GUVI disk imaging data in the 135.6 nm, LBH_S (140 − 150 nm) and LBH_L (165 − 180 nm) channels will be addressed. Dayglow data of interest are from the 135.6 nm and LBH_S channels recorded under quiet geomagnetic conditions in January and March 2002. Auroral data of interest are from these channels plus the LBH_L channel addressing observations in January, March, and April. Dayglow products are O/N_2 (column density ratio referenced to an N_2 column density of 10^{17} cm^2) and Q_{EUV} (integrated solar flux below 45 nm). Auroral products are O/N_2, E_o (characteristic energy in keV for either Gaussian or Maxwellian distributions being used to characterize electron precipitation), and Q (associated energy flux in ergs cm^{-2} s^{-1}). The products are derived from recently developed algorithms by Strickland [2002]. The sensitivity of dayside O/N_2 and Q_{EUV} to scalings of the N_2 LBH cross section and the Hinteregger spectrum below 20 nm will be shown. Comparisons will also be shown between GUVI and MSIS O/N_2. Q_{EUV} is under investigation and will be discussed in terms of a recommended scaling of the Hinteregger spectrum below 20 nm. Auroral products will be shown for observations made during weak and strong geomagnetic disturbances. Derived O/N_2 is significantly smaller within the auroral oval under the more highly disturbed conditions.

Strickland, D. J., Dayglow and auroral remote sensing algorithms for TIMED/GUVI, submitted to J. Geophys. Res., September, 2002.

URL: http://www.cpi.com

SA62B-0418 1330h POSTER

Data Visualization Tools and Techniques developed for the TIMED/GUVI Instrument

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The Global Ultraviolet Imager (GUVI) on the NASA Thermosphere Ionosphere Mesosphere Energetics and Dynamics (TIMED) spacecraft is a far-ultraviolet, scanning imaging spectrograph.

In this paper we present some of the tools and techniques that have been developed to visualize the GUVI data. These include and interactive data browser, summary thumb images and a variety of tools for creating animations suitable for Education and Public Outreach purposes.

The tools and techniques for rapidly producing high quality animations that show GUVI data overlayed on a photo-realistic rendering of the Earth will be demonstrated, together with methods of adapting the techniques to other TIMED data sets.

URL: http://guvi.jhuapl.edu

SA62B-0419 1330h POSTER

Exploiting Web-Based Systems to Provide Interactive Interpretation, Access and Display of Far Ultraviolet Data from the Global Ultraviolet Imager (GUVI) on TIMED

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The Global Ultra Violet Imager (GUVI) on the NASA TIMED spacecraft obtains horizon-to-horizon images of the aurora, dayglow and nightglow to routinely produce information about the space weather environment in the Earths upper atmosphere. This information is made available as soon as possible in a comprehensive web-based data system. This poster presents our design and implementation of an integrated web-based system which provides access to the GUVI instrument data as well as visualization tools to interactively display the GUVI data products. We will demonstrate how to access the data in its various forms, what tools are available for locating the appropriate and desired data set and various forms of summary images that are available.

URL: http://guvi.jhuapl.edu

SA71A MCC: 270 Sunday 0830h

Microscopic Processes in Solar System Atmospheres I *(joint with A, P)*

Presiding: **T G Slanger,** SRI International**; D L Huestis,** SRI International

SA71A-01 0835h INVITED

Laboratory Needs and Capabilities for Solar System Science

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A concerted effort has been made in the last year to begin to compile a comprehensive list of laboratory capabilities and needs specifically targeted toward solar system research. The NASA Laboratory Astrophysics Workshop held at NASA Ames Research Center in May 2002 provided a focus for these efforts: the solar system invited review by Dale Cruikshank and an informal working session at that meeting produced a draft list of needs and providers, a white paper for solar system science laboratory needs, and special sessions at several meetings such as this one. These materials have been distributed by email and posted on an existing laboratory web site (http://www.lpi.usra.edu/IJW/lab.html), and a more general web site for sharing such information is under development. This talk will give a brief overview of the solar system laboratory needs and capabilities identified in this process, with special focus on the needs for planetary atmospheres.

SA71A-02 0855h INVITED

Chemical Kinetics and Modeling the Flow of Energy in the Earth's Upper Atmosphere

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The fundamental physical difference between the radiative balance of the terrestrial mesosphere and thermosphere and that of the atmosphere below is the departure from local thermodynamic equilibrium (LTE) that occurs for all significant radiatively active gases. Under non-LTE the distribution of energy within the quantum states of these gases is no longer determined solely by collisions with other atmospheric constituents. Instead, radiative and chemical processes are competitive with collisional processes in determining the quantum state populations. In addition, the dominant collisional processes often involve atomic oxygen, a minor constituent whose abundance is virtually impossible to measure directly using satellite remote sensing techniques. The departure from LTE dramatically impacts the radiative balance of the upper atmosphere. In this talk we will review some of the major radiative cooling mechanisms of the terrestrial upper atmosphere and discuss the role chemical kinetics plays in determining the quantum state populations, the rates of radiative emission, the rates of radiative cooling, and hence the thermal structure. An illustration of these effects as dramatically demonstrated by the upper atmosphere's response to the solar storms of April 2002 will be presented.

SA71A-03 0915h

Infrared Backgrounds from Rotational Non-Equilibrium Processes in the Upper Atmosphere

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Many of the dominant features of the infrared spectrum of the mesosphere and thermosphere result from the production of radiating states of atmospheric species which are not in vibrational equilibrium with the local translational temperature. However, the analysis of high spectral resolution data collected during the CIRRIS 1A Space Shuttle and the Midcourse Space Experiment (MSX) missions showed that significant infrared spectral features of the upper atmosphere are due to states of radiating species which are not in rotational equilibrium with the local translational temperature. This paper will review the observational database collected by CIRRIS 1A and MSX on infrared emissions from highly rotationally excited OH, NO, and NO+ in the upper atmosphere. Laboratory measurements, state-to-state molecular dynamics calculations, and aeronomic models of chemical processes producing highly rotationally excited OH in the mesosphere and highly rotationally excited NO and NO+ in the thermosphere will also be reviewed. In addition, requirements for additional space-based observations, laboratory measurements, and chemical dynamical calculations of upper atmospheric rotational non-equilibrium processes will be identified.

SA71A-04 0930h

The Utility of NO 5.3 μm Radiation for Remote Sensing of Thermospheric Atomic Oxygen or Temperature

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A major mechanism for vibrational excitation of NO in the thermosphere is collisional energy transfer from atomic oxygen, $NO(\nu'' = 0) + O \rightarrow NO(\nu' = 1) + O$. Emission from $NO(\nu' = 1)$ produces the bright 5.3 μm band. At altitudes where this process dominates vibrational excitation during daylight or aurora, a relationship exists between atomic oxygen and ground state NO densities and temperature (due to the strong temperature dependence of the rate coefficient for vibrational excitation). Simultaneous measurements of ground state NO density, NO 5.3 μm volume emission rate, and either temperature or atomic oxygen density, would enable determination of the remaining quantity. This could provide a powerful remote sensing technique for temperature or atomic oxygen for altitudes where their determination is presently difficult. We will present a sensitivity analysis of this technique and discuss its limitations and range of applicability.

SA71A-05 0945h

The Photoabsorption Spectrum of N2 in 105-140 nm: The Tanaka and LBH systems and Production of the 2PB Fluorescence

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The absorption spectrum of N2 in 105-140 nm consists of forbidden electronic transitions of X 1S-C 3P (Tanaka system) and X1S-a 1P (LBH) with absorption cross sections in the order of 10-20 cm2 , and other weaker system involving the excited states B3U , a1U among others. Vibrational bands of v=0-3 in the Tanaka system and v=0-16 in the LBH (Lyman-Birge-Hopfield) were resolved. The absorption process in the C state produces UV fluorescence caused because of the transitions of C-B (2nd positive bands) with unity quantum yield. The process should contribute to the N2 dayglow in the thermosphere in addition to electron impact excitation.

SA71A-06 1020h INVITED

Laboratory Studies of Organic Polymer Particles: Implications for Early Earth

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In efforts to resolve the "Faint Young Sun" paradox, it has been suggested that early Earth may have had a reduced atmosphere similar to that present on the Saturn moon Titan. The N_2/CH_4 atmosphere of Titan is known to produce organic polymer particles. If similar particles were present on early Earth, they may have provided a UV-shield to allow greenhouse gases to accumulate. We are performing laboratory experiments to probe the formation and composition of Titan-like particles that might have formed on the early Earth. We are using a novel analysis technique based on detection of particles using an aerosol mass spectrometer (AMS). Using the AMS, we are able to determine the number, size and chemical composition of the particles in real time without first collecting and concentrating them. Our studies focus on characterizing the particles as a function of input trace gas composition. We are varying CH_4 concentrations from 10% CH_4 in N_2 to less than 1000 ppmv CH_4. We are also examining the influence of CO_2 on the particle characteristics. Results of our ongoing studies will be presented and implications for early Earth discussed.

SA71A-07 1040h

Photochemical formation rates and optical properties of organic aerosols through time-resolved *in situ* laboratory measurements

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The presence of photochemically-generated hazes has a significant impact on radiative transfer in planetary atmospheres. While the rates of particle formation have been inferred from photochemical or microphysical models constrained to match observations, these rates have not been determined experimentally. Thus, the fundamental kinetics of particle formation are not known and remain highly parameterized in planetary atmospheric models. We have developed instrumentation for measuring the formation rates and optical properties of organic aerosols produced by irradiating mixtures of precursor gases via *in situ* optical (633nm) scattering and online quadrupole mass spectrometry (1-200 amu). Results for the generation of particulate hydrocarbons from the irradiation of pure, gas-phase CH_4 with vacuum ultraviolet (120-160nm) light, along with simultaneous measurements of the evolution higher gas-phase hydrocarbons will be presented.

SA71A-08 1055h

Microphysics of Polar Mesosphere Summer Echoes: Electron Diffusion in the Vicinity of Charged Particles

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Since several years very strong radar echoes from the upper polar summer mesosphere called 'polar mesosphere summer echoes (PMSE) are observed. These PMSE are difficult to understand since electron density irregularities must have been produced in the D region at very small spatial scales of meters only. Neutral air turbulence was proposed as the key mechanism for this structuring earlier but in-situ measurements have frequently shown the absence of turbulence at PMSE altitudes. We reconsider microphysical processes of electron diffusion in the presence of positive ions and negatively charged aerosols. We obtain analytical solutions of the coupled diffusion equations and find that the main characteristics of these solutions are in line with available in situ measurements of electrons, ions, aerosols, and neutral air turbulence. The lifetime of the plasma perturbations is proportional to the square of the aerosol particle radius. For example, the presence of particles with radii larger than $\sim$10 nm allows for the existence of electron number density perturbations up to several hours after the creation mechanism has ceased. Contrary to other studies we find that this result is almost independent of the ratio between the aerosol charge number density and the number density of free electrons, again in agreement with observations. The electron perturbations potentially give rise to a radar reflectivity comparable to values observed with 50 MHz VHF radars. Our model readily explains why in situ measurements of neutral air turbulence have repeatedly shown active turbulence in some part of the PMSE layer whereas turbulence was basically absent at other parts. We compare our model results with ground-based observations of PMSE and find that the model yields the correct altitude profile of the mean PMSE occurrence frequency.

SA71A-09 1110h

Experimental Investigations of Oxygen Atom Loss on Mesospheric Dust Surrogates

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Inconsistencies have been noted between model predictions and observations of mesospheric composition in narrow regions of the mesosphere. Several arctic rocket campaigns between 1978 and 1993 have observed oxygen atom bite-outs, narrow layers just below 85 km depleted in atomic oxygen, correlated with NLC observations[1]. Separate observations from the HALOE instrument on UARS indicated the presence of a band of enhanced water vapor centered near 70 km at mid-latitudes that has not yet been adequately explained by current HO_x models[2]. Because the upper mesosphere and lower thermosphere (MLT) contains a variety of surfaces such as ice particles and ablated meteoric dust, heterogeneous reactions might influence these observed phenomena. Reactions currently being considered are the recombination of oxygen atoms to form molecular oxygen and the reaction of molecular hydrogen with atomic oxygen to form water.

To investigate these possible surface-mediated reactions, Knudsen cell experiments have been performed to quantify the oxygen atom recombination coefficient on mineral oxide powders representative of meteoritic composition. Oxygen atoms, produced by means of a microwave frequency discharge, and reagent gases are admitted to a low-pressure, well-mixed reactor in which the loss of the reactant species to a sample surface competes with escape through an exit aperture. Steady state reactant and product concentrations are measured by laser-induced fluorescence and mass spectrometry. By varying the area of the exit orifice in the presence or absence of the surface or reagent gases being investigated, atomic oxygen loss coefficients (γ) can be derived and then related to specific heterogeneous chemical reactions. Preliminary values will be reported for surface-mediated oxygen loss coefficients on several dust surrogates at room temperature and at pressures characteristic of the mesopause region.

[1] Gumbel, J., Murtagh, D. P. Espy, P. J., Witt, G., and Schmidlin, F. J., *J. Geophys. Res.*, **103**, 23,399-23,413 (1998).

[2] Summers, M. E, and Siskind, D. E., *Geophys. Res. Lett.*, **26**, 1937-1840 (1999).

This work is supported by the Aeronomy and Atmospheric Chemistry Programs of the National Science Foundation, the Ionospheric, Thermospheric and Mesospheric Physics Program of the National Aeronautics and Space Administration, and the Postdoctoral Program in Environmental Chemistry of the Henry and Camille Dreyfus Foundation.

SA71A-10 1125h INVITED

Ab Initio Theory of Water and Methane Frequencies and Opacities

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The prediction of frequencies and intensities for molecular ro-vibrational transitions by ab initio techniques is entering an exciting new era. Whereas the best twentieth century calculations of hydrogen containing molecules, such as water and methane, could predict fundamental frequencies with errors of several wave numbers, it is now possible to make predictions with errors of much less than one wave number. This level of accuracy is acheivable only when one uses an accurate electron correlation treatment, extrapolates the one-electron basis to the complete basis set limit, includes an accurate treatment of core-valence correlation, includes the scalar one and two electron relativistic effect, and accounts for the breakdown of the Born-Oppenheimer approximation.

These techniques are used with two different goals. First we have been honing these techniques to maximize our predictive ability. This will be especially important for methane, where spectral conjestion has made the assignment of the experimental spectrum an impossible task. It is the hope that our calculations will make the assignment possible.

Secondly we have studied the prediction of isotopic shifts for water. This requires accurate first and second order Born-Oppenheimer breakdown terms. It is hoped that this will enable us to leverage the large amount of data for the principle isotopomer to produce equal amounts of reliable data for all other isotopomers.

SA71A-11 1145h

Using Sensitivity Analysis to Identify Critical Rate Parameters for Jovian Planet Photochemistry

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A direct local sensitivity analysis technique, using the Senkin program from Sandia, has been applied to 0-D boxes of output from a 1-D Jupiter photochemistry model supplied by Dr. J. Moses using the Caltech-JPL CTM code. Results systematically and quantitatively

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predict each species variation with each rate parameter, along with terms for non-local effects. This procedure tracks chemically sensitive observations, and identifies steps and product ratios requiring further investigation; it can suggest field measurements, and the accuracies required of the kinetics. Key photolysis processes, H atom addition reactions to various hydrocarbon molecules and radicals, and methyl recombination to form ethane are identified. The use of kinetics rate theory approaches such as RRKM theory to provide low pressure and temperature rate constant values for these reactions will be described, noting uncertainties when relevant data are unavailable or limited.

Supported by NASA Planetary Atmospheres and NSF Planetary Astronomy Programs. D.A.N. was sponsored by an NSF Research Experiences for Undergraduates grant.

SA72A MCC: Hall D Sunday 1330h

Microscopic Processes in Solar System Atmospheres II Posters *(joint with A, P)*

Presiding: **T G Slanger,** SRI International**; D L Huestis,** SRI International

SA72A-0510 1330h POSTER

Recommended OH Vibrational Energy Transfer Rate Constants Based on Laboratory Studies

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Emission from vibrationally excited OH radicals is used to monitor the condition of the mesopause region and to trace the propagation of gravity waves through the nightglow layer. To extract information from the intensity of the emission, collisional energy transfer rate constants must be known or estimated for the temperature of the emitting layer. In addition to OH emission itself the energy from the reaction of hydrogen atoms with ozone can show up in CO_2, affecting the altitude profile of the infrared emission from this important species.[1]

Laboratory studies have attempted to measure these rate constants for over forty years with varying degrees of success. In this work the rate constants for the interaction of vibrationally excited OH with the important atmospheric colliders, O_2, N_2, and O atoms will be assembled and critically evaluated. Where conflicting measurements are available a recommended value will be presented and the justification for excluding specific results outlined. Where no experimental values have been measured, best estimates will be provided based on the behavior of similar chemical systems. Estimates of the temperature dependence will be undertaken based on the limited laboratory data. The reasons and basis for the estimates will be outlined.

This research is supported by the National Science Foundation Aeronomy Program under Grant No. ATM-9909807.

[1]M. Lopez-Puertas, R. H. Picard, M. Garcia-Comas, P. P. Wintersteiner, J. R. Winick, M. G. Mlynczak, C. J. Mertens, J. M. Russell, and L. L. Gordley, *Eos. Trans. AGU, 83(19)*, Spring Meet. Suppl. Abstract SA51A-06, 2002.

SA72A-0511 1330h POSTER

Quantum Mechanical Investigation of the O+H$_2$ → OH + H Reaction

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The reaction between $O(^3P)$ atoms and vibrationally excited H_2 molecules has been suggested as an important source of OH in the mesosphere. The reaction is dominated by tunneling at low temperatures and quantum mechanical calculations are needed for accurate calculation of its rate coefficient. We report quantum mechanical calculations of cross sections and rate coefficients for the $O+H_2 \rightarrow OH + H$ reaction on chemically accurate potential energy surfaces. We present rotational and vibrational energy distributions of the product OH molecule for different initial vibrational state of the reagent H_2 molecule and $O(^3P)$ atom kinetic energies.

SA72A-0512 1330h POSTER

The Role of the Quenching of O$_2$(1) by Atomic Oxygen on 6.3 μm Atmospheric Radiances and its Impact on the Retrieval of Water Vapour

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The high sensitivity of the new generation of atmospheric IR sounders has made the remote sensing of the upper atmosphere a reality. Emission from the high atmospheric layers is, however, quite often in non-local thermodynamic equilibrium (non-LTE). To retrieve the atmospheric parameters accurately, the excitation mechanisms of the emitting energy levels have to be well known. The emission of water vapor at 6.3 μm is one such example, that is in non-LTE above about 55-60 km. The major sources of uncertainty in this emission come from the vibrational-vibrational energy rate of transfer between $H_2O(010)$ and $O_2(1)$, the yield of $O_2(1)$ from O_3 photolysis and the thermal quenching of $O_2(1)$ by atomic oxygen. The latter has been measured only at high temperatures (1000-3500 K) until recently. Consequently, this posed a large uncertainty in $H_2O(010)$ populations and in its 6.3 μm atmospheric emission. The recent accurate measurements of this rate at room temperature (Kalogerakis et al., 2001) allow us to retrieve H_2O in the mesosphere more accurately. We discuss in this paper the importance of this rate for the water vapor retrieval and its application to the H_2O 6.3 μm measurements currently being taken by the SABER instrument on the TIMED satellite.

SA72A-0513 1330h POSTER

Temperature Dependence of the Collisional Deactivation Processes in Excited O$_2$: A Probe to the Relaxation Pathways and Energetics

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Emission from electronically excited O_2 is an important component of the nightglow of the Earth and Venus. Since these emissions occur at altitudes where the temperature is significantly below room temperature, understanding the temperature dependence of collisional removal is crucial to modeling the emission. Recent results have shown an unexpectedly large variation in the removal rates for nearby vibrational levels in the $a^1\Delta_g$, $b^1\Sigma_g^+$, and $c^1\Sigma_u^-$ states. As an example, the $b^1\Sigma_g^+(\nu = 13)$ removal rate constant for collisions with O_2 at 150 K is 4 to 60 times larger than that of the neighboring $\nu = 14$ and 12 levels, respectively. Such a large discrepancy can be caused by the presence of a resonant energy transfer pathway. A difference in behavior is also seen in how the magnitude of the rate constant varies with temperature. Knowledge of this behavior helps us to achieve a better understanding of the relaxation pathways and the relevant kinetic parameters in the collisional deactivation of the highly excited levels.

The removal rates for the $b^1\Sigma_g^+$ state $\nu = 14$ and 15 levels by collisions with O_2 were measured to be 2-4×10^{-12} cm^{3}s^{-1} and found to be almost independent of temperature over the entire atmospheric range (150-300 K), which points to a deactivation process with little or no energetic barrier. However, the rates for $\nu = 11$ and 12 at 150 K are an order of magnitude slower than those for ν = 13-15. We find that the $\nu = 12$ rate increases by a factor of 5 going from 150 to 240 K, indicative of a relaxation process with an activation barrier of about 350 ± 120 cm^{-1}.

For the $c^1\Sigma_u^-$ state at 155 K, the collisional removal rate constants in O_2 are $(2.6 \pm 0.3) \times 10^{-11}$ and $(7 \pm 3) \times 10^{-11}$ cm^{3}s^{-1} for $\nu = 10$ and 11, respectively. As the temperature is varied between 150 and 300 K, little or no change is observed in the magnitude of these rate constants. In contrast, the rate for $\nu = 9$ increases by more than a factor of 3 in the same temperature range, from 1.5 to 5.4×10^{-12} cm^{3}s^{-1}, perhaps indicating a process with a barrier.

These results will be compared with the collisional removal rates of other O_2 electronic states, namely $^5\Pi_g$ and $A^3\Sigma_u^+$, and the lower vibrational levels of the $b^1\Sigma_g^+$ state.

Overall, the magnitude of the collisional removal rate constants and their temperature dependence revealed interesting details of the specific relaxation processes. Experiments are currently underway to determine the involved relaxation pathways and energy transfer mechanisms to help explain the large differences observed from one vibrational level to the next.

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Theoretical and Experimental Studies of O-CO$_2$ Collisions

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Infrared emissions near 15 μm from bending-mode vibrationally excited carbon dioxide molecules control the rates of radiative cooling in key altitude regions of the upper atmospheres of Venus, Earth and Mars. The critical limiting process is excitation of $CO_2(v_2)$ in collisions with atomic oxygen. Laboratory measurements suggest rate coefficients about 3 times smaller than the values preferred by modelers.

Our theoretical investigations have developed improved potential energy surfaces for O + CO_2. A Diatomics-in-Molecules approach combines O-O and O-C repulsion and dispersion interactions, modeled by *ab initio* potential energy curves of the ArO molecule, with electrostatic interactions of the oxygen atom quadrupole moment with fractional charges on the CO_2 molecule, corresponding to its permanent quadrupole and instantaneous dipole moments. Nonadiabatic matrix elements are calculated by integrals over products of bending wavefunctions versus the CO_2 bond angle. Spin-orbit coupling is explicitly included. Results of Landau-Zener calculations will be presented. Calibration with *ab initio* O-CO_2 potential energy surfaces as well as quasiclassical trajectory calculations are underway.

The experimental approach is based on 248-nm photodissociation of ozone, followed by energy transfer of $O(^1D)$ to CO_2(vib), whose time evolution is followed by resonance-enhanced multiphoton ionization (REMPI). Preliminary work on the CO_2 REMPI spectrum will be presented.

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Diurnal Variations of Energetic O(3P) and O(1D) Atoms in the Thermosphere and Mesosphere

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