Table I. Predicted Spectra of Deuterated Ethanes, Based on Ethane-d_0[a]

m/e	d_0	d_1	d_2	d_3	d_4	d_5	d_6
28	187.30	53.07	9.02	0	0	0	0
29	12.67	126.66	84.90	27.06	0	0	0
30	100	10.56	78.51	95.52	54.13	0	0
31	0	100	8.44	42.84	84.85	90.20	0
32	0	0	100	6.33	19.66	53.06	135.32
33	0	0	0	100	4.22	8.97	0
34	0	0	0	0	100	2.11	10.77
35	0	0	0	0	0	100	0
36	0	0	0	0	0	0	100

[a] Ionization potential, 12 eV; gain, 10; pressure, 47 μ; current, 35 μA.

Table III. Recalculated Statistical Parameters

Current output (mA)	p	q	r	s
5.3	3.8	3.15	10.4	0.90
46	6.2	2.48	6.40	0.28
118	14.5	1.63	7.16	0.16
180	22.8	1.05	8.21	0.12
265	31.9	0.90	8.40	0.10
330	51.8	1.04	6.89	0.11

Table II. Corrected Ethane Product Distribution. Electrogenerative Hydrogenation of Ethylene with Deuterium[a]

Sample	0.514	A	B	C	D	E	F
E_{obsd}, V	Open	0.219	0.143	0.100	0.070	0.044	0.031
I, mA	circuit	5.3	46	118	180	265	330
% conversion	0	1.04	9.17	23.8	34.3	49.4	54.9
				Ethanes			
d_0	0	14.2	10.1	13.6	17.9	20.3	18.0
d_1	0	18.9	30.9	29.3	29.4	30.1	30.4
d_2	0	23.0	27.1	23.5	21.8	21.4	22.5
d_3	0	17.2	9.4	11.8	11.5	12.5	12.4
d_4	0	12.5	9.7	11.4	10.5	9.6	10.0
d_5	0	9.4	9.6	7.9	6.9	4.9	5.2
d_6	0	4.7	3.3	2.5	2.2	1.3	1.5

[a] Run D54, temp 24°, pressure 746 mm, R_{int} = 0.25 ohm, gas flow = 4.5 ml/min.

Table IV. Comparison of Observed and Calculated Distribution of Deuterated Products from Ethylene and Deuterium in Electrogenerative Reaction with D_2O–2N Perchloric Acid-d_1 Electrolyte Recalculated

	A		B		C		D		E		F	
	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd	Calcd	Obsd
						Ethylenes						
d_1	33.5	34.4	21.4	21.2	12.8	12.4	10.5	9.1	8.2	6.6	4.5	2.6
d_2	19.1	11.8	12.4	8.5	8.5	5.3	6.5	3.8	4.9	3.0	2.8	1.5
d_3	8.1	8.7	5.2	5.4	3.9	3.3	2.5	2.2	1.8	1.6	1.7	0.9
d_4	1.9	6.0	1.2	3.4	0.8	1.7	0.4	1.1	0.3	0.6	0.2	0.4
						Ethanes						
d_0	2.1	5.6	5.9	6.2	9.2	10.5	13.3	15.0	15.9	17.9	15.4	17.1
d_1	10.0	7.4	20.2	19.0	23.9	22.6	26.9	24.6	29.2	26.5	30.8	28.7
d_2	12.5	9.0	17.5	16.6	20.6	18.2	21.9	18.3	22.8	18.8	25.0	21.3
d_3	7.6	6.8	10.2	5.8	13.0	9.1	12.4	9.6	12.1	11.0	14.1	11.8
d_4	3.7	4.9	4.6	6.0	5.8	8.8	4.6	8.8	4.0	8.4	5.1	9.5
d_5	1.3	3.7	1.3	5.9	1.5	6.1	0.9	5.8	0.7	4.3	1.0	4.9
d_6	0.2	1.8	0.2	2.0	0.13	2.0	0.06	1.8	0.04	1.1	0.06	1.4

given in Table II. With the new ethane distributions, we have recalculated statistical parameters for the addition of hydrogen or deuterium to ethylene as shown in Table III. Because of the qualitative nature of our earlier discussion, the new statistical parameters are consistent with the argument there. The only significant change is in the value of q which is indicative of a high probability of addition of deuterium from the electrolyte in the initiating step of hydrogenation (see eq 12).

A corrected comparison of observed and calculated values of labeled ethylenes and ethanes is given in Table IV. Agreement between observed and calculated values is improved.

Ground States of Molecules. XXV. MINDO/3. An Improved Version of the MINDO Semiempirical SCF-MO Method [*J. Am. Chem. Soc.*, **97**, 1285 (1975)]. By RICHARD C. BINGHAM, MICHAEL J. S. DEWAR,* and DONALD H. LO, Department of Chemistry, The University of Texas at Austin, Austin, Texas 78812.

The first summation in eq 2 should be:

$$\sum_{k \neq i}^{(m)} q_k(g_{ik} - 0.5h_{ik})$$

Equation 3 should be:

$$F_{ik}(mm) = 0.5p_{ik}(3h_{ik} - g_{ik})$$

These errors were due to an uncorrected page from an earlier draft being accidentally included in the final manuscript. The correct version was given in the original MINDO paper (N. C. Baird and M. J. S. Dewar, *J. Chem. Phys.*, **50**, 1262 (1969)) and has been used in all our calculations.

Radical Production from the Interaction of Closed Shell Molecules. II. The Reaction of Organic Sulfides with *tert*-Butyl Peroxybenzoates [*J. Am. Chem. Soc.*, **97**, 1580 (1975)]. By WILLIAM A. PRYOR* and WILLIAM H.