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ATOMIC AND MOLECULAR DATA FOR OPACITY CALCULATIONS

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RESUMEN. Se intenta producir listas de líneas espectrales de todos los átomos y moléculas que son importantes en las estrellas. Se recolectan todos los datos publicados sobre análisis espectral y valores gf. Se calculan los niveles de energía, las longitudes de onda, los valores gf y las constantes de amortiguamiento no disponibles en la literatura. Se han calculado listas de líneas para las moléculas diatómicas H_2, CH, NH, OH, MgH, SiH, CN, C_2, CO, SiO y TiO y para los átomos Ca I-IX a Ni I-IX del grupo del hierro. En total, las listas cuentan con 58 millones de líneas. Estos cálculos se revisan a medida que se dispone de nuevos datos de laboratorio. Este trabajo se está extendiendo a otras moléculas diatómicas, a elementos más y menos pesados, así como a especies de mayor nivel de ionización.

ABSTRACT. I am attempting to produce line lists for all atoms and diatomic molecules that are important in stars. I collect all published data on spectrum analysis and oscillator strengths. I compute the energy levels, wavelengths, gf values, and damping constants that are not available from the literature. Line lists have been computed for diatomic molecules H_2, CH, NH, OH, MgH, SiH, CN, C_2, CO, SiO, and TiO, and for the iron group atoms Ca I-IX to Ni I-IX. These lists total 58 million lines. These calculations are being revised as new laboratory data become available. The work is being extended to other diatomic molecules, to lighter and heavier elements, and to higher stages of ionization.

Key words: ATOMIC PROCESSES – MOLECULAR PROCESSES – TRANSITION PROBABILITIES

I. HISTORY

My early model calculations used the distribution-function line opacity computed by Kurucz (1979ab) from the line data of Kurucz and Peytremann (1975). We had 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 has provided the basic data and has since been combined with a list of additional lines, corrections, and deletions with the help of Barbara Bell and Terry Varner at the Center for Astrophysics. The line data are being continually, but slowly, improved. We collect all published data on gf values and include them in the line list whenever they appear to be more reliable than the current data. I have also completely recomputed Fe II (Kurucz 1981).

After the Kurucz-Peytremann calculations were published, I started work on line lists for diatomic molecules beginning with H_2, CO (Kurucz 1977), and SiO (Kurucz 1980). Next, Lucio Rossi of the Istituto Astrofisica Spaziale in Frascati, John Dragon of Los Alamos, and I computed line lists for electronic transitions of CH, NH, OH, MgH, SiH, CN, C_2, and TiO. We generally had to repeat the rotational and vibrational fits to the laboratory measurements because the published data were usually mutually inconsistent. For example energy levels determined from FTS spectra could be taken as fixed when reducing less reliable observations, but had been free parameters in the original reductions. We adopted published transition moments, lifetimes, or f values. We generated RKR potentials, transition moments or Frank-Condon factors, and Hönl-London factors, and then the whole line list. In addition to lines between known levels, these lists include lines whose wavelengths are predicted and are not good enough for detailed spectrum comparisons but are quite adequate for statistical opacities. All these data are listed in Table I.

Table I. Line lists

FILE	NUMBER OF LINES	WAVELENGTH (NM)		COMMENT
		FIRST	LAST	
NLTELINES	39554	22.7838	99962.750	Elements that can be NLTE
GFIRONLAB	4906	188.0389	2239.4669	Iron group laboratory data
NBSMFW	7259	10.0856	2056.8400	Martin, Fuhr, Wiese iron group
BELLHEAVY	38456	33.3324	9946.0622	Elements heavier than Ni
BELLLIGHT	66792	2.4898	65101.683	Elements lighter than Ca
PREDKP	696704	6.6681	9995.4359	Kurucz-Peytremann predicted
H2	28486	84.4941	184.4573	Lyman and Werner
HYDRIDES	331268	203.6264	3245.1715	CH,NH,OH,MgH,SiH all isotopes
COAX	396004	111.3365	460.6524	CO 4th Pos all isotopes
COIR	118920	963.5078	9998.8853	CO vib-rot all isotopes
SIOAX	760378	177.3128	546.2833	SiO A-X all isotopes
SIOEX	947015	143.0468	462.4214	SiO E-X all isotopes
CNAX12	484709	292.5406	99912.800	$^{12}C^{14}N$ Red
CNAX13	503631	295.1871	99924.784	$^{13}C^{14}N$ Red
CNAX15	289887	341.5994	99776.188	$^{12}C^{15}N$ Red
CNBX	323818	201.9947	715.7552	CN Violet all isotopes
C2AX	406236	271.8071	9999.6289	C_2 Phillips all isotopes
C2BA12	462803	389.6061	99957.754	$^{12}C^{12}C$ Ballik-Ramsay
C2BA13	387809	511.6587	99980.746	$^{12}C^{13}C$ Ballik-Ramsay
C2BA33	313319	527.1495	80319.395	$^{13}C^{13}C$ Ballik-Ramsay
C2DA12	329771	344.9621	2541.6874	$^{12}C^{12}C$ Swan
C2DA13	253014	374.0201	991.5625	$^{12}C^{13}C$ Swan
C2DA33	217545	376.2757	959.4157	$^{13}C^{13}C$ Swan
C2EA12	487232	176.0052	862.4585	$^{12}C^{12}C$ Fox-Herzberg
C2EA13	332214	177.3769	560.9010	$^{12}C^{13}C$ Fox-Herzberg
C2EA33	260883	178.6938	543.2282	$^{13}C^{13}C$ Fox-Herzberg
TIOAX6	325116	528.5640	1875.4212	$^{46}Ti^{16}O\ \gamma$
TIOAX7	327496	528.7059	1771.6149	$^{47}Ti^{16}O\ \gamma$
TIOAX8	647203	490.4263	2146.0045	$^{48}Ti^{16}O\ \gamma$
TIOAX9	332113	528.9757	1864.4024	$^{49}Ti^{16}O\ \gamma$
TIOAX0	334222	529.1046	1860.9887	$^{50}Ti^{16}O\ \gamma$
TIOBX6	343598	246.6118	1232.9218	$^{46}Ti^{16}O\ \gamma'$
TIOBX7	345990	246.3570	1209.4093	$^{47}Ti^{16}O\ \gamma'$
TIOBX8	861488	235.9828	1362.8784	$^{48}Ti^{16}O\ \gamma'$
TIOBX9	350530	246.7795	1187.2650	$^{49}Ti^{16}O\ \gamma'$
TIOBX0	352802	247.3491	1186.9649	$^{50}Ti^{16}O\ \gamma'$
TIOCX6	232718	350.0947	1562.0368	$^{46}Ti^{16}O\ \alpha$
TIOCX7	234318	350.0471	1554.5985	$^{47}Ti^{16}O\ \alpha$
TIOCX8	503950	257.0800	1316.1735	$^{48}Ti^{16}O\ \alpha$
TIOCX9	237430	350.0113	1540.7715	$^{49}Ti^{16}O\ \alpha$
TIOCX0	238827	349.9744	1534.3348	$^{50}Ti^{16}O\ \alpha$
TIOEX6	241398	630.6768	2002.6215	$^{46}Ti^{16}O\ \epsilon$
TIOEX7	242954	631.0335	1997.7022	$^{47}Ti^{16}O\ \epsilon$
TIOEX8	510074	549.4411	2273.1493	$^{48}Ti^{16}O\ \epsilon$
TIOEX9	245978	631.7067	1988.4477	$^{49}Ti^{16}O\ \epsilon$
TIOEX0	247466	632.0252	1984.0965	$^{50}Ti^{16}O\ \epsilon$
TIOBA	310376	541.4458	2250.2486	TiO δ all isotopes
TIOCA	223850	446.7588	1669.0456	TiO β all isotopes
TIOFA	153496	432.0083	816.6252	TiO f-a all isotopes
TIOBD	158000	593.4372	2662.9648	TiO ϕ all isotopes
TIOED	102107	332.9690	562.5112	TiO e-d all isotopes

In 1983 I recomputed the opacities using the additional atomic and molecular data described above. These new opacities were used to produce improved empirical solar models (Avrett, Kurucz, and Loeser 1984), but were found to still not have enough lines. For example, there were 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 theoretical model this error is balanced by a flux error in the red. The model thus 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 these lines in absorption without difficulty. Including these additional lines produces 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 are large effects from third and higher iron group ions. Envelope opacities that are used in interior and pulsation models are also strongly affected.

II. RECENT CALCULATIONS

I was granted a large amount of computer time at the San Diego Supercomputer Center by NSF to carry out new calculations. To compute the iron group line lists I determined 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,

	22 even configurations				16 odd configurations			
$d^6 4s$	$d^6 4d$		$d^5 4s^2$	$d^5 4s4d$	$d^6 4p$	$d^6 4f$	$d^5 4s4p$	$d^5 4s4f$
$d^6 5s$	$d^6 5d$	$d^6 5g$	$d^5 4s5s$	$d^5 4s5d$	$d^6 5p$	$d^6 5f$	$d^5 4s5p$	
$d^6 6s$	$d^6 6d$	$d^6 6g$	$d^5 4s6s$	$d^5 4s6d$	$d^6 6p$	$d^6 6f$	$d^5 4s6p$	
$d^6 7s$	$d^6 7d$	$d^6 7g$			$d^6 7p$		$d^5 4s7p$	
$d^6 8s$	$d^6 8d$		$d^5 4p^2$		$d^6 8p$		$d^5 4s8p$	
$d^6 9s$			d^7		$d^6 9p$			$d^4 s^2 4p$
	5723 levels				5198 levels			
	largest Hamiltonian 1102 x 1102				largest Hamiltonian 1049 x 1049			
	729 Slater parameters				541 Slater parameters.			

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 can be computed as well. Radiative, Stark, and van der Waals damping constants and Landé g values are automatically produced for each line.

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. The files fill 28 6250-bpi VAX tapes. Most of these lines have uncertain wavelengths because they go to predicted rather than measured levels. I have produced a single tape edition of these data for distribution that has all the lines with reliable wavelengths between laboratory determined energy levels.

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 12% shorter than observed (Biémont et al. 1991). 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.

Several of these calculations have already been revised. Fe II has been repeated several times in collaboration with Sveneric Johansson from Lund (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 given me revised levels for Fe I (Brown et al. 1988) so I will also repeat those calculations. Ti I has been repeated based on the thesis by Forsberg (1987). This process will continue into the future. I will recompute the energy levels and line lists when new analyses become available and I will make the predictions available to laboratory spectroscopists. I plan to do the heavier and lighter elements as a background project.

III. FUTURE WORK

Returning to the diatomic molecules, all the line lists are in need of revision. Diatomic molecules in general are poorly analyzed. Stars are very high-temperature sources by laboratory standards. High-V and high-J levels are populated and produce significant opacity, but in current laboratory studies only low-V and low-J levels have been observed. Many excited electronic states that could produce significant opacity have not been analyzed at all. Thorough laboratory analyses are required. I have obtained James Brault's FTS CN spectra but have not yet reduced them. They will provide a tremendous advance in our knowledge of CN and should account for many weak features in the solar spectrum (and for stronger features in cool stars). I plan to work on the electronic and vibration-rotation spectra of all the significant diatomic molecules.

I eventually need line lists for the triatomic molecules so that I can work on M stars, but I hope that other people will do the work before I have to learn the physics. I am working on the low-temperature bands now, however, for atmospheric transmission.

I now distribute my computed line data on tapes. I plan to publish the line lists on CD-ROMs. These will include both a replacement for Kurucz-Peytremann (1975) listing all lines with good wavelengths for use in spectrum synthesis calculations, and a highly packed version of the whole line list that has all the data needed for opacity calculations on two CD-ROMs. This would allow anyone to compute opacities or opacity-sampled model atmospheres for arbitrary abundances. For each major atomic calculation I expect to publish a CD-ROM on which I will provide tables of all laboratory measurements, together with my computed energy levels, damping constants, Landé g values, lifetimes, branching ratios, and line gf values. These should be of value to both laboratory and astronomical spectroscopists.

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