in the three stomachs, one of which contained a 1974 Lincoln-head penny. The liver was wrapped around the inferior vena cava. Cut sections of the kidneys revealed that they are composed of multiple separate nodules, each with individual cortices and medullae.

Light microscopic tissue examinations of lung showed bronchial cartilage extending to peripheral bronchi (Fig. 1b,c,d). Alveolar spaces were filled with a pale eosinophilic proteinaceous material and polymorphonuclear cells. Multiple abscesses were present, containing necrotic cellular debris, polymorphonuclear cells, and numerous large colonies of gram-positive and gram-negative bacilli and gram-positive cocci. Lymph node sections showed areas of abscess formation with numerous polymorphonuclear cells, basophilic bacterial colonies and cellular debris. There was dilatation of sinusoids which were filled with pale eosinophilic proteinaceous material, polymorphonuclear cells, lymphocytes and reticuloendothelial cells. Liver sections showed a fibrinous eosinophilic capsular exudate, Kupfer cells were filled with golden-brown pigment and intrasinusoidal extramedullary hematopoiesis was present.

Blood and urine drug screens were negative. Urine arsenic, lead and mercury levels were negative, and the blood typed as Group A2B, Rho(D) negative.

DISCUSSION

This case is not typical of most deaths associated with swimming pools which are referred to the Medical Examiner's office. Drowning is the fourth leading cause of accidental death in the United States. Approximately two-thirds of these drowning deaths are accidental, the remaining third are suicide, with rare instances of homicide. It is interesting to speculate whether death occurred with or without drowning, the decedent's compromised pulmonary function leaving him susceptible to (in this case) salt-water drowning. Whether or not drowning played a role in his death, it is the authors' opinion that this death is the result of a mixed bacterial pneumonia.

LITERATURE CITED

Bell, J. S., and Harlan, C. W., 1979. Forensic Autopsy Sampling. *The Tennessee Pathologist* 1(1): 21-23.

Bell, J. S., Autopsy Sampling. U.T.C.H.S. Forensic Seminar, 9/22/76.

Wells, G.G. 1958. *Histologic Technique,* U.T. Institute of Pathology, Memphis, TN.

American Association of Blood Banks. 1974. *Technical Methods and Procedures.* 374 pp.

JOURNAL OF THE TENNESSEE ACADEMY OF SCIENCE

VOLUME 60, NUMBER 4, OCTOBER 1985

ROTATIONAL TRANSITION PROBABILITIES IN TWO DIMENSIONS. II. SEMICLASSICAL APPROACH.

JOHN W. WILSON AND DAVID J. WILSON
Vanderbilt University
Nashville, Tennessee 37235

ABSTRACT

Rotational transition probabilities are calculated for argon-nitrogen collisions by means of a semiclassical method in which the classical trajectory is used to calculate the force acting on a quantum-mechanically treated driven rotor. The dependences of the transition probabilities on initial energies, relative orientation of the rotor, and impact parameter are studied.

INTRODUCTION

The problem of calculating rotational transition probabilities is one of long standing, dating back to Zener's work in 1930. (1931). The older literature is well reviewed by Takayanagi (1963) and by Gordon, Klemperer and Steinfeld (1968). A variety of approaches has been used, including the adiabatic (Ben-Reuven, 1965) and sudden (Kramer and Bernstein, 1964) approximations, and the method of distorted waves. (Brout, 1954; Davison; 1962; Dalgarno and Henry, 1964; Dalgarno, Henry, and Roberts, 1966; Roberts, 1963). Arthurs and Dalgarno (1960) used Racah's formalism to couple the rigid rotor states with the colliding particle's orbital angular momentum states, with which they then considered several approximations, Takayanagi and Nishimura (1960) used the modified wave number method (Takayanagi, 1963) and Allison and Dalgarno (1967) did close-coupling calculations for the 0 → 2 rotational transitions of H_2 and D_2. Of particular relevance to our work are the semiclassical approaches of Raff (1967) and of Lawley and Ross. (1965)

In the semiclassical approach, the classical collision trajectory is computed, and this is used to obtain a time-dependent driving force which acts on the quantized system; the behavior of this system is then analyzed by means of a time-dependent quantum mechanical treatment. The approach has been used effectively for the calculation of vibrational transition probabilities. (Widom and Bauer, 1953; Rapp and Sharp, 1963, Zelechow, et al. 1968, Locker and Wilson, 1970; Locker and Endres, 1969).

ANALYSIS

We consider the problem of planar collisions of an atom with a rigid rotor; see Fig. 1. We take our origin at the center of mass of the system. Coordinates R, Θ and ϕ are as indicated in Fig. 1; m_1 and m_2 are the atomic masses of the rotor; m_3 is the mass of the bombarding atom; r_o is the interatomic distance in the rotor; $a = r_o m_2/(m_1 + m_2)$; $b = r_o m_1/(m_1 + m_2)$; U_1 and U_2 are the distances between the bombarding atom 3 and the atoms 1 and 2 comprising the rotor. These distances are given by Eq. (1).

$$U_1^2 = R^2 + a^2 - 2Ra\cos(\theta - \phi) \tag{1}$$

$$U_2^2 = R^2 + b^2 + 2Rb\cos(\theta - \phi)$$

The kinetic energy is given by

$$T = \frac{\mu r_o^2}{2}\dot{\theta}^2 + \frac{M}{2}(\dot{R}^2 + R^2\dot{\phi}^2), \tag{2}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2};\ M = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$$

We assume that the potential energy is given by

$$V = \sum_{i=1}^{2} 4\epsilon_i\left[\left(\frac{\sigma_i}{U_i}\right)^{12} - \left(\frac{\sigma_i}{U_i}\right)^{6}\right], \tag{3}$$

the sum of two Lennard-Jones 6-12 potentials.

The classical equations of motion are then given by

$$M\ddot{R} = MR\dot{\phi}^2 - \frac{\partial V}{\partial U_1}\frac{\partial U_1}{\partial R} - \frac{\partial V}{\partial U_2}\frac{\partial U_2}{\partial R} \tag{4}$$

$$MR^2\ddot{\phi} = -2MR\dot{R}\dot{\phi} - \frac{\partial V}{\partial U_1}\frac{\partial U_1}{\partial \phi} - \frac{\partial V}{\partial U_2}\frac{\partial U_2}{\partial \phi}$$

$$\mu r_o^2\ddot{\theta} = -\frac{\partial V}{\partial U_1}\frac{\partial U_1}{\partial \theta} - \frac{\partial V}{\partial U_2}\frac{\partial U_2}{\partial \theta}$$

$$\frac{\partial U_1}{\partial R} = \frac{1}{U_1}[R - a\cos(\theta - \phi)]$$

$$\frac{\partial U_2}{\partial R} = \frac{1}{U_2}[R + b\cos(\theta - \phi)]$$

$$\frac{\partial U_1}{\partial \theta} = \frac{Ra}{U_1}\sin(\theta - \phi)$$

$$\frac{\partial U_2}{\partial \theta} = -\frac{Rb}{U_2}\sin(\theta - \phi)$$

$$\frac{\partial U_1}{\partial \phi} = -\frac{\partial U_1}{\partial \theta}$$

$$\frac{\partial U_2}{\partial \phi} = -\frac{\partial U_2}{\partial \theta}$$

Initial conditions are handled as follows. Without loss of generality we set $\phi(t = 0) = 0$. We choose an initial quantum level, *l*, for the rotor; from this we calculate

$$\dot{\theta}(t = 0) = \ell h/\mu r_o^2,\ E_{rot} = \frac{\hbar^2\ell^2}{2\mu r_o^2}$$

We let T_{rt} be the initial relative translation energy,

$$T_{rt} = \frac{M}{2}(\dot{R}^2 + R^2\dot{\phi}^2),$$

and b_{ip} be the impact parameter. Then

$$\dot{R}(t = 0) = -\left[\frac{2T_{rt}}{MR_o^2}(R_o^2 - b_{ip}^2)\right]^{\frac{1}{2}}$$

and

$$\dot{\phi}(t = 0) = \pm\frac{\dot{R}(t = 0)b_{ip}}{R_o(R_o^2 - b_{ip}^2)^{\frac{1}{2}}}$$

The initial values of θ may range from 0 to π (symmetric rotor) or 2π (asymmetric rotor); the initial value of R, R_O, is taken to be somewhat larger than $r_0 + \max(\sigma_1 \sigma_2)$.

The motion of the rotor is then reanalyzed by means of a time-dependent quantum mechanical formulation as follows.

$$\left[-\frac{\hbar^2}{2\mu r_o^2}\frac{\partial^2}{\partial\theta^2} + V(\theta,\phi(t),R(t))\right]\Psi(\theta,t) = i\hbar\frac{\partial\Psi}{\partial t} \tag{5}$$

Here $\phi(t)$ and R(t) are the classical numerical values of ϕ and R at the time t.

In the usual way (Pauling and Wilson, 1935) we write

$$\Psi = \sum_n A_n(t)\exp\left(\frac{-iE_n t}{\hbar}\right)\exp(in\theta), \tag{6}$$

which on substitution in Eq. (5), multiplication by $\exp(-im\theta)$, and integration over θ, yields

$$\dot{A}_m(t) = \frac{1}{i\hbar}\sum_n \exp[i(E_m - E_n)t/\hbar]V_{mn}(t)A_n, \tag{7}$$

where

$$V_{mn}(t) = \frac{1}{2\pi}\int_0^{2\pi}\exp[i(n - m)\theta]V(\theta,t)d\theta$$

On writing $V(\theta,t)$ as a Fourier series,

$$V(\theta,t) = \sum_k b_k(t)\exp(ik\theta),$$

we obtain from Eq. (7) the following:

$$\dot{A}_m = (i\hbar)^{-1} \sum_n \exp[i(E_m - E_n)t/\hbar] b_{m-n}(t) A_n \tag{8}$$

The Fourier coefficients $b_m(t)$ are calculated by a procedure very similar to that used by Dillon (1974) on a related problem. We proceed as follows. Let

$$F(k,n,R,a,\phi) = \int_0^{2\pi} \frac{\exp(-ik\theta)d\theta}{[R^2 + a^2 - 2Ra\cos(\theta - \phi)]^n} \tag{9}$$

Letting $\theta - \phi = \delta$, using a binomial expansion on the denominator, and employing a trigonometric identity for $\cos^r\delta$ then yields

$$F(k,n,R,a,\phi) = \frac{\exp(-ik\phi)}{(R^2 + a^2)^n} \sum_{r=0}^{\infty} \binom{n + r - 1}{n - 1} \left(\frac{2Ra}{R^2 + a^2}\right)^r \cdot \int_{-\phi}^{2\pi-\phi} (\cos k\delta - i \sin k\delta) \sum_{\ell=0}^{r} \binom{r}{\ell} \frac{\cos(r - 2\ell)\delta}{2^r} d\delta \tag{10}$$

This, on carrying out the integration, yields

$$F = 2\pi \left(\frac{Ra}{R^2 + a^2}\right)^k \frac{\exp(-ik\phi)}{(R^2 + a^2)^n} \cdot \sum_{r=0}^{\infty} \binom{n + k + 2r - 1}{n - 1} \binom{k + 2r}{r} \left(\frac{Ra}{R^2 + a^2}\right)^{2r} \tag{11}$$

The expression for the Fourier coefficients of the interaction potential, the $b_k(t)$, is then given by

$$b_k[R(t),\phi(t)] = 4\varepsilon_1[\sigma_1^{12}F(k,6,R,a,\phi) - \sigma_1^{6}F(k,3,R,a,\phi)] + 4\varepsilon_2[\sigma_2^{12}F(k,6,R,-b,\phi) - \sigma_2^{6}F(k,3,R,-b,\phi)] \tag{12}$$

Equations (4) and (8) were then integrated forward in time from the given initial conditions (as specified previously for Eqs. (4); $A_n = \delta_{n,no}$ for Eqs. (8)) until the magnitude of R indicated that the collision was over. A fourth-order Runge-Kutta-Gill method with variable Δt was used for the numerical integration, with rates of loss of classical energy conservation and normalization of the wave function the criteria for adjusting Δt. (Ralston and Wilf, 1960)

RESULTS

Transition probabilities were calculated on an XDS Sigma 7 computer; up to 21 rotational states were included. Argon-nitrogen collisions were modeled; Lennard-Jones parameters were estimated from data for argon and neon (Hirshfelder, et al., 1954), and r_0 was taken from Herzberg's tabulation (1950).
($E_1 = E_2 = 4.416 \times 10^{-15}$ erg, $\sigma_1 = \sigma_2 = 3.12$ Å, $r_0 = 1.094$ Å).

In Fig. 2 we see the effect of varying impact parameter on the transition probabilities; as with our earlier approach (a strong-coupling fully quantum method), |Δm|values larger than 2 contribute very significantly for impact parameters < 5 Å at an initial relative translational energy of 8.83×10^{-15}erg. The initial value of the rotational quantum number, m_0, is zero for these runs.

The effect of initial relative translational energy upon the transition probabilities is illustrated in Fig. 3. At low energies |Δm| values >2 are not very important; but, for an initial relative translational energy of 8.83×10^{15}erg |Δm| = 4 transitions are quite significant. Qualitatively, we would expect that the more violent collisions would have contributions from transitions involving larger values of Δm. In this figure the initial rotor state is the ground state, $m_0 = 0$. In Fig. 4 we see the same type of runs made at various initial relative kinetic energies. Here, however, the initial rotor state has $m_0 = 2$. The magnitudes of the transition probabilities are comparable to what we found for $m_0 = 0$.

Figure 5 shows the effects of varying the initial orientation of the rotor in the calculation of the classical trajectories. To compare results obtained by this method with the results of our strong coupling fully quantal treatment requires integrating the transition probabilities over θ_0 (from 0 to π for N_2).

We conclude that this semi-classical approach produces results in reasonably good agreement with our strong coupling fully quantal calculation (Dillon, Wilson, and Wilson, 1984), and that both indicate that the collisional selection rule of |Δm| + 2 for collisions of a homonuclear diatomic is an artifact of the perturbation theory approach, and is generally not a good approximation for real collisions.

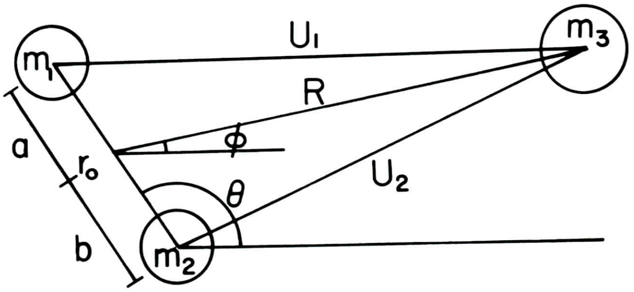

FIG. 1 *Model and notation.*

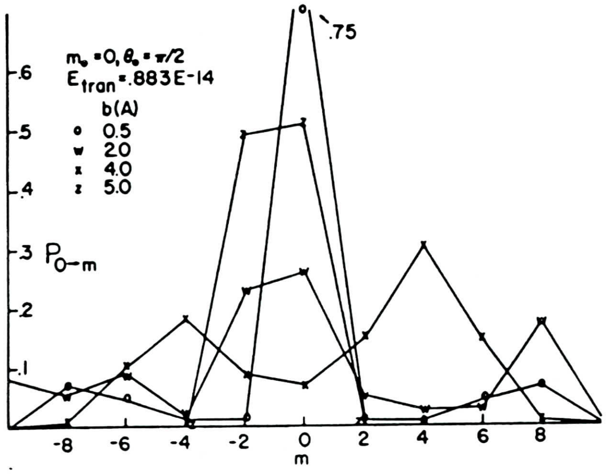

FIG. 2. *Dependence of rotational transition probabilities on impact parameter, b.*

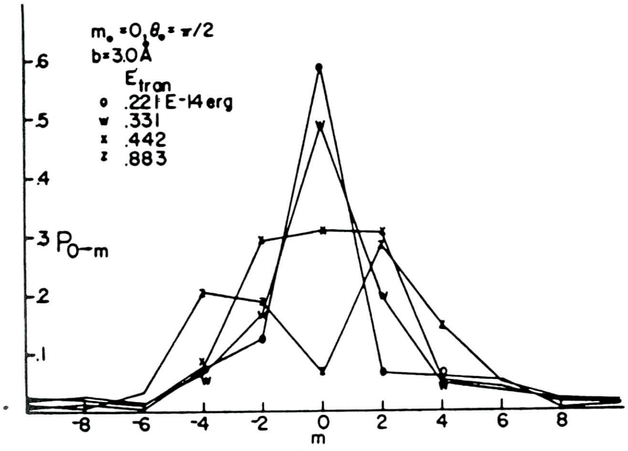

FIG. 3. *Dependence of rotational transition probabilities on initial relative translational energy, $E_{tran'}$ for m_O = 0.*

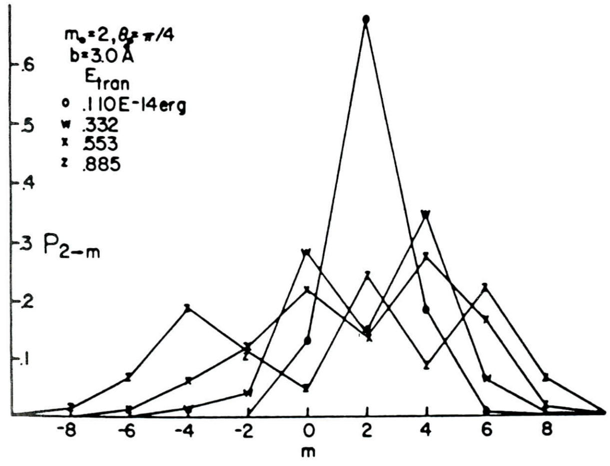

FIG. 4. *Dependence of ratational transition probabilities on E_{tran} for m_O = 2.*

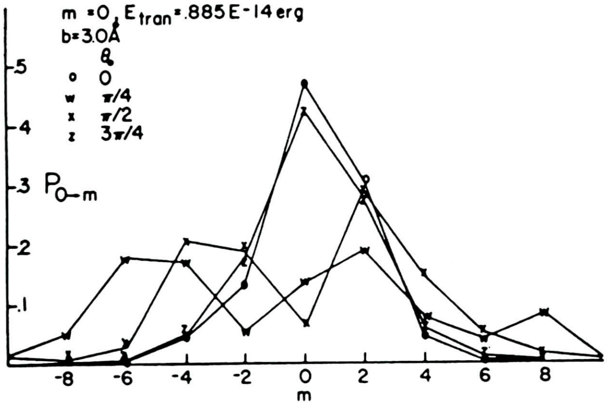

FIG. 5. *Dependence of rotational transition probabilities on the initial orientation angle,* Θ_O' of the rotor.

LITERATURE CITED

Allison, A. C., and A. Dalgarno. 1967. The rotational excitation of molecular hydrogen. proc. Phys. Soc. 90: 609.

Arthurs, A. M., and A. Dalgarno. 1960. The theory of scattering by a rigid rotor. Phys. Rev. 131:209.

Ben-Reuven, A. 1965. Shift of the R(O) and P(1) infrared lines of HCl perturbed by noble gases. J. Chem. Phys. 42:2037.

Brout, R. 1954. Rotational energy transfer in hydrogen. J. Chem. Phys. 22:934.

Dalgarno, A., and R. J. W. Henry. 1964. Atomic Collision Processes. Ed. M. R. C. McDowell. North-Holland Publishing Co., Amsterdam. pp. 91-120.

Dalgarno, A., R. J. W. Henry, and C. S. Roberts. 1966. Rotational excitation of H2 and D2 by H impact. proc. Phys. Soc. 88:611.

Davison, W. D. 1962. Rotational energy transfer in molecular collisions. Transitions in parahydrogen. Disc. Faraday Soc. 33:71.

Dillon, H. K. 1974. Atom-diatomic molecule collisions: a two-dimensional quantum mechanical treatment. Ph. D. Dissertation. Vanderbilt University. 117. pp.

Dillon, H. K., J. W. Wilson, and D. J. Wilson. 1984. Rotational transition probabilities in two dimensions. A strong-coupling approach. Jour. Tenn. Acad. Sci. 59:78.

Gordon, R. G., W. Klemperer, and J. I. Steinfeld. 1968. Vibrational and rotational relaxation. Ann. Rev. Phys. Chem. 19:215.

Herzberg, G. 1950. Molecular spectra and molecular structure. I. Spectra of diatomic molecules. D. Van Nostrand Co., New York.

Hirschfelder, J. O., C. F. Curtiss, and R. B. Bird. 1954. Molecular theory of gases and liquids. John Wiley and Sons, New York.

Kramer, K. H., and R. B. Bernstein. 1964. Sudden approximation applied to rotational excitation of molecules by atoms. I. J. Chem. Phys. 40:200.

Lawley, K. P., and J. Ross. 1965. Semiclassical theory of rotational excitation of a diatomic molecule by an atom. J. Chem. Phys. 43:2930.

Locker, D. J., and P. F. Endres. 1969. Semiclassical transition probabilities for collinear collisions between an atom and a Morse oscillator. J. Chem. Phys. 51:5482.

Locker, D. J., and D. J. Wilson. 1970. Exact semiclassical transition probabilities for collinear collisions. J. Chem. Phys. 52:271.

Pauling, L., and E. B. Wilson, Jr. 1935. Introduction to quantum mechanics. McGraw-Hill Book Co., New York. p. 294.

Raff, L. M. 1967. Theoretical investigation of translation-rotation energy transfer. II. J. Chem. Phys. 47:4789.

Ralston, A., and H. S. Wilf. 1960. Mathematical methods for digital computers. Vol. 1. John Wiley and Sons, New York. p. 115.

Rapp, D., and T. E. Sharp. 1963. Vibrational energy transfer in molecular collisions involving large transition probabilities. J. Chem. Phys. 38:2641.

Roberts, C. S. 1963. Inelastic scattering from a diatomic molecule: Rotational excitation. Phys. Rev. 131:209.

Takayanagi, K. 1963. Vibrational and rotational transitions in molecular collisions. Progr. Theoret. Phys. (Japan) Suppl. 25:1

Takayanagi, K., and S. Nishimura. 1960. Cooling of the interstellar clouds in region of neutral hydrogen. Publ. Astron. Soc. (Japan). 12:77.

Widom, B. and S. H. Bauer. 1953. Energy exchange in molecular collisions. J. Chem. Phys. 21:1670.

Zelechow, A., D. Rapp, and T. E. Sharp. 1968. Vibrational-vibrational-translational energy transfer between two diatomic molecules. J. Chem. Phys. 49:286.

Zener, C. 1931. Interchange of translational, rotational, and vibrational energy in molecular collisions. Phys. Rev. 37:556.

JOURNAL OF THE TENNESSEE ACADEMY OF SCIENCE
VOLUME 60, NUMBER 4, OCTOBER, 1985

OCCURRENCE OF THE COTTONMOUTH *(AGKISTRODON PISCIVORUS)* IN COFFEE COUNTY, TENNESSEE

RONALD R. BINGHAM
Central High School
Manchester, Tennessee 37355

ABSTRACT

On 12 and 15 May 1984, cottonmouths (*Agkistrodon piscivorus*) were collected in backwater sloughs of Morton's Lake in Manchester, Coffee County, Tennessee. Both snakes were females (975mm and 690mm SVL). Specimens were deposited in the Central High School Science Department Vertebrate Collection (CHS-RO15 and CHS-RO16). Identification followed Conant (1975) and Barbour (1971).

This find constitutes the first record of cottonmouths in Coffee County. This is approximately 165 km southeast of the Montgomery County record of Scott and Snyder (1968) and 265 km to the east of A. *piscivorus* found in Hardeman County by Norton and Harvey (1975). There is an additional previously unreported specimen in the Herpetological Collection at Tennessee Technological University which was also collected at Morton's Lake on 16 August 1981 (O. Ray Jordan, unpublished data). In Tennessee, the range of A. *piscivorus* has been limited to the western half of the state (Conant, 1975). Gentry (1956) indicated the same general distribution with the exception of two isolated reports in Anderson County and Campbell County in eastern Tennessee. The range reported by Conant (1975) indicates a possible existence of the species in this area.

It is widely believed cottonmouths of Morton's Lake were purposely introduced early this century to discourage poaching. This could not be confirmed. Local residents report cottonmouths to occur commonly in this part of the state and county. After examination of numerous specimens and talking with knowledgeable people, it is believed most reports are false. Most cottonmouths are usually found to be water snakes (*Nerodia* sp.)

ACKNOWLEDGEMENTS

I wish to thank Dr. George Murphy, Middle Tennessee State University, for his assistance in identification of the snakes.

LITERATURE CITED

Barbour, R. 1971. Amphibians and reptiles of Kentucky. Univ. Ky. Press, Lexingtron.

Conant, R. 1975. A field guide to reptiles and amphibians. Houghton Mifflin Co., Boston.

Gentry, G. 1956. An annotated check list of the reptiles and amphibians of Tennessee. J. Tenn. Acad. Sci. 31:242-251.

Norton, V. and M. Harvey. 1975. Herpetofauna of Hardeman County, Tennessee. J. Tenn. Acad. Sci. 50:131-136.

Scott, F. and D. Snyder. 1968. The amphibians and reptiles of Montgomery County, Tennessee. J. Tenn. Acad. Sci. 43:79-84.

SIXTH CENTRAL HARDWOOD CONFERENCE SCHEDULED AT UT

The sixth hardwood forest conference will be held at the University of Tennessee, Knoxville, Tennessee on February 24-26, 1987. the Conference will be sponsored by the UT Department of Forestry, Wildlife and Fisheries, Society of American Foresters, UT Department of Botany, and the Southern Forest Experiment Station. Papers pertaining to hardwood forests and forestry are invited. Abstracts should be submitted by March 1, 1986. All correspondence and inquiries should be addressed to:

Dr. Ronald Hay, Chairman
Sixth Central Hardwood Forest Conference
Department of Forestry, Wildlife and Fisheries
UT Box 1071
Knoxville, TN 37901