Table II. ^{13}C Enrichment of Antibiotic Carbons by Precursors

			enrichment[a]							
car-bon	δ[b,c]		sodium [1-^{13}C]-acetate		sodium [2-^{13}C]-acetate		sodium [1-^{13}C]-propionate		L-[*methyl*-^{13}C]-methionine	
	1	**2**	1	**2**	**1**	**2**	**1**	**2**	**1**	**2**
1	173.5	172.7		3.6	1.3	0.8				
2	85.6	83.4	0.7	1.1	2.7	3.8	1.0	1.2	1.1	2.0
3	35.7	34.3	3.7	4.2	0.7	1.1	0.9	1.1	0.6	1.8
4	43.5	43.0	0.9	1.0	2.2	3.4	0.9	0.7	1.4	1.6
5	133.3	132.8	3.7	4.4	1.4	0.9	1.5	1.1	0.7	1.4
6	129.1	127.5	1.0	1.2	3.9	3.4	1.5	1.5	1.0	1.8
7	39.0	39.0	4.0	4.8	1.0	1.1	1.2	1.4	1.1	1.7
8	83.4	81.2	0.7	1.2	3.4	3.4	0.9	1.1	0.9	2.4
9	72.7	73.7	6.0	8.7	0.7	1.1	9.7	17.4	0.9	2.3
10	36.3	34.8	0.8	1.2	0.7	1.0	1.2	1.6	0.9	2.2
11	75.6	76.0	2.9	4.5	0.6	1.1	1.2	2.0	1.0	1.7
12	50.4	49.1	0.8	0.6	2.2	3.3	1.0	1.0	0.7	1.2
13	89.4	89.1	6.3	6.1	1.1	0.6	7.3	8.0		
14	136.1	134.3			0.7	0.8				
15	131.3	131.3	5.6	6.9	0.8	0.7	8.8	11.4	0.8	1.5
16	33.5	32.7	0.8	1.0	1.4	1.1	1.0	1.1	1.0	1.9
17	79.1	79.0	5.9	6.6	1.3	0.8	9.4	11.2	0.7	2.0
18	66.0	66.4	0.7	1.1	0.7	1.1	0.9	1.3	1.2	1.7
19	21.7	20.6	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
20	13.6	12.9	0.7	0.9	1.0	1.0	0.8		0.6	1.5
21	17.5	17.0	0.4	0.8	0.6	0.9	0.5	0.9	0.7	1.2
22	16.0	15.5	0.7	0.8	0.9	1.0	0.7	1.0	1.1	1.3
23	57.5	57.7	1.0	1.0	0.6	0.7	1.3	0.9	27.2	21.4

[a] Peak height times natural abundance, based on peak height of 1.0 for C-19 as an internal standard. [b] Parts per million from Me_4Si; nodusmicin spectra taken in acetone, nargenicin spectra taken in $CDCl_3$. [c] Resonances of the pyrrole carbonyl group have been omitted for nargenicin. No enrichment of these carbons was observed.

level of incorporation of succinate than acetate (Table I). From the ^{14}C incorporation data it appears that most of the acetate incorporated is first processed through the TCA cycle, rather than being directly incorporated as malonyl-CoA. However, the extent to which acetate was converted into propionate varied considerably in four experiments employing different soil stocks. For example, in the experiment with [2-^{13}C]acetate in Tables I and II very little labeling of propionate by acetate was observed.

^{13}C NMR spectra were obtained on a Varian XL 200 spectrometer using a 5-mm probe with identical operating parameters for each set of antibiotics. Samples were diluted with unenriched nargenicin or nodusmicin, as desired.

Radiolabel Determination. Samples of the two antibiotics were first dissolved in methanol to a final concentration of 1 mg/mL and each methanolic solution (1.0 mL) was diluted with 15 mL of Aquasol II (New England Nuclear). Disintegrations per minute (corrected for background) were determined on a Tracor Analytic BetaTrac, Model 6895, liquid scintillation counter.

Simultaneous Production of 1, 3, and 4: A seed medium [TY medium, consisting of Tryptone (Difco), 0.5%; yeast extract (Gibco), 0.3%; and tap water, 100 mL in a 500-mL Erlenmeyer flask] was inoculated from a dried soil stock of *Nocardia argentinensis* Huang (ATCC 31306) and incubated at 30 °C on a rotary shaker at 250 rpm. After 72 h, 5-mL aliquots were removed and inoculated into 100-mL portions of the production medium [glucose, 2.2%; Peptone (Difco), 0.5%; beef extract, 0.5%; yeast extract, 0.5%; N-Z amine type B (Sheffield), 0.3%; NaCl, 0.5%, with tap water] in 500-mL flasks. The medium was incubated for 120 h then filtered through glass wool. The clarified broth was extracted with two half-volumes of ethyl acetate and the combined organic layers were taken to dryness. After trituration with hexane, the remaining solids were dissolved in chloroform and separated on silica gel with a gradient of chloroform–methanol. Fractions were combined on the basis of TLC (Merck silica gel 60, $CHCl_3$:MeOH, 9:1, visualized by spraying with EtOH:H_2SO_4:*p*-anisaldehyde, 90:5:5, followed by warming).[17] The respective R_f values for **1**, **2**, **3**, and **4** in this system are 0.44, 0.62, 0.66, and 0.87.

Production of nodusmicin and nargenicin was achieved by the same procedure as in the preceding paragraph except for the production medium (soluble starch, 2%; corn steep liquor, 2%; corn meal, 2%; $CaCO_3$, 0.3%, 100 mL in 500-mL flasks). After a 12-h incubation (30 °C, 250 rpm), precursors were added, and fermentation was continued for 132 h. The antibiotics were isolated from the filtered broth by extracting twice with quarter-volumes of ethyl acetate followed by evaporating the combined organic phases. After hexane trituration of the resulting syrups, the remaining chloroform-soluble materials were processed over Brinkmann silica gel ($CHCl_3$:MeOH 98.5:1.5 for nargenicin and $CHCl_3$:MeOH 97:3 for nodusmicin). Fractions were pooled on the basis of TLC. Yields of pure nargenicin ranged from 20 to 40 μg per mL of fermentation medium and of pure nodusmicin from 10 to 20 μg per mL.

Acknowledgment. This work was supported in part by a grant (AI 01278) from the National Institute of Allergy and Infectious Diseases. We thank A. Dietz and Drs. J. E. Grady and H. A. Whaley, The Upjohn Co., Kalamazoo, MI, for their advice and assistance throughout this project.

Registry No. 1, 76265-48-0; **2**, 70695-02-2; **3**, 88343-90-2; **4**, 74686-27-4; propionic acid, 79-09-4; methionine, 63-68-3; acetic acid, 64-19-7; malonic acid, 141-82-2; succinic acid, 110-15-6; glutaric acid, 56-86-0; proline, 147-85-3.

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(17) This reagent, a modification of that used by Calton et al. (Calton, G. J.; Ranieri, R. L.; Espenshade, M. A. *J. Antibiot.* **1978**, *31*, 38–42), was quite useful in that all compounds containing the pyrrole carbonyl unit developed as bright yellow spots while those lacking the unit became bright pink.

(18) Cane, D. E.; Yang, C.-C. *J. Am. Chem. Soc.*, preceding paper in this issue.

A Novel Cubane-Type Mo_4S_4 Cluster

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The cubane-type Fe_4S_4[1] and $MoFe_3S_4$[2] clusters have been attracting much interest as the synthetic analogues of the active site in the ferredoxine[3] and FeMo protein of the nitrogenases.[4]

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(1) (a) Averil, B. A.; Herskovitz, T.; Holm, R. H.; Ibers, J. A. *J. Am. Chem. Soc.* **1973**, *95*, 3523. (b) Que, L.; Bobrik, M. A; Ibers, J. A.; Holm, R. H. *Ibid.* **1974**, *96*, 4168. (c) Bobric, M. A.; Hodgson, K. O.; Holm, R. H. *Inorg. Chem.* **1977**, *16*, 1851. (d) Carrel, H. L.; Gluster, J. P.; Job, R.; Bruice, T. C. *J. Am. Chem. Soc.* **1979**, *99*, 3683. (e) Laskowski, E. J.; Frankel, R. B.; Gillum, W. O.; Papaefthymiou, G. C.; Renaud, J.; Ibers, J. A.; Holm, R. H. *Ibid.* **1978**, *100*, 5322. (f) Kanatzidis, M. G.; Ryan, M.; Coucouvanis, D.; Simopoulus, A.; Kostikas, A. *Inorg. Chem.* **1983**, *22*, 179. (g) Stephan, D. W.; Papaefthymiou, G. C.; Frankel, R. B.; Holm, R. H. *Ibid.* **1983**, *22*, 1550.

(2) (a) Palermo, R. E.; Holm, R. H. *J. Am. Chem. Soc.* **1983**, *105*, 4310. (b) Wolff, T. E.; Berg, J. M.; Hodgson, K. O.; Frankel, R. B.; Holm, R. H. *Ibid.* **1979**, *101*, 4140. (c) Mascharak, P. K.; Armstrong, W. H.; Mizobe, Y.; Holm, R. H. *Ibid.* **1983**, *105*, 475. (d) Christou, G.; Mascharak, P. K.; Armstrong, W. H.; Papaefthymiou, G. C.; Frankel, R. B.; Holm, R. H. *Ibid.* **1982**, *104*, 2820. (e) Christou, G.; Garner, C. D.; Mabbs, F. E.; King, T. J. *J. Chem. Soc., Chem. Commun.* **1978**, 740. (f) Christou, G.; Garner, C. D.; Mabbs, F. E.; Drew, M. G. B. *Ibid.* **1979**, 91. (g) Acott, S. R.; Christou, G.; Garner, C. D.; King, T. J.; Mabbs, F. E.; Miller, R. M. *Inorg. Chim. Acta* **1979**, *35*, L337. (h) Armstrong, W. H.; Mascharak, P. K.; Holm, R. H. *Inorg. Chem.* **1982**, *21*, 1669; (i) *J. Am. Chem. Soc.* **1982**, *104*, 4373.

(3) Holm, R. H. *Endeavor* **1975**, *34*, 38.

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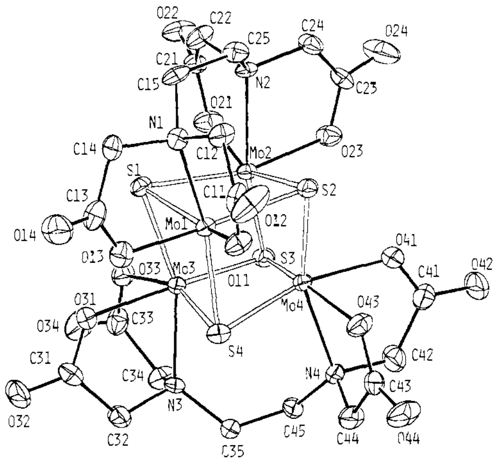

Figure 1. Perspective view of $[Mo_4S_4(edta)_2]^{3-}$. Bond distances (Å): Mol-Mo2, 2.775 (2); Mol-Mo3, 2.794 (2); Mol-Mo4, 2.880 (2); Mo2-Mo3, 2.845 (2); Mo2-Mo4, 2.755 (2); Mo3-Mo4, 2.796 (2); Mol-S1, 2.352 (3); Mol-S2, 2.364 (4); Mol-S4, 2.355 (3); Mol-O11, 2.139 (8); Mol-O13, 2.151 (10); Mol-N1, 2.284 (11); Mo2-S1, 2.369 (4); Mo2-S2, 2.363 (3); Mo2-S3, 2.351 (3); Mo2-O21, 2.145 (8); Mo2-O23, 2.129 (10); Mo2-N2, 2.283 (11); Mo3-S1, 2.351 (3); Mo3-S3, 2.357 (4); Mo3-S4, 2.353 (3); Mo3-O31, 2.131 (11); Mo3-O33, 2.153 (9); Mo3-N3, 2.290 (11); Mo4-S2, 2.351 (4); Mo4-S3, 2.355 (3); Mo4-S4, 2.358 (4); Mo4-O41, 2.143 (11); Mo4-O43, 2.136 (9); Mo4-N4, 2.300 (11).

We have recently prepared a novel mixed-valence molybdenum complex, $[Mo_4S_4(edta)_2]^{3-}$ (edta, ethylenediaminetetraacetate^{4-}), which contains a cubane-type $Mo_4S_4^{5+}$ core, and report here its structure and properties.

Recently Müller and co-workers[5] reported the synthesis and characterization of $K_8[Mo_4S_4(CN)_{12}]\cdot 4H_2O$, although no detail of the preparation was described in their paper. The complex comprises a $Mo_4S_4^{4+}$ core and is diamagnetic, all the Mo's being in tervalent oxidation state. In contrast with the Müller's complex, the present $[Mo_4S_4(edta)_2]^{3-}$ has one unpaired electron and is a $Mo_3^{III}Mo^{IV}$ mixed-valence complex. The Mo_4S_4 cluster[6] is situated at one extreme of the $Mo_nFe_{4-n}S_4$ cluster series. A complete investigation of the Mo_4S_4 core will serve for developing the chemistry of inorganic metal–sulfur cluster and furthermore for disclosing the role of Mo ion in the mixed-metal clusters.

A solution of $Na_2[Mo_2O_2S_2(edta)]\cdot 2H_2O$[7] (2 g) in 0.03 M HCl (200 mL) was poured upon $NaBH_4$ (1 g) under a dinitrogen atmosphere to give a brown solution. Then this solution was subjected to air oxidation; the color of the solution turned gradually to dark green. The purification of the green solution was effected by Sephadex G-10 column chromatography by elution with water. Addition of acetone to the eluate gave dark green crystals of sodium salt; these were dissolved in water and, from the solution, recrystallized in the form of calcium salt by the addition of solid $CaCl_2$. The crystals were analyzed to be $Ca_3[Mo_4S_4(edta)_2]_2\cdot 26H_2O$[8] (**1**). Ammonium salt of the anion has also been isolated in the similar way.

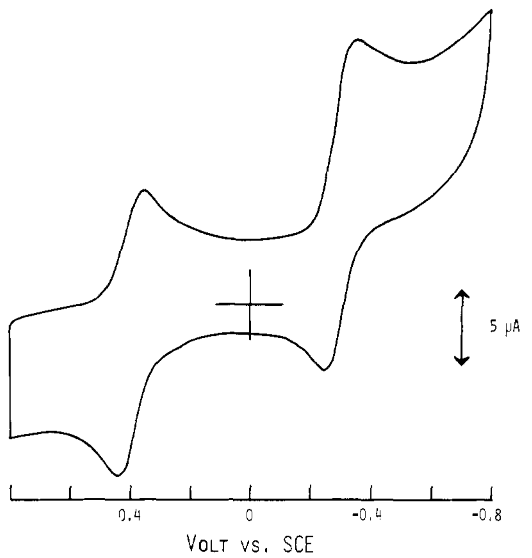

Figure 2. Cyclic voltammogram of $[Mo_4S_4(edta)_2]^{3-}$ (0.8 mM) in 0.1 M $HClO_4$ at a glassy carbon electrode; scan rate, 100 mV/s; reference electrode, SCE; temperature, 25 °C.

The crystal of **1** used for X-ray measurement was sealed in a thin-walled glass capirally to prevent dehydration. Crystal data: monoclinic system, space group $P2_1/c$, $a = 15.726$ (8) Å, $b = 12.447$ (4) Å, $c = 28.10$ (2) Å, $\beta = 123.16$ (3)°, $Z = 4$ (for $Ca_{1.5}[Mo_4S_4(edta)_2]\cdot 13H_2O$), $D_c = 2.00$, $D_m = 2.00$ g cm^{-3}, μ(Mo Kα) = 14.8 cm^{-1}. Intensity data were collected on an automated four-circle diffractometer by use of graphite-monochromated Mo Kα radiation in the $2\theta_{max} \leq 46.0°$ range. The coordinates of Mo and S atoms were determined by means of MULTAN, and the remaining non-hydrogen atoms were located from difference maps. The current R value is 0.059 for 5658 reflections ($F_o^2 \geq 3\sigma(F_o^2)$).

Figure 1 shows the structure of $[Mo_4S_4(edta)_2]^{3-}$ (**2**), which has an approximate symmetry of S_4. The $Mo_4S_4^{5+}$ core is cubane typed, and the edta^{4-} spans two Mo atoms at Mo_2S_2 face. Every Mo atom has a distorted octahedral coordination by three S, two O, and N atoms, the three S atoms being in a facial disposition. The four Mo atoms have an approximately regular-tetrahedral configuration. Important bond distances are given in the caption to Figure 1. The Mo–Mo–Mo, N–Mo–O, and O–Mo–O angles lie in the 58.29–62.76 (4)°, 75.7–77.6 (4)°, and 76.8–79.7 (4)° ranges, respectively. The Mo–Mo distances are not much different from those (2.855, 2.853 Å) in $[Mo_4S_4(CN)_{12}]^{8-}$.[5] The Mo–S distances are comparable to the corresponding one in $[MoFe_3S_4Cl_3(al_2cat)(THF)]^{2-}$[2a] and $[Mo_2Fe_6S_8(SEt)_9]^{3-}$[2b] but slightly shorter than those in $[Mo_4S_4(CN)_{12}]^{8-}$,[5] $[MoFe_3S_4(S\text{-}p\text{-}C_6H_4Cl)_4(al_2cat)]^{3-}$,[2c] and $[Mo_2Fe_6S_8(SPh)_9]^{5-}$,[2d] a 3+ oxidation state being assigned to Mo in the double-cubane cluster cited for the reference.[2d] The mean S–Mo–S angle (104.5°) in the $Mo_4S_4^{5+}$ core is slightly larger than those in the $MoFe_3S_4$ core.[2a–d]

Formally, the four Mo's in the $Mo_4S_4^{5+}$ core are in the oxidation state of $Mo_3^{III}Mo^{IV}$. The way of bonding is, however, indistinguishable between the four Mo atoms, as far as the corresponding bond lengths are compared, and this is indicative of the absence of any valence trapping. As a matter of fact, the volumes of coordination octahedra around respective Mo's are, in the order of Mo1–Mo4, 14.92 (6), 14.86 (6), 14.88 (6), and 14.93 (6) Å^3, which might be regarded as identical in view of the estimated standard deviations. Thus every Mo has, in the first approximation, an average oxidation state of +3.25, and the present mixed-valence complex should be classified as belonging to class III.[9]

The room-temperature magnetic moment per Mo_4 is 2.0 μ_B, indicating the presence of one unpaired electron. However, no ESR signal was observed on the powder sample even at 150 K.

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(4) For example: Antonio, M. R.; Teo, B. K.; Cleland, W. E.; Averill, B. A. *J. Am. Chem. Soc.* **1983**, *105*, 3477.

(5) Müller, A.; Eltzner, W.; Bogge, H.; Jostes, R. *Angew. Chem., Int. Ed. Engl.* **1982**, *21*, 795.

(6) The first Mo_4S_4 cluster was reported in the study of $[Mo^V(N\text{-tol})(\mu\text{-}S)(S_2P(OEt)_2)]_4$ by Wentworth and co-workers. This tetranuclear complex is, however, considered to be composed of two $[Mo(N\text{-tol})(\mu\text{-}S)(S_2P(OEt)_2)]_2$ dimers that interact with each other in such a way that the μ-S ligands in one dimer are linked weakly to the Mo atoms in the other. Indeed the tetramer readily dissociates into the dimers in polar solvents. In contrast to their complex, the present $[Mo_4S_4(edta)_2]^{3-}$ is stable even in water. (a) Edelblut, A. W.; Wentworth, R. A. D. *Inorg. Chem.* **1980**, *19*, 1110. (b) Edelblut, A. W.; Folting, K.; Huffman, J. C.; Wentworth, R. A. D. *J. Am. Chem. Soc.* **1981**, *103*, 1927. (c) Wall, K. L.; Folting, K.; Huffman, J. C.; Wentworth, R. A. D. *Inorg. Chem.* **1983**, *22*, 2366.

(7) Otto, V. R.; Swieter, D. S.; Schultz, F. A. *Inorg. Chem.* **1977**, *16*, 2538.

(8) Anal. Calcd for $Ca_3Mo_8S_8N_8C_{40}H_{100}O_{58}$: Ca, 4.35; N, 4.05; C, 17.37; H, 3.64. Found: Ca, 4.14; N, 3.99; C, 17.23; H, 3.40.

(9) Day, P. In "Mixed-Valence Compounds"; Brown, D. B., Ed.; Reidel: Dordrecht, Holland, 1979; "Introduction to Mixed-Valence Chemistry", p 3.

The electronic spectrum of **2** measured in aqueous solution showed peaks at 258 (ϵ(M^{-1} cm^{-1}) = 20 000), 300(sh, 7500), 450(sh, 750), 636(630), 900(sh, 86), and 1150 nm (260).

The most remarkable feature of **2** is its high stability to acid (up to 1 M HCl) and atomospheric oxygen. It should be noted that all Fe_4S_4 and $MoFe_3S_4$ cluster compounds so far reported[10] are decomposed by acids to give hydrogen sulfide, while oxygen-bridged di-,[11a] tri-,[11b] and tetranuclear[11c] Mo$^{III/IV}$ compounds are readily air oxidized.

A cyclic voltammogram of **2** (0.8 mM in 0.1 M $HClO_4$) shows two quasi-reversible, one-electron waves (Figure 2). The controlled potential Coulometry of **2** at 0.50 V (vs. SCE) in 0.1 M $HClO_4$ and at -0.40 V (vs. SCE) in 0.5 M KCl gave an electron stoichiometry of 0.25e per molybdenum. The reversibility indicates that one electron is added to or removed from **2** without drastic change in structure. The large comproportionation constant (K = 7.3 × 10^{11}) for the following equilibrium

$$[Mo_4S_4(edta)_2]^{4-} + [Mo_4S_4(edta)_2]^{2-} \rightleftharpoons 2[Mo_4S_4(edta)_2]^{3-}$$

indicates that the trivalent anion is the overwhelmingly dominant species in solution.

Recently the oxidized and reduced species, $[Mo_4S_4(edta)_2]^{2-}$ and $[Mo_4S_4(edta)_2]^{4-}$, have been successfully isolated as single crystals in combination with appropriate cations. Comparisons of the structure and property of **2** with those of $[Mo_4S_4(edta)_2]^{2-}$ and $[Mo_4S_4(edta)_2]^{4-}$ will disclose the electronic structure for each of the $Mo_4S_4{}^{n+}$ cores.

Acknowledgment. We are grateful to Dr. I. Kinoshita of Osaka City University for his help in the cyclic voltammometry measurement.

Supplementary Material Available: Lisitng of atomic coordinates, thermal parameters, and bond angles and electronic spectrum (4 pages). Ordering information is given on any current masthead page.

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[10] Lippard, S. J. In "Mixed-Valence Compounds"; Brown, D. B., Ed.; Reidel: Dordrecht, Holland, 1979; "Polymetalic Centers in Biology", p 427.

[11] For example: (a) Shibahara, T.; Sykes, A. G. *J. Chem. Soc., Dalton Trans.* **1978**, 95. (b) Richens, D. T.; Sydes, A. G. *Inorg. Chem.* **1982**, *21*, 418. (c) Shibahara, T.; Sykes, A. G. *J. Chem. Soc., Dalton Trans.* **1978**, 100.

"Hyperconjugation Transitions" in Radical Cation Optical Spectra

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Murrell has stated that alkyl substituents are spectroscopically rather inert and only produce a large change in the absorption spectrum of a molecule when the shape of the absorbing group is appreciably changed by the substitution.[1] In contrast, when *tert*-butyl cation was believed to show a strong absorption band at 290-295 nm,[2] the absorption was attributed to charge-transfer configurations caused by electron transfer from the methyl groups toward the central carbon, which bears a formally empty 2p orbital. This band was called the "hyperconjugation transition", and approximate MO calculations agreed fully with this rationalization.[3] When Olah and co-workers prepared a purer sample of *tert*-butyl cation, the 290-295 nm band was shown to be absent, and Olah, Pittman, and Symons concluded that "the theory that the "hyperconjugation transitions" can contribute to the optical spectra is, therefore returned to the realm of fancy: apparently possible, they do not seem to have been detected experimentally".[4] The strained σ bonds in three- and four-membered rings, which have high p character relative to unstrained σ bonds, are known to provide significant σ,π interactions leading to interesting spectral and chemical behavior,[5] but we are not aware of previous observations of such transitions involving unstrained alkyl groups. We report here the observation of bands involving unstrained alkyl group interactions with both olefin radical cations (1-electron, 2-atom π orbitals) and hydrazine radical cations (1-electron, 2-atom π^* orbitals).

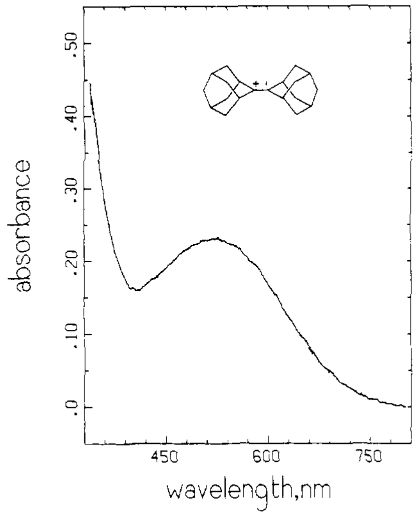
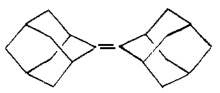


Figure 1. Visible spectrum of $1^{+\cdot}$ in CH_2Cl_2, -78 °C.

Monoolefins **1** and **2** give radical cations that are long-lived on the cyclic voltammetry time scale at room temperature[6] because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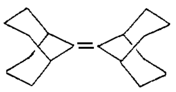
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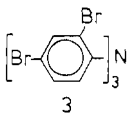

3

they are "Bredt's Rule" protected—their α hydrogens are held near the nodal plane of the formally spin-bearing π system. We have found that both $1^{+\cdot}$ and $2^{+\cdot}$ are colored. We had considerable difficulty generating solutions of these species that last for minutes, because low temperatures are required and their oxidation potentials are rather high. This problem was solved by employing tris(o,p-dibromophenyl)aminium hexachloroantimonate ($3^{+\cdot}$ $SbCl_6{}^-$),[7] a powerful enough oxidant that the electron transfer gives the olefin radical cation (cyclic voltammetry shows the electron transfer is 1.5 kcal/mol exothermic with **1** at -78 °C in methylene chloride, and under the conditions of the experiment, 10^{-2} M **1**, 10^{-3} M $3^{+\cdot}$ initially, the electron transfer is over 99% complete at equilibrium). Solutions of $1^{+\cdot}$ are deep purple, and the color lasts for tens of minutes at -78 °C, at millimolar concentration. The ESR spectrum of $1^{+\cdot}$ fades as the purple color fades upon warming. Because $1^{+\cdot}$ disappears more rapidly at higher concentration as well as at higher temperature, we believe that it is destroyed by self-electron-transfer disproportionation. The second oxidation wave of **1** is totally irreversible at all scan rates in cyclic voltammetry experiments, indicating a very short lifetime for the dication. The visible spectrum of $1^{+\cdot}$ shows a very broad absorption centered at λ_m ca. 530 nm (Figure 1). The

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[1] Murrell, J. N. "The Theory of the Electronic Spectra of Organic Molecules"; Wiley: New York, 1963; p 238.

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