molina and Pimentel | JCPA6-1972-56-3988  |

## B. $HCl^{\ddagger}$ (DCl<sup>+</sup>) Energy Transfer and Quenching

### 1. $HCl^{\ddagger}$ (DCl<sup>+</sup>) Energy transfer

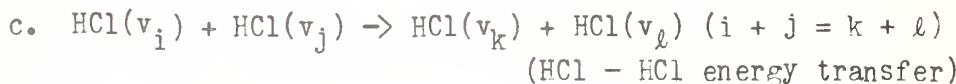


|                  |                            |
|------------------|----------------------------|
| Ahl and Cool     | JCPA6-1973-58-5540         |
| Blauer, et al.   | JCPA6-1972-57-3277         |
| Chen, et al.     | CHPLBC-1968-2-593          |
| Moore and Zittel | SCIEAS-1973-182-541 (rev.) |



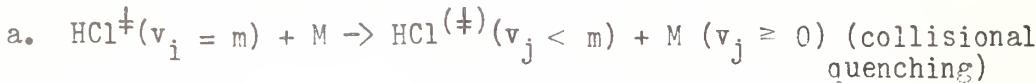
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|----------------------|--------------------|
| Ahl and Cool         | JCPA6-1973-58-5540 |
| Airey, J. R.         | IEJQA7-1970-6-175  |
| Airey, J. R.         | JCPA6-1970-52-156  |
| Bott and Cohen       | JCPA6-1973-58-4539 |
| Bowen and Overholser | ASACAW-1969-14-475 |
| Chen and Moore       | IEJQA7-1970-6-175  |

|                       |                                      |
|-----------------------|--------------------------------------|
| Chen and Moore        | JCPA6-1971-54-4072                   |
| Chen and Moore        | JCPA6-1971-54-4080                   |
| Chen, et al.          | CHPLBC-1968-2-593                    |
| Cool, et al.          | IJCKBO-1969-1-495 (r. p.)            |
| Cool, et al.          | JAPIAU-1970-41-4038 (r. p.)          |
| Dillon and Stephenson | JCPA6-1973-58-2056 (calc.,cr. sect.) |
| Hopkins, et al.       | JCPA6-1973-59-836                    |
| Hopkins and Chen      | JCPA6-1972-57-3161                   |
| Moore, C. B.          | ACHRAY-1969-2-103 (rev.)             |
| Moore and Zittel      | SCIEAS-1973-182-541 (rev.)           |
| Sentman, L. H.        | CHPLBC-1973-18-493 (calc.,model.)    |
| Stephenson, et al.    | JCPA6-1972-56-5214                   |
| Zittel and Moore      | JCPA6-1973-58-2004                   |



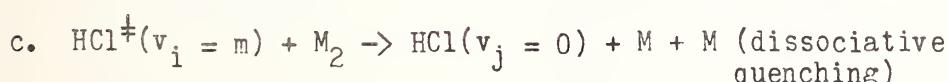
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|-----------------------|-----------------------------------|
| Bowen and Overholser  | ASACAW-1969-14-475                |
| Chen and Moore        | JCPA6-1971-54-4072                |
| Chen and Moore        | JCPA6-1971-54-4080                |
| Chen, et al.          | CHPLBC-1968-2-593                 |
| Cohen, et al.         | IJCKBO-1969-1-551                 |
| Corneil and Kasper    | IEJQAT-1970-6-170 (calc.)         |
| Findlay and Polanyi   | CJCHAG-1964-42-2176               |
| Findlay and Polanyi   | DFSOAW-1962-33-274                |
| Gorshkov, et al.      | APOPAI-1971-10-1781               |
| Hopkins and Chen      | IEJQAT-1973-9-196                 |
| Hopkins and Chen      | JCPA6-1972-57-3816                |
| Igoshin and Oraevskii | HIECAP-1971-5-357 (calc.)         |
| Leone and Moore       | CHPLFC-1973-19-340                |
| Moore and Zittel      | SCIEAS-1973-182-541 (rev.)        |
| Polanyi, J. C.        | JQSRAE-1963-3-471 (rev.)          |
| Sentman, L. H.        | CHPLBC-1973-18-493 (calc.,model.) |
| Sharma, et al.        | JCPA6-1973-58-3519 (calc.)        |

## 2. $\text{HCl}^\ddagger(\text{DCl}^\ddagger)$ Quenching



|                      |  |
|----------------------|--|
| Ahl and Cool         | JCPA6-1973-58-5540                     |
| Bott and Cohen       | JCPA6-1973-58-4539                     |
| Bowen and Overholser | ASACAW-1969-14-475                     |
| Chen and Moore       | JCPA6-1971-54-4072                     |
| Chen, et al.         | CHPLBC-1968-2-593                      |
| Cohen, et al.        | IJCKBO-1969-1-551                      |
| Corneil and Kasper   | IEJQAT-1970-6-170 (calc.)              |
| Craig and Moore      | JPCCHAX-1971-75-1622                   |
| Gorshkov, et al.     | APOPAI-1971-10-1781                    |
| Hopkins and Chen     | JCPA6-1972-57-3161                     |
| Kapralkova, et al.   | CHPLBC-1968-2-581 (calc.,trans. prob.) |
| Letokhov, V. S.      | SCIEAS-1973-180-451                    |

|   |  |
|---|--|
| Moore and Zittel  | SCIEAS-1973-182-541 (rev.)                   |
| Ridley and Smith  | CHPLBC-1971-9-457                            |
| Ridley and Smith  | JCFBTS-1972-68-1231                          |
| Seery, D. J.  | JCPA6-1973-58-1796                           |
| Sentman, L. H.  | CHPLBC-1973-18-493 (calc.,model.)            |
| Smith and Wood  | MOPHAM-1973-25-441                           |
| Zittel and Moore  | JCPA6-1973-58-2004                           |
| b. $\text{HCl}^{\pm}(v_i = m) + \text{HCl} \rightarrow \text{HCl}^{(\pm)}(v_j < m) + \text{HCl} (v_j \geq 0)$ | (HCl - HCl self-quenching)                   |
| Ahl and Cool  | JCPA6-1973-58-5540                           |
| Borrell, P.   | CSSPAD-1966-20-263                           |
| Bowen and Overholser  | ASACAW-1969-14-475                           |
| Bowman and Seery  | JCPA6-1969-50-1904                           |
| Breazeale and Kneser  | JASMAN-1960-32-885                           |
| Breshears and Bird  | JCPA6-1969-50-333                            |
| Cabre and Henry   | JCPQAY-1967-64-119 (pop. distr.)             |
| Chen, H-L.  | JCPA6-1971-55-5551                           |
| Chen and Moore  | JCPA6-1971-54-4072                           |
| Chen, et al.  | CHPLBC-1968-2-593                            |
| Cohen, et al.   | IJCKBO-1969-1-551                            |
| Corneil, P. H.  | DABSA9-1968-28-4524 (r. p.)                  |
| Corneil and Kasper  | IEJQA7-1970-6-170                            |
| Ferguson and Read   | TFSOA4-1967-63-61 (calc.)                    |
| Kapralova, et al.   | CHPLBC-1968-2-581 (calc.,trans. prob.)       |
| Letokhov, V. S.   | SCIEAS-1973-180-451                          |
| Margottin-Maclou, et al.  | APOPAI-1971-10-1768                          |
| Molina and Pimentel   | IEJQA7-1973-9-64                             |
| Moore, C. B.  | JCPA6-1965-43-297 (calc.,model.)             |
| Ridley and Smith  | JCFBTS-1972-68-1231                          |
| Sentman, L. H.  | CHPLBC-1973-18-493 (calc.,model.)            |
| Shin, H. K.   | CHPLBC-1970-6-494 (calc.)                    |
| Shin, H. K.   | JPCCHAX-1971-75-1079 (calc.)                 |
| Stephenson, et al.  | JCPA6-1972-56-5214                           |
| Thommanson and Berend   | IJCKBO-1973-5-629 (calc.,pot. surf., traj.)  |
| Thompson, D. L.   | JCPA6-1972-56-3570 (calc.,pot. surf., traj.) |
| Thompson, D. L.   | JCPA6-1972-57-2589                           |
| Zittel and Moore  | JCPA6-1973-58-2004                           |



|                               |                            |
|-------------------------------|----------------------------|
| Anlauf, et al.                | JCPA6-1969-51-5716         |
| Slootmaekers and Van Tiggelen | BSCBAG-1958-67-135 (r. p.) |

C.  $\text{HCl}^\ddagger$  ( $\text{DCl}^\ddagger$ ) Theoretical papers

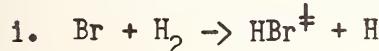
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|-----------------------|--|
| Anlauf, et al.        | JCPA6-1970-53-4091 (calc., pop. distr.)                    |
| Anlauf, et al.        | JCPA6-1972-57-1561 (calc., d. r.)                          |
| Anlauf, et al.        | JCPA6-1968-49-5189 (pop. distr.)                           |
| Ben-Shaul, et al.     | CHPLBC-1972-15-160 (pop. distr.)                           |
| Ben-Shaul, et al.     | JCPA6-1972-57-5427 (calc., pop. distr.)                    |
| Dillon and Stephenson | JCPA6-1973-58-2056 (calc., cr. sect.)                      |
| Kaprалова, et al.     | CHPLBC-1968-2-581 (calc., trans. prob.)                    |
| Levine, et al.        | CHPLBC-1973-19-1 (pop. distr.)                             |
| Miller and Light      | JCPA6-1971-54-1643 (calc., pot. surf.)                     |
| Moore, C. B.          | JCPA6-1965-43-2979 (calc., model.)                         |
| Parr and Truhlar      | JPCHAX-1971-75-1844 (calc., pot. surf.)                    |
| Parr, et al.          | JCPA6-1973-58-5 (calc., pop. distr.,<br>pot. surf., traj.) |
| Polanyi, J. C.        | APOSAR-1965-2-109 (pot. surf.)                             |
| Polanyi, J. C.        | JCPA6-1959-31-1338 (pop. distr.)                           |
| Polanyi and Rosner    | JCPA6-1963-38-1028 (r. p.)                                 |
| Polanyi and Woodall   | JCPA6-1972-56-1563 (calc., pop. distr.)                    |
| Raff, et al.          | JCPA6-1970-53-1606 (calc.)                                 |
| Rankin and Light      | JCPA6-1969-51-1701 (calc., pop. distr.,<br>pot. surf.)     |
| Russell and Light     | JCPA6-1969-51-1270 (calc., pop. distr.,<br>traj.)          |
| Sentman, L. H.        | CHPLBC-1973-18-493 (calc., model.)                         |
| Sharma, et al.        | JCPA6-1973-58-3519 (calc.)                                 |
| Shin, H. K.           | CHPLBC-1970-6-494 (calc., model.)                          |
| Shin, H. K.           | JPCHAX-1971-75-1079 (calc.)                                |
| Stern, et al.         | JCPA6-1973-58-5697 (calc., model.)                         |
| Wei and Yankwich      | JCPA6-1973-58-5552 (calc.)                                 |

Part III. Hydrogen bromide (HBr, DBr)

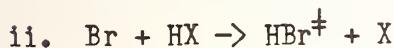
A. Formation of HBr<sup>‡</sup>(DBr<sup>‡</sup>)

1. Bimolecular reactions (abstraction lasers)

a. Abstraction of H (D) atom by Br atom



|                     |                                  |
|---------------------|----------------------------------|
| Bodenstein and Jung | ZEPCAC-1926-121-127 (r. p.)      |
| Deutsch, T. F.      | APPLAB-1967-10-234 (r. p.)       |
| Deutsch, T. F.      | IEJQA7-1967-3-419 (r. p.)        |
| Fettis and Knox     | PRKNAZ-1964-2-2 (r. p.)          |
| Jost, W.            | ZPCBAL-1929-3-95 (r. p.)         |
| Raff, et al.        | JCPSA6-1970-53-1606 (calc.)      |
| Truhlar, D. G.      | JCPSA6-1972-56-3189 (pot. surf.) |
| Wood and Chang      | APPLAB-1972-20-77 (r. p.)        |

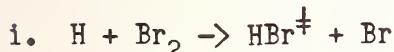


|                  |                                   |
|------------------|-----------------------------------|
| Anlauf, et al.   | DFSOAW-1967-44-183 (calc.)        |
| Blauer, et al.   | XADRCA-1972-AD 738296             |
| Maylotte, et al. | JCPSA6-1972-57-1547 (pop. distr.) |



|                 |                         |
|-----------------|-------------------------|
| Fettis and Knox | PRKNAZ-1964-2-2 (r. p.) |
|-----------------|-------------------------|

b. Abstraction of Br Atom by H(D) Atom



|                     |  |
|---------------------|--|
| Airey, et al.       | SYMCAQ-1967-11-85  |
| Anlauf, K. G.       | DABPBA-1970-31-1195  |
| Anlauf, et al.      | JCPSA6-1970-53-4091 (calc., pop. distr.)                     |
| Anlauf, et al.      | JCPSA6-1972-57-1561 (calc., d. r.)                           |
| Anlauf, et al.      | DFSOAW-1967-44-183 (calc., pop. distr.)                      |
| Anlauf, et al.      | PYLAAG-1967-24-208 (pop. distr.)                             |
| Ben-Shaul, et al.   | JCPSA6-1972-57-5427 (calc., pop. distr.)                     |
| Bodenstein and Jung | ZEPCAC-1926-121-127 (r. p.)                                  |
| Cashion and Polanyi | PRLAAZ-1960-258-570  |
| Chester, A. N.      | JCPSA6-1970-53-3595 (calc., pop. distr.)                     |
| Cool and Stephens   | JCPSA6-1970-52-3304 (r. p.)                                  |
| Fass, et al.        | JPCHAX-1972-76-2801  |
| Jost, W.            | ZPCBAL-1929-3-95 (r. p.)                                     |
| Mayer, et al.       | SYMCAQ-1967-11-837 (r. p.)                                   |
| Pimentel, G. C.     | PACHAS-1969-18-275 (rev.)                                    |
| Polanyi, J. C.      | IEJQA7-1970-6-168 (r. p.)                                    |
| Polanyi, J. C.      | JCPSA6-1959-31-1338 (rev.)                                   |
| Wagner and Wolfrum  | ACIEAY-1971-10-604 (rev.)                                    |
| White, J. M.        | JCPSA6-1973-58-4482 (calc., cr. sec.,<br>pop. distr., traj.) |



Ben-Shaul, et al.

JCPA6-1972-57-5427 (calc., pop. distr.)

Mayer, et al.

SYMCAQ-1967-11-837 (r. p.)

B.  $HBr^{\pm}$  ( $DBr^{\pm}$ ) Energy Transfer and Quenching

1.  $HBr^{\pm}$  ( $DBr^{\pm}$ ) Energy Transfer

a.  $HBr(v_i = 0) + M^{\pm} \rightarrow HBr^{\pm}(v_j > 0) + M$  ( $M \neq HBr$ )

(energy transferred to HBr from  $M^{\pm}$ )

Ahl and Cool

JCPA6-1973-58-5540

Airey, J. R.

IEJQA7-1970-6-175

Airey, J. R.

JCPA6-1970-52-156

Bott and Cohen

JCPA6-1973-58-4539

Chen and Moore

IEJQA7-1970-6-175

Chen and Moore

JCPA6-1971-54-4080

Cool, et al.

JAPIAU-1970-41-4038

Donovan, et al.

TFSOA4-1970-66-2148

Moore and Zittel

SCIEAS-1973-182-541 (rev.)

b.  $HBr^{\pm}(v_i = m) + M \rightarrow HBr^{(\pm)}(v_j < m) + M^{\pm} (v_j \geq 0)$

(energy transferred from  $HBr^{\pm}$  to  $M$ )

Ahl and Cool

JCPA6-1973-58-5540

Bott and Cohen

JCPA6-1973-58-4539

Chen, H-L.

JCPA6-1971-55-5551

Chen, H-L.

JCPA6-1971-55-5557

Cool and Stephens

JCPA6-1970-52-3304 (r. p.)

Donovan, et al.

TFSOA4-1970-66-2148

Hopkins, et al.

JCPA6-1973-59-836

Hopkins and Chen

JCPA6-1973-59-1495

Sentman, L. H.

CHPLBC-1973-18-493 (calc., model.)

Stephenson, et al.

JCPA6-1972-56-5214

c.  $HBr(v_i) + HBr(v_j) \rightarrow HBr(v_k) + HBr(v_{\ell})$  ( $i + j = k + \ell$ )

(HBr - HBr energy transfer)

Chen, H-L.

JCPA6-1971-55-5551

2.  $HBr^{\pm}$  ( $DBr^{\pm}$ ) Quenching

a.  $HBr^{\pm}(v_i = m) + M \rightarrow HBr^{(\pm)}(v_j < m) + M$  ( $v_j \geq 0$ )

(collisional quenching)

Ahl and Cool

JCPA6-1973-58-5540

Bott and Cohen

JCPA6-1973-58-4539

Chen and Chen

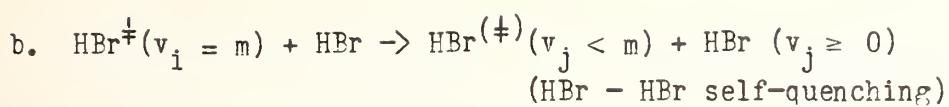
JCPA6-1972-56-3315

Hopkins and Chen

JCPA6-1973-59-1495

Sentman, L. H.

CHPLBC-1973-18-493 (calc., model.)



|                    |   |
|--------------------|---|
| Ahl and Cool       | JCPA6-1973-58-5540                      |
| Borrell, P.        | CSSPAD-1966-20-263                      |
| Breshears and Bird | JCPA6-1970-52-999                       |
| Chen and Chen      | JCPA6-1972-56-3315                      |
| Ferguson and Read  | TFSOA4-1967-63-61                       |
| Kaprалова, et al.  | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Kiefer, et al.     | JCPA6-1969-50-3641                      |
| Moore, C. B.       | JCPA6-1965-43-2979 (calc., model.)      |
| Sharma, et al.     | JCPA6-1973-58-3519 (calc.)              |
| Shin, H. K.        | JPCHAX-1971-75-1079 (calc.)             |
| Shin, H. K.        | JCPA6-1968-49-3964 (r. p.)              |
| Stephenson, et al. | JCPA6-1972-56-5214                      |

c.  $\text{HBr}^\ddagger (\text{DBr}^\ddagger)$  Theoretical papers

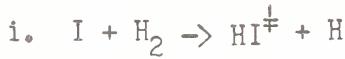
|                   |   |
|-------------------|---|
| Anlauf, et al.    | JCPA6-1972-57-1561 (d. r.)                                  |
| Ben-Shaul, et al. | JCPA6-1972-57-5427 (calc., pop. distr.)                     |
| Chester, A. N.    | JCPA6-1970-53-3595 (calc.)                                  |
| Kaprалova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.)                     |
| Moore, C. B.      | JCPA6-1965-43-2979 (calc., model.)                          |
| Parr and Truhlar  | JPCHAX-1971-75-1844 (calc., pot. surff.)                    |
| Pirkle and McGee  | JCPA6-1968-49-3532 (calc., cr. sect.,<br>pot. surff.)       |
| Polanyi, J. C.    | JCPA6-1959-31-1338 (rev.)                                   |
| Raff, et al.      | JCPA6-1970-53-1606 (calc.)                                  |
| Sentman, L. H.    | CHPLBC-1973-18-493 (calc., model.)                          |
| Sharma, et al.    | JCPA6-1973-58-3519 (calc.)                                  |
| Shin, H. K.       | JPCHAX-1971-75-1079 (calc.)                                 |
| Shin, H. K.       | JCPA6-1968-49-3964 (r. p.)                                  |
| White, J. M.      | JCPA6-1973-58-4482 (calc., cr. sec.,<br>pop. distr., traj.) |

## Part IV. Hydrogen iodide (HI, DI)

### A. Formation of $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$

#### 1. Bimolecular Reactions (abstraction lasers)

##### a. Abstraction of H(D) Atom by I Atom



Fettis and Knox

PRKNAZ-1964-2-2 (r. p.)

Henry, et al.

CHPLBC-1973-20-138 (r.p., traj.)

Parr and Truhlar

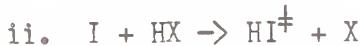
JPCHAX-1971-75-1844 (calc., pot. surf.)

Raff, et al.

JCPA6-1970-53-1606 (calc.)

Truhlar, D. G.

JCPA6-1972-56-3189 (pot. surf.)



Anlauf, et al.

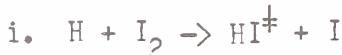
JCPA6-1969-51-5716



Wagner and Wolfrum

ACIEAY-1971-10-604 (rev.)

##### b. Abstraction of I Atom by H(D) Atom



Anderson and Kung

JCPA6-1973-58-2477 (pop. distr., traj.)

Ben-Shaul, et al.

JCPA6-1972-57-5427

Mayer, et al.

SYMCAQ-1967-11-837 (r. p.)

Penzhorn and Darwent

JPCHAX-1968-72-1639 (r. p.)

Sullivan, J. H.

JCPA6-1963-39-3001 (r. p.)



Ben-Shaul, et al.

JCPA6-1972-57-5427 (calc., pop. distr.)

Johnson, et al.

JPCHAX-1973-77-2499 (calc., pot. surf., traj.)

Mayer, et al.

SYMCAQ-1967-11-837 (r. p.)

### B. $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$ Energy Transfer and Quenching

#### 1. $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$ Energy Transfer



(energy transferred to HI from  $M^{\ddagger}$ )

Ahl and Cool

JCPA6-1973-58-5540

Chen, H-L.

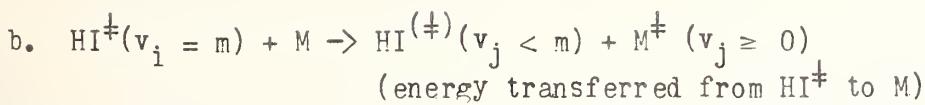
JCPA6-1971-55-5551

Chen and Moore

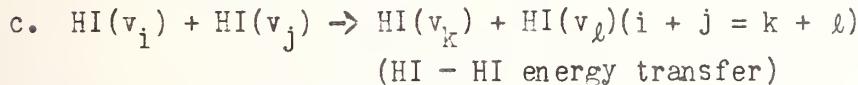
JCPA6-1971-54-4080

Chen, et al.

CHPLBC-1968-2-593

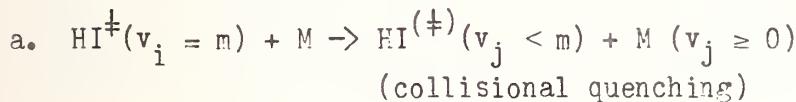


|                    |                    |
|--------------------|--------------------|
| Ahl and Cool       | JCPA6-1973-58-5540 |
| Breshears and Bird | JCPA6-1971-54-2968 |
| Chen, H-L.         | JCPA6-1971-55-5551 |
| Stephenson, et al. | JCPA6-1972-56-5214 |

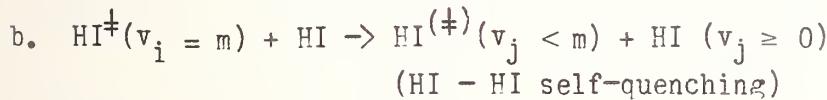


|                 |                                    |
|-----------------|------------------------------------|
| Chow and Greene | JCPA6-1965-43-324                  |
| Sentman, L. H.  | CHPLBC-1973-18-493 (calc., model.) |

## 2. $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$ Quenching



|                    |   |
|--------------------|---|
| Ahl and Cool       | JCPA6-1973-58-5540                      |
| Breshears and Bird | JCPA6-1971-54-2968                      |
| Chen, H-L.         | JCPA6-1971-55-5551                      |
| Chow and Greene    | JCPA6-1965-43-324                       |
| Kapralkova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Kiefer, et al.     | JCPA6-1969-50-3641                      |



|                    |   |
|--------------------|---|
| Ahl and Cool       | JCPA6-1973-58-5540                      |
| Breshears and Bird | JCPA6-1971-54-2968                      |
| Chen, H-L.         | JCPA6-1971-55-5551                      |
| Chow and Greene    | JCPA6-1965-43-324                       |
| Kapralkova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Moore, C. B.       | JCPA6-1965-43-2979                      |
| Sentman, L. H.     | CHPLBC-1973-18-493 (calc., model.)      |
| Shin, H. K.        | JPCHAX-1971-75-1079                     |

## c. $\text{HI}^{\ddagger}(\text{DI}^{\ddagger})$ Theoretical papers

|                    |   |
|--------------------|---|
| Anderson and Kung  | JCPA6-1973-58-2477 (pop. distr., traj.) |
| Ben-Shaul, et al.  | JCPA6-1972-57-5427 (calc., pop. distr.) |
| Henry, et al.      | CHPLBC-1973-20-138 (r.p., traj.)        |
| Kapralkova, et al. | CHPLBC-1968-2-581 (calc., trans. prob.) |
| Moore, C. B.       | JCPA6-1965-43-2979                      |
| Sentman, L. H.     | CHPLBC-1973-18-493 (calc., model.)      |
| Shin, H. K.        | JPCHAX-1971-75-1079                     |

|                         |                        |
|-------------------------|------------------------|
| Arnold and Rojeska      | AFOPAI-1973-12-169     |
| Borreli, P.             | BOOKA7-1969-2-180      |
| Carrington and Garvin   | CCHKAZ-1969-3-174      |
| Carrington and Polanyi  | 26BMAD-1972-9-135      |
| Chester, A. N.          | LSRVAN-1971-7-25.      |
| Chester and Hess        | IEJQAT-1972-8-1        |
| Cohen, N.               | XADRCA-1972-AD 763715  |
| Cool, T. A.             | BOOKA7-1971-197        |
| Cool, T. A.             | IEJQA7-1973-9-72       |
| Dobratz, B. M.          | XERLAR-1972-UCRL 51285 |
| Dzhidzhoev, M. S.       | SPUSBI-1970-13-237     |
| Emanuel, et al.         | XADRCA-1972-AD 746685  |
| Fettis and Knox         | PRKNAZ-1964-2-2        |
| Kerber, et al.          | IEJQA7-1973-9-94       |
| Kompa, K. L.            | ACIEAY-1970-9-773      |
| Kompa, K. L.            | CITEAH-1970-42-573     |
| Moore, C. B.            | ADCPAA-1973-23-41      |
| Moore, C. B.            | ARPLAP-1971-22-387     |
| Moore, C. B.            | ACHRAY-1969-2-103      |
| Moore, C. B.            | BOOKA7-1967-133        |
| Pimentel, G. C.         | DAKEAT-1969-50-1       |
| Pimentel, G. C.         | PACHAS-1969-18-275     |
| Rabinovitch and Flowers | QRCSAL-1964-18-122     |
| Shuler, et al.          | APOSAR-1965-2-81       |
| Wagner and Wolfrum      | ACIEAY-1971-10-604     |

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Airey, J. R., Pacey, P. D., and Polanyi, J. C., "Infrared Chemiluminescence in the Systems H + Br<sub>2</sub> and H + Br," *Symp. Combust.* 11 (Combustion Institute, Pittsburgh, 1967) 85

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Morosov, I. I., and Tal'roze, V. L., "Mass-Spectrometric  
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with Cl<sub>2</sub> and F<sub>2</sub>," J. Chem. Phys. 50, 3632 (1969)

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Inversion in Hydrogen Iodide From H + I<sub>2</sub> → HI + I,"  
J. Chem. Phys. 58, 2477 (1973)

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from the Systems H + Cl<sub>2</sub>, H + Br<sub>2</sub>, and H + ClNO," Diss.  
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Tardy, D. C., and Woodall, K. B., "Translational  
Energy-Distribution in the Products of Some Exothermic  
Reactions," J. Chem. Phys. 53, 4091 (1970)

Anlauf, K. G., Dawson, P. H., and Herman, J. A., "Relaxation  
of vibrationally excited HF in Levels v=1 and v=2. II.  
By Cl<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>2</sub>H<sub>2</sub>, and C<sub>2</sub>H<sub>4</sub>," J. Chem. Phys. 58,  
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and Woodall, K. B., "Energy Distribution among Reaction  
Products. V. H + X<sub>2</sub> (X ≡ Cl, Br), D + Cl<sub>2</sub>," J. Chem.  
Phys. 57, 1561 (1972)

Anlauf, K. G., Kuntz, P. J., Maylotte, D. H., Pace, P. D.,  
and Polanyi, J. C., "Energy Distribution among Reaction  
Products. Part 2. H + X<sub>2</sub> and X + HY," Discussions  
Faraday Soc. 44, 183 (1967)

Anlauf, K. G., Maylotte, D. H., Pace, P. D., and  
Polanyi, J. C., "Vibrational Population-Inversion and  
Stimulated Emission from the Continuous-Mixing of  
Chemical Reagents," Phys. Ltrs. A 24, 208 (1967)

Anlauf, K. G., Maylotte, D. H., Polanyi, J. C., and Bernstein,  
R. B., "Rates of the Endothermic Reactions HCl + X (X ≡ I, Cl)  
as a Function of Reagent Vibration, Rotation, and Trans-  
lation," J. Chem. Phys. 51, 5716 (1969)

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| <b>16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)</b><br><br>A bibliography, a reaction oriented list of references, is provided for published papers and reports containing rate data for reactions of halogen atoms with hydrogen-containing compounds, or of H (D, or T) atoms with halogen-containing compounds to form vibrationally chemiexcited hydrogen halides. The reactions for vibroexcitation of hydrogen halides through unimolecular or photochemical elimination, as well as the processes for vibrational energy transfer between hydrogen halides and various second bodies are also included. In addition, four lists of theoretical papers and a list of critical reviews and bibliographies are provided. Over 300 papers covering 50 types of reactions are listed. The period covered extends from 1958 through 1973. |  |  |                                   |                                     |
| <b>17. KEY WORDS (six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)</b><br><br><b>Bibliography; chemical kinetics; chemiexcitation; gas phase; halogens; hydrogen; hydrogen halides; laser; quenching; vibrational energy transfer.</b>  |  |  |                                   |                                     |
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