limit for the asymmetry parameter might be, and further experiments are planned.

Because of crystallographic disorder, one of the complexes studied, $[(Ph_3P)_2N][^2HW_2(CO)_{10}]$, has an unknown M–H–M geometry.[15] The solid-state deuterium NMR parameters are similar to those found for $[Ph_4P][^2HW_2(CO)_{10}]$ and suggest a similar structure. Some refinement of the structural prediction is possible with the aid of the modified point charge model. The most likely M–H–M angle is more obtuse than for $[Ph_4P][^2HW_2(CO)_{10}]$, possibly about 135°, based upon the asymmetry parameter of 0.201 (3).

Conclusions

Solid-state deuterium NMR powder patterns were acquired for six bridging metal hydrides to obtain structural information on the $M{-}^2H{-}M$ structure. The complexes studied have both eclipsed and bent staggered metal–carbonyl geometries. The observed deuterium powder patterns are a result of the deuterium quadrupole coupling constant, the asymmetry parameter, and, for sites with an eclipsed metal–carbonyl geometry, possible rapid four-site jump motion in the $M{-}^2H{-}M$ unit. The temperature dependence of the deuterium spectrum was examined for $[Et_4N][^2HCr_2(CO)_{10}]$ and $[Ph_4P][^2HCr_2(CO)_{10}]$ which have eclipsed and bent staggered metal–carbonyl geometries, respectively. The former shows little temperature dependence beyond a slight increase in the quadrupole coupling constant. Most importantly, the apparent axial symmetry of the eclipsed metal carbonyl structure was preserved to the lowest temperature studied, 140 K, but does not necessarily indicate rapid four-site jump motion. The latter complex shows a significant increase in the asymmetry parameter, possibly correlated with the same line-broadening mechanism noted in Raman and infrared spectroscopy of the bridging metal hydrides. The deuterium quadrupole coupling constants and asymmetry parameters were related to the M–H–M bond distance and the M–H–M bond angle with a point charge model and by assuming that the sign of the quadrupole coupling constant is positive.

This work shows that solid-state deuterium NMR spectroscopy has the potential to investigate structure in metal hydrides. In particular, μ_2-bridging hydrides on surfaces should have quadrupole coupling constants and asymmetry parameters similar to those found herein for metal dimers where the important factors are the $M{-}^2H$ bond length, the $M{-}^2H{-}M$ bond angle, the effective charge on the metal, and the mobility of the deuteron across a metal surface.[58] An extension of μ_3-bridging hydrides on surfaces is possible by a change in the model presented in eq 7; briefly, the asymmetry parameter should be zero and the z-axis of the electric field gradient aligned along the C_3 axis of the triply bridging site. Otherwise, the same factors should again determine the deuterium NMR parameters.

Acknowledgment. The support of the National Science Foundation (CHE-8715517) is gratefully acknowledged. The purchase of the Bruker MSL 200 NMR spectrometer was made possible by NSF Grant CHE-8711788. Leslie G. Butler is a Fellow of the Alfred P. Sloan Foundation (1989–1991). We gratefully acknowledge Prof. J. L. Petersen for an introductory sample of $[K(crypt\text{-}222)][^2HCr_2(CO)_{10}]$. Dr. C. E. Bronnimann and the Colorado State University Regional NMR Center, funded by National Science Foundation Grant CHE-8616437, are gratefully acknowledged for providing the ^1H CRAMPS results.

Supplementary Material Available: Listings of bond distances and angles for $[Ph_4P][^2HCr_2(CO)_{10}]$, coordinates of hydrogen atoms, least-squares planes for the two sets of $Cr{-}(C_{eq})_4$ units, and anisotropic thermal parameters (7 pages); listing of observed and calculated structure factors (30 pages). Ordering information is given on any current masthead page.

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(58) Kara, A.; DePristo, A. E. *J. Chem. Phys.* **1990**, *92*, 5653–60.

Evidence for Nucleophilic Addition by Muonium to Pyrazine in Water: Contrast with Ordinary Hydrogen

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Abstract: The presence of heterocyclic N atoms in an aromatic solute enhance its rate of reaction toward muonium, and the free radicals formed are seen to have muonium attached to a C atom of the ring. This contrasts the behavior of ^1H in water, where addition to N-heterocyclic rings occurs an order of magnitude slower and with H attaching to N, at least in acid solution. Muonium evidently shows nucleophilic character while ordinary hydrogen atoms are electrophilic. Pyrazine (1,4-diazine) was used for this comparison with benzene because it has the advantage over pyridine of forming only two possible radicals.

Introduction

When H atoms in acid solution react with nitrogen heterocyclic aromatic molecules like pyrazine, free radicals are formed by addition to the ring. These radicals have been identified by ESR to result from H attaching to an N atom of the ring,[1] and the rate of reaction was reduced relative to benzene.[2] Such results were taken as an indication of the electrophilic nature of H, because N has a higher electronegativity than C, and this agrees with Hammett ρ studies with substituted benzenes.[2,3]

In the case of hydrogen's light radioactive isotope muonium (Mu), with a short-lived positive muon as its nucleus, there is evidence that electron-withdrawing groups on benzene enhance the reaction rate—suggesting Mu is nucleophilic.[4] That con-

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(1) (a) Baron, B. L.; Fraenkel, G. F. *J. Chem. Phys.* **1964**, *41*, 1455. (b) Zeldes, H.; Livingston, R. *J. Phys. Chem.* **1972**, *76*, 3348.

(2) (a) Neta, P.; Schuler, R. H. *J. Am. Chem. Soc.* **1972**, *94*, 1056. (b) Neta, P. *Chem. Rev.* **1972**, *72*, 533.

(3) Pryor, W. A.; Lin, T. H.; Stanley, J. P.; Henderson, R. W. *J. Am. Chem. Soc.* **1973**, *95*, 6993.

0002-7863/91/1513-9096$02.50/0

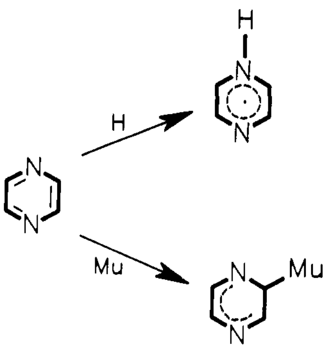

Figure 1. Structure of pyrazine (1,4-diazine) and its Mu and H reactions to give free radicals.

clusion was based on the overall rate of reaction and invoked the presumption that a similar ortho:meta:para product distribution would apply regardless of substitutent; but there is now evidence that Mu shows strong selectivity for the ortho position, at least with benzoic acid.[5]

In order to test further this intrinsic difference between ^1H and Mu we studied the effect of nitrogen atoms within an aromatic ring on the selectivity of Mu. Pyrazine, $C_4H_4N_2$, a *p*-diaza heterocyclic aromatic (see Figure 1), was chosen for this initial study because its symmetry should make it relatively simple to identify and measure the yields of radicals using muon level crossing resonance spectroscopy.

Experimental Section

Three types of muon spin polarization experiments were performed on aqueous solutions of pyrazine in order to determine (a) the reaction rate with muonium, (b) the precession frequencies of its muonated radicals, and (c) their yield and hyperfine coupling constants.

(a) Muon spin rotation (μSR) studies in low transverse magnetic fields (<10 G)[6] were used to determine the time dependence of free muonium atoms as a function of concentration of pyrazine (abbreviated to Pz) in aqueous solutions. The bimolecular rate constant k_M for the reaction is given by $k_M = (\lambda - \lambda_0)/[S]$, where λ is the exponential decay constant of Mu at solute concentration [S] and λ_0 that at zero solute concentration. λ is one of the fitted parameters from a μSR lifetime histogram.[6] Pz was used at concentrations of $\sim 10^{-4}$ M for maximum experimental accuracy.

(b) Muon spin rotation experiments in high transverse magnetic fields (2–5 kG) were then used to detect all muonated free radicals formed by the reaction of Mu with Pz, and thus to determine their muon–electron hyperfine coupling constants (A_μ).[7] This was done in aqueous solution at neutral pH to ensure Mu was the precursor. Due to the requirement for initial phase coherence in the precession of muon spins, the rate of formation of the radicals detected must be very high, so 1 M solutions of Pz were used to evaluate A_μ.

(c) Muon level crossing resonance spectroscopy (μLCR)[8] with very high longitudinal magnetic fields was used to determine the actual yields of each free radical formed, and to evaluate all their proton hyperfine coupling constants (hfs).

In addition, π-electron densities were calculated with a Hückel molecular orbital (HMO) computing program with ω charge iteration provided by Chong.[9]

Pyrazine was of best Reagent grade quality manufactured by Aldrich and was used without further purification. The solutions were made from triply distilled water and deoxygenated by bubbling with pure N_2 prior to being exposed to high energy muon beams for measurement at $\sim$295 K. All μSR and μLCR experiments were carried out at the TRIUMF cyclotron using the M20 channel—with "surface" muons for μLCR, spin-rotated for A_μ, and "backward" muons for low-field μSR. The experimental details were similar to those described previously.[4,10,11]

Table I. Comparison of Rate Constants for the Reactions of Mu and H with Pyrazine and Benzene: Overall and Partial Kinetic Isotope Effects (k_M/k_H)

rate constants/10^9 M^{-1} s^{-1}	pyrazine	benzene	pyrazine/ benzene
overall k_M obsed	7.7 (±0.5)	3.3[a]	2.3
overall k_H obsed	0.33[b]	1.1[c]	0.3
overall ratio, k_M/k_H	23	3.0	7.7
k_M/k_H for reaction at C atoms	>70[d]	3.0	>20
k_M/k_H for reaction at N atoms	<6[e]		

[a] From ref 4. [b] From ref 2. [c] From ref 12. [d] Assumes less than ~30% of the observed k_H reaction occurred at C atoms. [e] Assumes less than ~25% of our observed k_M corresponds to reaction at N atoms of Pz.

Table II. Parameters Obtained from the FFT Analysis of High-Field μSR Spectra of 1 M Pyrazine in Water

field/kG	ν_D/MHz	ν_{12}/MHz	ν_{34}/MHz	A_μ/MHz
2.076	28.13	200.5	276.6	477.1
4.786	64.84	169.5	307.0	476.5

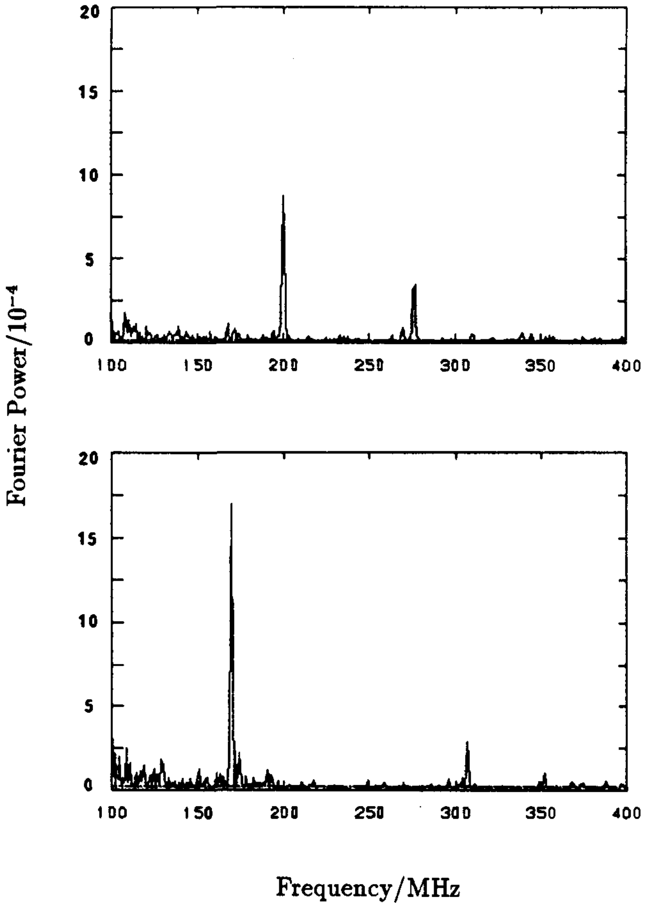

Figure 2. The FFT of the μSR spectra of 1 M pyrazine in water, presented as Fourier power against frequency: (a) at about 2 kG; (b) at about 4.8 kG.

Results

1. Rate Constant. μSR measurements at 8 G for the reaction of Mu with Pz in neutral water at concentrations of 0.10 and 0.20

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(4) Stadlbauer, J. M.; Ng, B. W.; Ganti, R.; Walker, D. C. *J. Am. Chem. Soc.* **1984**, *106*, 3151.

(5) Stadlbauer, J. M.; Barnabas, M. V.; Wu, Z.; Walker, D. C. *Hyperfine Interact.* **1990**, *65*, 939.

(6) (a), Brewer, J. H.; Crowe, K. M. *Annu. Rev. Nucl. Part. Sci.* **1978**, *28*, 239. (b) Fleming, D. G.; Garner, D. M.; Vaz, L. C.; Walker, D. C.; Brewer, J. H.; Crowe, K. M. *Adv. Chem. Ser., ACS* **1979**, *175*, 279.

(7) (a) Roduner, E.; Percival, P. W.; Fleming, D. G.; Hochmann, J.; Fischer, H. *Chem. Phys. Let.* **1978**, *57*, 37. (b) Roduner, E.; Fischer, H. *Chem. Phys.* **1981**, *54*, 261.

(8) (a) Kiefl, R. F.; Kreitzman, S. R.; Celio, M.; Keitel, R.; Brewer, J. H.; Luke, G. M.; Noakes, D. R.; Percival, P. W.; Matsuzaki, T.; Nishiyama, K. *Phys. Rev. A* **1986**, *34*, 681. (b) Kiefl, R. F. *Hyperfine Interact.* **1986**, *32*, 707.

(9) Chong, D. P., private communication.

(10) Venkateswaran, K.; Barnabas, M. V.; Kiefl, R. F.; Stadlbauer, J. M.; Walker, D. C. *J. Phys. Chem.* **1989**, *93*, 388.

(11) Venkateswaran, K.; Barnabas, M. V.; Wu, Z.; Stadlbauer, J. M.; Ng, B. W.; Walker, D. C. *Chem. Phys.* **1989**, *137*, 239.

Table III. μLCR Positions (B_R), Line Widths (ΔB), Amplitudes (ampl), and Calculated Fractional Yields (P_R) for 20 mM Pyrazine in Water

B_R/kG	ΔB_{obs}/kG	ampl/%	P_R
19.545	0.1214	0.676	0.24 ± 0.03
26.646	0.033	0.16	0.23 ± 0.05
27.628	0.050	0.25	0.24 ± 0.05

mM gave the bimolecular rate constant (k_M) as 7.6 (±0.5) × 10^9 M^{-1} s^{-1}. This value is compared in Table I with published data on the Mu reaction with benzene[4] and the analogous rate constants for H reactions (k_H).[2,12]

2. Muon-Electron Hyperfine Coupling Constant. Figure 2 shows the fast Fourier transform (FFT) power spectra recorded for reaction of Mu with 1 M Pz in water at transverse magnetic fields of 2 and 4.8 kG. There is only one pair of peaks (ν_{12} and ν_{43}) at each field and they are seen to separate with increasing field as in eq 1, where ν_D is the diamagnetic muon precession

$$\nu_{12} = 0.5A_\mu - \nu_D \qquad \nu_{43} = -0.5A_\mu - \nu_D \tag{1}$$

frequency and proportional to field[7]—so only one type of radical is observed for the reaction. Its computer-determined FFT peak frequencies are recorded in Table II. These produce a muon hyperfine coupling constant of A_μ = 476.8 ± 0.3 MHz for the radical from $A_\mu = |\nu_{12}| + |\nu_{43}|$.

3. Radical Yield. The μLCR technique was used to search for the radical's resonance field (B_R) when Mu reacted with 20 mM Pz in aqueous solution at neutral pH. A strong resonance signal at 19 545 G was found and two weaker signals appeared at higher fields (26 646 and 27 628 G). These spectra are presented in Figure 3, and Table III lists their three computer-fitted μLCR parameters, B_R, ampl (amplitude), and ΔB (line width).

The yield of a free radical, P_R, given as the fraction of incident muons observed in that state, was evaluated using eq 2,[10] where

$$P_R = \text{ampl}(\Delta B)^2(\gamma_\mu - \gamma_p)^2/A_{bf}\nu_r^2 \tag{2}$$

γ_μ and γ_p are magnetogyric ratios for muon and proton respectively, A_{bf} is the experimental backward to forward asymmetry determined with neat benzene, and ν_r is the μLCR transition frequency (equal to $A_\mu A_H/2B_R\gamma_e$, where A_H is the resonant H atom coupling constant and γ_e the magnetogyric ratio of the electron). The yield obtained for the intense peak at 19.5 kG was P_R = 0.24, with an estimated overall error ±15%.

4. π-Electron-Density Distributions. The ω-HMO method gave π-electron densities at the two N and four C sites of Pz as 1.084 and 0.958, respectively, relative to 1.000 on the C atoms of benzene.

Discussion

The comparison given in Table I shows that the presence of p-N heteroatoms in an aromatic ring enhances the rate of reaction of Mu by a factor of ~2.3 (3.5 per C atom). This increase coincides with the N atoms reducing the electron density on C from 1.000 in benzene to 0.958 in pyrazine, as shown by the results of HMO calculations (MNDO results are similar).[9] Furthermore, adducts involving N-Mu are shown to be unimportant by the failure to observe appropriate μSR-FFT or μLCR spectra and by the fact that the yield of C-centered radicals equals most of the full Mu yield expected. These data therefore show Mu to be nucleophilic in character.

This 3.5-fold increase in rate greatly exceeds that seen for ^{1}H, where the overall rate actually decreased 3-fold for pyrazine relative to benzene[2]—though the rate per active site (unprotonated ring N atoms)[13] showed no significant change. For both isotopes the reactions involved are "addition" reactions, because strong signals of free radical products are found. In the case of H atoms in acid solution there is ESR proof that the principal radical formed is that arising from addition to a N atom of the ring,[1] as in Figure 1. For Mu, however, attachment occurs at C.

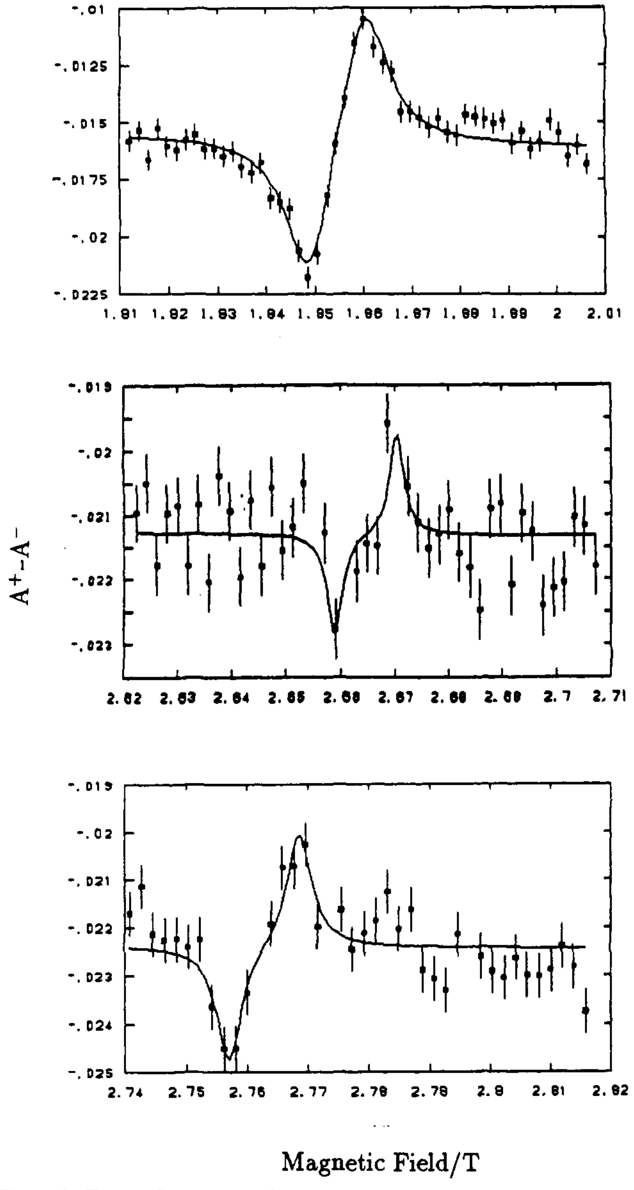

Figure 3. The μLCR spectra of 20 mM pyrazine in water: shown as the normalized forward-to-backward asymmetry difference (A^+, with a small modulation field applied with the main magnetic field, A^-, with it opposed) as a function of longitudinal magnetic field (in Tesla, 10^4 G). (The top spectrum is due to the proton attached to the same C as Mu; the middle spectrum is due to the proton ortho to Mu; and the bottom spectrum due to the para proton).

Our reasons for drawing this latter conclusion are based on the hyperfine parameters and yields of the muonated free radicals formed:

(i) First, the very high muon hyperfine coupling constant, A_μ = 476.8 MHz, is characteristic of muonium addition to C in aromatic rings. Muonated cyclohexadienyl radicals themselves have A_μ values of 514.6 MHz, and with NH_2, OH, CN, COOH, etc. groups at ortho, meta, or para positions relative to Mu, the A_μ values all lie in the range 460–520 MHz.[14] These differ from corresponding H adducts (A_p) by the ratio of nuclear moments (3.18-fold favoring μ) and by a factor of ~1.25, which is a typical isotope effect (of the first kind) arising from the higher vibrational zero point motion of Mu relative to H.[7,14,15] Our value of 476.8

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[12] Sauer, M. C., Jr.; Ward, B. *J. Phys. Chem.* **1967**, *71*, 3971.

[13] The H atom kinetic data were obtained at pH ~ 1,[2] where some 30% of the Pz molecules will be monoprotonated Pz since its pK_a is 0.65. On the basis of the assumption that protonated N atoms react much more slowly with Mu we take k_H per active site (unprotonated N) to be about 0.20 × 10^9 M^{-1} s^{-1}.

[14] Roduner, E.; *The Positive Muon as A Probe of Free Radical Chemistry*; Springer: Berlin, 1988.

Table IV. Proton Hyperfine Coupling Constants for the Various H Atoms (A_H) in the $C_4H_4N_2Mu^\bullet$ Radical, As Assigned Here[a]

	A_H/MHz	
site of the H	$C_4H_4N_2Mu^\bullet$	$C_6H_6Mu^{\bullet b}$
H on same C as Mu	111.5	126.1
H on C ortho to Mu	−20.0	−25.1
H on C meta to Mu		+7.5
H on C para to Mu	−38.2	−36.2

[a] Assignment based on the published data for analogous H atom positions in the cyclohexadienyl radical ($C_6H_6Mu^\bullet$) as shown in the table. [b] Data published in ref 19.

MHz for Pz thus falls in the very range one would anticipate for an aromatic radical with Mu attached to C and out of plane. The fields of the LCR spectra, being in the 20 kG region, also show that A_μ must be in the 400–500 MHz range for the only radical observed.

This high A_μ is in sharp contrast to the proton hyperfine coupling constants of planar heterocyclic free radicals with H adding to N. These are typically only 15–25 MHz, as found by ESR in acidified pyrazine[1] and in picolines and pyridines.[16] If our 476.8 MHz coupling constant were to be attributed to >N–Mu, we would have to try to explain an unreasonably large isotope effect of ~7 (rather than the usual ~1.3). Furthermore, for neat aliphatic compounds containing –N=N– groups, where only N-bonded Mu atoms were possible, the Mu radicals observed by μSR had A_μ values of only 21–35 MHz.[17] Consequently we conclude that in Pz Mu attaches to C.

(ii) Confirmation of this comes from the μLCR data through the internal consistency of its assignments and yields, as follows. When the parameters of the three peaks of Figure 3 are each analyzed according to eq 2 using A_μ = 476.8 MHz (and the A_H values assigned later), the values of P_R given in the last column of Table III were obtained. The fact that each peak has the same yield very strongly suggests that all three correspond to different proton resonances of the *same* radical. Furthermore, this one radical is the *major* reaction product because its fractional yield of 0.24 accounts for a large fraction of available Mu atoms. Specifically, with $k_M = 7.6 \times 10^9\ M^{-1}\ s^{-1}$ (some 3-fold less than the diffusion controlled limit[15]), 20 mM Pz allows Mu in water a mean lifetime of ~7 ns—by which time a significant "missing fraction" (~0.07) has occurred from the initial Mu yield of 0.38, due to nonhomogeneous track effects.[18] The addition reaction observed thus arises from a fractional yield of 0.24 of the ~0.31 scavengable muonium atoms available (i.e. ~78%).

Assignment of these three LCR peaks to specific protons utilizes eq 3, where n stands for "another" nucleus (^1H or ^{14}N here), A_n

$$B_R = 0.5[(A_\mu - A_n)/(\gamma_\mu - \gamma_n) - (A_\mu^2 - 2MA_n^2)/\gamma_e(A_\mu - A_n)] \quad (3)$$

is its hfs, γ_n is its magnetogyric ratio, and M is the total spin quantum number of the resonant state.[8] The second term is quite small due to the large value of γ_e, so eq 3 can be approximated for ^1H to $B_R = (476.8 - A_H)/18.58$ in kG with A_H in MHz. Consequently, we have A_H values of +111.5, −20.0, and −38.2 MHz for the μLCRs of three of the H atoms of this radical. They are assigned, as in Table IV, from their closeness to the A_H values of the H atoms in muonated cyclohexadienyl radicals.[19] (We presume that the weak couplings expected with ^1H meta to Mu, and both ^{14}N nuclei, are not observable above the experimental μLCR noise level in our dilute aqueous solutions of Pz.)

The strongest and lowest field peak at 19.5 kG is thus attributed to the H attached to the same C as Mu (the only H_β, see Figure 1) with A_H = 111.5 MHz. We can now calculate an isotope effect *of the second kind*[20] to be 476.8/(111.5 × 3.18) = 1.34. A very similar isotope effect for Mu compared to H, on the same C of a given radical, was found for the meta-muonated free radical of benzoic acid.[5]

Summary and Conclusion

Mu and ^1H are excellent comparative isotopes, with only slightly different (0.4%) Bohr radii and ionization energies, but with Mu having much greater zero point vibrational motion due to its 9-fold smaller mass. Here we have seen a further difference: Mu preferring to react at the points of lower electron density (C) while ^1H reacts at the higher (N). In absolute terms there is not a large difference because both ^1H and Mu have apparent Hammett ρ parameters close to zero (approximately −0.4 for $^1H^{2,3}$ and +0.5 for Mu[4]); but they are on opposite sides of zero, so it is a difference *in kind*.

There are also considerable kinetic isotope effects emerging from these contrary electrophilicities. As seen in Table I, the k_M/k_H ratio is 23 for pyrazine, in contrast to only 3 for benzene, based on overall observed reaction rates. When one takes account of the fact that Mu and H are seen to react at different points on the Pz molecule, then this kinetic isotope effect of 23 increases to >70 for reaction at the C atoms of Pz and falls to <6 for reaction at its N atoms.[21]

Acknowledgment. We are particularly grateful to Prof. D. P. Chong for initiating the HMO calculations on this molecule and for his help. We appreciate, as ever, the continued assistance of Curtis Ballard and Keith Hoyle with the experiments. JMS wishes to thank the Hood College Board of Associates for financial assistance. NSERC of Canada is thanked for providing most of the funding required for this research.

Registry No. $C_4H_4N_2$, 290-37-9; C_4H_4-μ-$N_2^\bullet$, 136675-72-4; Mu, 12587-65-4.

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(15) Walker, D. C. *Muon and Muonium Chemistry*; Cambridge University Press: Cambridge, UK, 1983.

(16) (a) Rakowsky, Th.; Dohrmann, J. K. *Ber. Bunsenges. Phys. Chem.* **1975**, *79*, 18. (b) Dohrmann, J. K.; Kieslich, W. *J. Magn. Reson.* **1978**, *31*, 69. (c) Dohrmann, J. K.; Kieslich, W. *J. Magn. Reson.* **1978**, *32*, 353.

(17) Louwrier, P. W. F.; Brinkman, G. A.; Bakker, C. N. M.; Roduner, E. *Hyperfine Interact.* **1986**, *32*, 753.

(18) Venkateswaran, K.; Barnabas, M. V.; Wu, Z.; Walker, D. C. *Can. J. Phys.* **1990**, *68*, 957.

(19) Percival, P. W.; Kiefl, R. F.; Kreitzmann, S. R.; Garner, D. M.; Cox, S. F. J.; Luke, G. M.; Brewer, J. H.; Nishiyama, K.; Venkateswaran, K. *Chem. Phys. Lett.* **1987**, *133*, 465.

(20) Isotope effects of the first kind are ratios of A_μ/A_p where A_p is the hfs for the same radical with H replacing Mu, as in (i) in the text; but isotope effects of the second kind are A_μ/A_H, where A_H is the hfs of H attached to the same C as Mu.[5]

(21) As in the footnote to Table I, these values are merely lower and upper limits based on the assumption that the dominant addition was at least 70–75% dominant. In practice the other reaction path was simply not observed for Mu or H. A search for μLCR bands from 0 to 5 kG, where N–Mu would be expected, showed nothing observable.