

COMMISSION No. 14
ATOMIC AND MOLECULAR DATA
(DONNEES ATOMIQUES ET MOLECULAIRES)

Report of Meetings 3 and 9 August 1988

PRESIDENT: R.W. Nicholls

Business Session, 3 August 1988

1. Activities and Scope of the Commission

A brief review was given of the substance of the discussion of the previous business meeting of Nov. 21 1985 on the subject matter of the commission. There was general endorsement of the view of that meeting that the purpose of the Commission was to keep a watching brief on the energy exchange processes of atomic and molecular physics, and of related spectral and structure data of atomic and molecular species. Such information is essential to the use of astronomical observations for astrophysical diagnosis and modelling.

In the discussion which followed it was emphasised that many research communities (including chemical physics, laser physics, plasma physics, atmospheric physics and chemistry and astrophysics) produced data of importance to the commission, some of whose members were also members of the commission.

The research areas of particular interest to the commission include:

- Photon phenomena (spectral wavelengths, intensities and transition probability data)
- Particle phenomena (atomic, molecular, ionic and electronic collision phenomena and cross sections)
- Line broadening phenomena

Accordingly the following working groups were established for 1985-88:

- Atomic Spectra and Wavelength Standards (W.C. Martin)
- Atomic Transition Probabilities (W.L. Wiese)
- Collision Processes (A. Dalgarno)
- Line Broadening (N. Feautrier)
- Molecular Structure and Transition Data (W.H. Parkinson)

2. Appointment of Officers for the period 1988-91

The following committee was approved:-

President: S. Sahal-Brechot

Vice President: W.L. Wiese

Organizing Committee:

A.H. Gabriel

T. Kato

F.J. Lovas

S.L. Mandel'shtam

R.W. Nicholls

H. Nussbaumer

W.H. Parkinson

Z.R. Rudzigas

W.L. Wiese

The commission expressed its gratitude to A. Dalgarno for his outstanding services for a number of years as chairman of the working group on collision processes.

Working Groups and their Chairmen for 1988-91 were approved as follows:

- 1: Atomic Spectra and Wavelength Standards
(W.C. Martin)
- 2: Atomic Transition Probabilities
(W.L. Wiese)
- 3: Collision Processes (S. Sahl-Brechot and W.L. Wiese to discuss appointment of new Chairman)
- 4: Line Broadening (N. Feautrier)
- 5: Molecular Structure and Transition Data:
(W.H. Parkinson)

Scientific Session, 9 August 1988

SPECTROSCOPIC CONSTANTS AND FRANCK CONDON FACTORS FOR THE MOLECULES
OBSERVED IN THE COMETARY SPECTRUM OF HALLEY

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Spectroscopic constants have been reviewed for the molecules observed recently in the spectrum of comet Halley. Franck-Condon factors have been calculated for these molecules.

SURVEY OF THE NEEDS OF ASTRONOMERS FOR NEW OR IMPROVED ATOMIC AND
MOLECULAR PARAMETERS

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In 1984, the "Committee on Line Spectra of the Elements - Atomic Spectroscopy" [CLSE-AS] of the U.S. National Research Council, began some informal surveys of the requirements for new and improved atomic data in a number of fields. As a member of that committee, I agreed to enquire about such needs, as well as for molecular parameters for "optical" wavelength (30nm to 10 μ) astronomy. Notice of the survey was mailed to 440 astronomers, who had demonstrated an interest in optical wavelength astronomical spectroscopy, distributed to all registrants at the June 1988 meeting of the American Astronomical Society, and published as letters to the editors of Newsletters of the American and Canadian Astronomical Societies. A poster paper that described the survey was presented at the January 1988 meeting of the American Astronomical Society [see Bull. Am. Astron. Soc. 19, p.1064, 1987]. Those who responded to the notices were asked to document their data needs in a particular format that was intended to enable producers of such data rapidly to understand the requirements and to be stimulated into providing them.

About 35 requests for atomic and molecular data were received. Some were well considered, documented, multipage summaries. Others were brief electronic mail statements. A number of the requests were from workshop chairs, working groups, satellite instrument teams, groups of collaborators etc., and therefore represented the collected opinions of a number of researchers. All requests will be collated, reproduced, and distributed, especially to producers of atomic and molecular data, both theorists and experimenters.

In this brief summary of the survey, it is impossible to provide a comprehensive review of the many types of data that are needed. However, one type of request stood out. A significant fraction of the responses requested greatly improved wavelength and energy level data, accurate to one part in 10⁶ to 10⁷ for common species, such as singly or doubly ionized iron peak and rare-earth elements, as well as Li-like and Be-like ions.

There have been some encouraging improvements in laboratory capabilities for this sort of work in recent years, in particular, the development of the Imperial College (UK) and the Los Alamos National Laboratory (USA) Fourier transform spectrometers. It is likely that these instruments will be frequently employed in obtaining better atomic and (molecular) wavelength and energy-level data for astronomical spectroscopy. Much of the progress in astronomical research depends upon knowledge or expertise from other scientific fields; atomic and molecular data are typical. Astronomers who need such information must support activities by making their needs known, by collaborating in obtaining funds for research, by participating in the collection and analysis of the data, and by encouraging publication of the results in the astronomical literature.

Those who wish to obtain a copy of the compilation of requests for new atomic and molecular data should contact the author at the above

address. Scientists with an interest in encouraging the acquisition of more and better atomic data for use in all areas of research, development and manufacturing, are referred to the proceedings of a related workshop on atomic data needs for analytical chemistry: "Needs for Fundamental Reference Data for Analytical Atomic Spectroscopy", edited by P. Boumans and A. Scheeline [Spectrochimica Acta, 43B pp 1-127, 1988]. Consideration of this report will show the considerable overlap between the atomic data needs of astronomers and those of analytical chemists.

I thank W.H. Parkinson, A. Dalgarno and R.E. Stencel for their advice and comments when this survey was being planned, and J.W. Linsky, S.J. Shawl and C.D. Scarfe for their assistance in publicizing it.

The work was supported in part by NASA Grant NSG-7304 to Harvard University.

ATOMIC SPECTRA - AN UPDATE

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A few forthcoming papers can be cited here to update the 1988 report of Working Group 1. The issue of J. Opt. Soc. Am. B for October 1988 (Vol. 5, No. 10) features a group of papers submitted as a tribute to Charlotte E. Moore-Sitterly on the occasion of her ninetieth birthday. Included are a review by S. Johansson and C.R. Cowley of research on the first three spectra of the iron-group elements, with special emphasis on the completeness of the line lists and analyses in view of astrophysical needs; a paper by C.M. Brown *et al.* on Fe I absorption in the 1550-3215 Å region that includes some 3000 lines; new high-accuracy measurements by R.C.M. Learner and A.P. Thorne of 300 Fe I lines in the 3830-5760 Å range; and accurate wavelengths for 558 Pt II lines over the range 1032-5223 Å as determined by J. Reader *et al.* The Pt I and Pt II spectra are of special interest for wavelength standards and will be used for calibration of spectra obtained with the High-Resolution Spectrograph of the Hubble Space Telescope.

The Atomic Energy Levels Data Center at the National Bureau of Standards has begun a program of compilations of wavelengths and energy-level classifications for spectral lines of elements in all ionization stages. A paper by V. Kaufman and J. Sugar giving these data for all the Sc spectra (Sc I - Sc XXI) will appear in J. Phys. Chem. Ref. Data 17, No. 4 (1988), and a similar compilation for the Si spectra is underway. Reference (87) of the Working-Group 1 report was cited incorrectly; the correct reference for the compilation of spectral data and Grotrian diagrams for Ni IX - Ni XXVIII is T. Shirai *et al.*: 1987, At. Data Nucl. Data Tables 37, p.235.

ATOMIC TRANSITION PROBABILITY MEASUREMENTS WITH THE NSO 1-m FTS

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The simplest method for measuring atomic transition probabilities is a two step process requiring (1) the radiative lifetime of the upper level of the transition and (2) the branching fraction, the probability that the upper level decays via the particular transition of interest. This latter probability is found by measuring the relative intensity of all of the decay channels that contribute significantly to the total decay strength of the upper level.

The first step has been greatly advanced by modern pulsed tunable UV lasers combined with nanosecond electronics. Atomic lifetimes are now measured routinely with 5% precision, and much better in special cases. This report deals with efforts to achieve similar precision and reliability in the spectrophotometry of branching ratios and with the exploration of a technique that would avoid the necessity to measure lifetimes for all levels.

Fourier transform spectroscopy has proven to be the best way to measure branching ratios. It has long been noted for its high accuracy, resolution and throughput, but for branching measurements the most important characteristic is that all of the decay channels can be measured at the same time. Any change in the brightness of the source while the spectrum is being recorded affects all branches equally, so branching ratios are unaffected. The 1-m. FTS at the McMath Solar Telescope on Kitt Peak is the best instrument currently available for these measurements, with a broad spectral range (250-1100 nm in a single spectrum; to 5500 nm in two) that extends far enough into the UV to encompass the great majority of atomic transitions and many lines of the singly-charged ion.

Recently we have explored a scheme that would take advantage of another feature of the FTS that has not been exploited in the work mentioned above: its awesome data-collection capability. This work used an inductively coupled argon plasma (ICP) source containing a trace amount of the atom to be studied. The ICP source is widely used by analytical chemists, and many papers in the spectrochemical literature have reported that excitation conditions in the ICP closely approximate thermodynamic equilibrium. This claim was tested by measuring the relative intensity in the ICP spectrum of 659 emission lines of Mo I of known transition probability (from lifetimes/branching fractions) to find the relative population of 67 levels in the ICP source. The measured level populations fit a Boltzmann distribution with an RMS

deviation of 7.5%, which is consistent with the uncertainty of the transition probabilities used in evaluating the populations. From this exponential distribution of measured level populations, the population of 204 levels for which the lifetime is not known could be interpolated. Once the population of a level is determined, the relative intensity of any emission line from that level determines the transition probability for that line. Transition probabilities for all other decay channels from the same upper level are then found from the emission branching ratios; it is not necessary to measure complete branching fractions.

Transition probabilities for 2176 lines were determined in this way with a precision limited by the 8% uncertainty in the level population, whereas for strong branches the branching fraction/lifetime method can achieve 3%, the uncertainty of the best lifetime values. However, the population method gives access to many more lines - virtually all of the classified lines in the 250 -1150 nm. range of these spectra.

In practice, the branching ratios were measured in the hollow cathode (HC) spectrum as well as in the ICP spectrum; both spectra were recorded with the D 1-m FTS. Comparison of the branching ratios in the two spectra helps eliminate difficulties with blends (in the ICP) and self-absorption (in the HC). This technique is now being applied to the MO II lines in the same spectra in collaboration with J.E. Lawler (U. Wis.), who is measuring Mo II level lifetimes needed to investigate the population distribution of ionic levels in the ICP source.

SEMIEMPIRICAL CALCULATION OF gf VALUES FOR THE IRON GROUP

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ABSTRACT: Lines of iron group elements that go to excited configurations that have not yet been studied in the laboratory produce considerable opacity in stars. I have computed new line lists for the first nine spectra of the iron group elements, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, and Ni including as many configurations as practical at the present time. Next I will compute opacities for the temperature range 2000K to 200000K, for abundances ranging from 0.0001 solar to 10 times solar, for microturbulent velocities 0, 1, 2, 4, and 8 km/s. Then I will compute corresponding grids of models, fluxes, colors, and spectra.

In 1970 Kurucz and Peytremann (1975) computed gf values for 1.7 million atomic lines for sequences up through nickel using scaled-Thomas-Fermi-Dirac wavefunctions and eigenvectors determined from least squares Slater parameter fits to the observed energy levels. That line list provided basic data for computing opacities (Kurucz 1979a), model stellar atmospheres (Kurucz 1979a;b), and spectra (Kurucz and Avrett 1981), and produced tremendous improvement in the comparison between theory and observation (Relyea and Kurucz 1978; Buser and Kurucz 1978).

However, it failed for cool stars and the sun because it does not include molecules.

In 1983 working with Lucio Rossi from Frascati and with John Dragon and Rod Whitaker at Los Alamos I finally completed line lists for all diatomic molecules that produce important opacity in G and K stars. Those data were combined with all existing theoretical and laboratory data, a newer calculation for Fe II (Kurucz 1981), and series extrapolations for the light elements, to produce input for computing new distribution function opacity tables. The calculations involved 17,000,000 atomic and molecular lines, 3,500,000 wavelength points, 50 temperatures and 20 pressures, and took a large amount of computer time.

As a test the opacities were used to compute a theoretical solar model and to predict solar fluxes and intensities from empirical models. There are several regions between 200 and 350 nm where the predicted solar intensities are several times higher than observed, say 85% blocking instead of the 95% observed. The integrated flux error of these regions is several per cent of the total. In a flux constant model this error is balanced by a flux error in the red. The model predicts the wrong colors. In detailed ultraviolet spectrum calculations half the intermediate strength and weak lines are missing. After many experiments, I determined that this discrepancy is caused by missing iron group atomic lines that go to excited configurations that have not been observed in the laboratory. Most laboratory work has been done with emission sources that cannot strongly populate these configurations. Stars, however, show lines in absorption without difficulty. Including these additional lines will produce a dramatic increase in opacity, both in the sun and in hotter stars. A stars have the same lines as the sun but more flux in the ultraviolet to block. In B stars and in O stars there will be large effects from third, fourth and fifth iron group ions. Envelope opacities that are used in interior and pulsation models will also be strongly affected.

I am fortunate to have been granted a large amount of computer time at the San Diego Supercomputer Center by NSF (AST-8518900) to carry out new calculations. To compute the iron group line lists I determine eigenvectors by combining least squares fits for levels that have been observed with computed Hartree-Fock integrals (scaled) for higher configurations including as many configurations as I can fit into a Cray. My computer programs have evolved from Cowan's (1968) programs. All configuration interactions are included. The following table is an example for Fe II,

even					odd			
d6 4s	d6 4d		d5 4s2	d5 4s4d	d6 4p	d6 4f	d5 4s4p	d5 4s4f
5s	5d	d6 5g	4s5s	4s5d	5p	5f	4s5p	
6s	6d	6g	4s6s	4s6d	6p	6f	4s6p	
7s	7d	7g			7p		4s7p	
8s	8d		d5 4p2		8p		4s8p	
9s			d7		9p			d4s2 4p

22 Configurations 5723 levels 16 Configurations 5198 levels
 largest Hamiltonian 1102 x 1102 1049 x 1049
 Slater parameters 729 541
 (many fixed at scaled Hartree-Fock)

The laboratory data are from the computer tapes that NBS uses to print its energy level compilations (Sugar and Corliss 1985). Transition integrals are computed with scaled-Thomas-Fermi-Dirac wavefunctions and the whole transition array is produced for each ion. The forbidden transitions are computed as well. Radiative, Stark, and van der Waals damping constants and Lande g values are automatically produced for each line.

The least squares fits to determine the energy levels are now complete for the first 10 ions of the Fe group. The most complex spectra were done first before moving toward the simpler Ca end of the iron group. Fe II has been redone several times in collaboration with Svereric Johansson from Lund who was been visiting Goddard (Johansson and Baschek 1988). We have added many more known levels, so the line lists will include many more Fe II lines with accurate positions. Johansson has just given me revised levels for Fe I so I will also redo those calculations. I will continue to revise these calculations for the iron group as new laboratory analyses become available, and I will continue on to other elements as time permits.

The following table shows the line lists completed at the present time, with the number of electric dipole lines saved for each ion,

	I	II	III	IV	V	VI	VII	VIII	IX
Ca	48573	4227	11740	113121	330004	217929	125560	30156	22803
Sc	191253	49811	1578	16985	130563	456400	227121	136916	30587
Ti	867399	264867	23742	5079	37610	155919	356808	230705	139356
V	1156790	925330	284003	61630	8427	39525	160652	443343	231753
Cr	434773	1304043	990951	366851	73222	10886	39668	164228	454312
Mn	327741	878996	1589314	1033926	450293	79068	14024	39770	147442
Fe	789176	1264969	1604934	1776984	1008385	475750	90250	14561	39346
Co	546130	1048188	2198940	1569347	2032402	1089039	562192	88976	15185
Ni	149926	404556	1309729	1918070	1971819	2211919	967466	602486	79627

The forbidden lines have not yet been tabulated. I have sorted all the lines and they will fill approximately thirty tapes by the time I complete writing them out. Most of these lines have uncertain wavelengths

because they go to predicted levels. I have produced a single tape edition of these data that has all the lines with reliable wavelengths between laboratory determined energy levels.

I have not yet made exhaustive comparisons with laboratory measurements. In general the calculations are greatly improved over my earlier work and show considerably less scatter. Some of the calculated lifetimes agree perfectly with the best measurements. Fe II lifetimes are about 15% shorter than observed. There can still be considerable scatter for lines that occur only because of configuration interactions. I found a few typographical errors in the input energy data because the output line list had lines in the wrong positions. Those spectra were recomputed.

I am now combining all these new data with my earlier atomic and molecular data to prepare the input files for my opacity calculations. I will compute opacities for the temperature range 2000K to 200000K, for abundances ranging from 0.0001 solar to 10 times solar, for microturbulent velocities 0, 1, 2, 4, and 8 km/s. I hope to finish the solar abundance models. Then I will continue with lower abundance Population II opacities and models in the coming year, and I also hope to get to enhanced abundances as well. I estimate that it will take one hundred Cray hours per abundance. I will compute grids of models, fluxes, colors, and spectra for each abundance.

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IDENTIFICATION ATLASES OF MOLECULAR SPECTRA

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In astrophysics, as in all research fields in which molecular spectra play important roles, there has been a continuing need for compendia of information on individual band systems. Firstly there is a requirement by observers and experimenters for aids to definitive identification of observed spectral features. Secondly there are needs by observers, by those who make diagnostic interpretations of spectral profiles, and also by theorists, for definitive critical compilations of appropriate molecular data with reference to the relevant literature. The continued popularity of various editions to Pearse and Gaydon's Identification of Molecular Spectra (1) and to Huber and Herzberg's Constants of Diatomic Molecules (2) are clear evidence of this.

In recognition of the need to augment the information in Pearse and Gaydon's compilation, the author and his colleagues established in the decade starting with 1964 an Identification Atlas of Molecular (3) series. Each of these roughly 20 page documents were devoted to one (diatomic) band system. It included a general description of the band system, its appearance and occurrence, an historical survey, tables of critically compiled molecular data, and plates of vibrationally identified spectra at low, medium and high resolution. These atlases were professionally printed, and because of cost the print runs were not large.

The more than a decade hiatus in Phase 1 of this project due to lack of funds (granting agencies do not look on such scholarly compilations as research !) has recently ended and Phase 2 has been initiated. This is a direct result of the formation of the Province of Ontario Centre of Excellence, The Institute for Space and Terrestrial Science and its support.

Phase 2 atlases have the same *raison d'être* as those of phase 1. However the spectra will be presented as intensity plots rather than as photographic plates. The plots will be numerically derived using our extensive realistic spectral synthesis facility (4). The atlases will be published "in house" inexpensively using desktop published facilities. The early atlases in the Phase 2 series will be devoted to atmospheric and astrophysical band systems.