

## Supplementary Materials

### Amorphous nanosized Al-Ti-Mn trimetal hydrous oxide: Synthesis, characterization and the enhanced performance in arsenic removal

Dong Nguyen Thanh<sup>a\*</sup>, Zdeněk Bastl<sup>b</sup>, Karla Černá<sup>a</sup>, Pavel Ulbrich<sup>c</sup>, Jaromír Lederer<sup>a</sup>

<sup>a</sup> Unipetrol Centre of Research and Education, Chempark Litvínov, Záluží – Litvínov, 436 70, Czech Republic

<sup>b</sup> J. Heyrovský Institute of Physical Chemistry, Academy of Science of the Czech Republic, Dolejškova 3, CZ-182 23 Prague 8, Czech Republic

<sup>c</sup> Department of Biochemistry and Microbiology, Institute of Chemical Technology, Technická 5, 166 28 Prague 6, Czech Republic

\*Corresponding author: Dong Nguyen Thanh

Tel: +420 471122287, Fax: +420 475 212 079, E-mail address: dong.nguyen@unicre.cz

Keywords: As(III) oxidation, trimetal hydrous oxide; nanosized; arsenic; adsorption

#### 1.1. Determination of the density of –OH groups

The surface -OH density of the ATM was determined by using thermogravimetric analysis developed by Mueller et al.[1]. The heating profile was set under a nitrogen atmosphere: the materials were stabilized at 25 °C for 5 min then subjected to a heating ramp of 10 °C min<sup>-1</sup> to a T<sub>1</sub> isotherm for 30 min. The materials were then heated to T<sub>2</sub> with a heating ramp of 20°C min<sup>-1</sup>. The surface hydroxyl group density (D<sub>OH</sub>, OH nm<sup>-2</sup>) was calculated based on weight loss (g) between T<sub>1</sub> and T<sub>2</sub> using the following equation.

$$D_{OH} = \alpha \left( \frac{wt_{T_1} - wt_{T_2}}{wt_{T_1}} \right) \frac{2N_A}{SA_{BET} \times M_{w_{H_2O}}} \quad (S1)$$

where  $\alpha=0.625$  (calibration factor),  $N_A$  is Avogadro's number and  $SA_{BET}$  (nm<sup>2</sup> g<sup>-1</sup>) is the BET surface area and  $M_{w_{H_2O}}$  is the molecular weight of water. For titanium and aluminum, it is assumed that at T<sub>2</sub> = 500 °C the powder surface is free of OH surface groups [1, 2] while manganese hydrous oxide, the –OH groups remains on the surface up to T<sub>2</sub> = 800 °C [2]. Thus, the TGA data were evaluated in the temperature range from T<sub>1</sub>=120 °C to T<sub>2</sub>=800 °C. The OH content was determined as:  $OHg^{-1} = D_{OH} \times SA_{BET}$ .

## 1.2. Tables and figures

Tab. S1. Elemental concentrations (in atomic %) calculated from XP spectra

Element Sample	Al	Ti	Mn	As
<b>ATM</b>	41.9	43.9	14.2	0
<b>ATM+As(III)</b>	34.1	37.7	5.3	22.9
<b>ATM +As(V)</b>	34.9	37.5	4.2	23.4

Tab. S2. Measured core level binding energies (eV) for the samples  
ATM, ATM +As(III) and ATM +As(V) ( $\pm 0.2$  eV)

Photoemission line Sample	Al 2p	Ti 3p	Ti 2p <sub>3/2</sub>	Mn 3p	Mn 2p <sub>3/2</sub>	As 3d	O 1s
<b>ATM</b>	74.5	37.1	458.6	50.1	642.6	-	530.2 532.1
<b>ATM+As(III)</b>	74.3	37.1	458.4	50.2	641.9	45.5	530.2 531.9
<b>ATM +As(V)</b>	74.3	37.2	458.4	50.4	642.4	45.5	530.3 531.8

Tab. S3. Langmuir and Freundlich isotherm parameters for As(V) and As(III) adsorption on ATM

As species and pH	Langmuir model			Freundlich model		
	q <sub>m</sub> (mg/g)	K <sub>L</sub> (L/mg)	R <sup>2</sup>	K <sub>F</sub> (mg/g) (L/mg)	n	R <sup>2</sup>
As(III) pH 7.0	110.582	0.0771	0.9884	30.286	0.257	0.9159
As(V) pH 7.0	51.143	0.0268	0.9068	7.384	0.345	0.9852

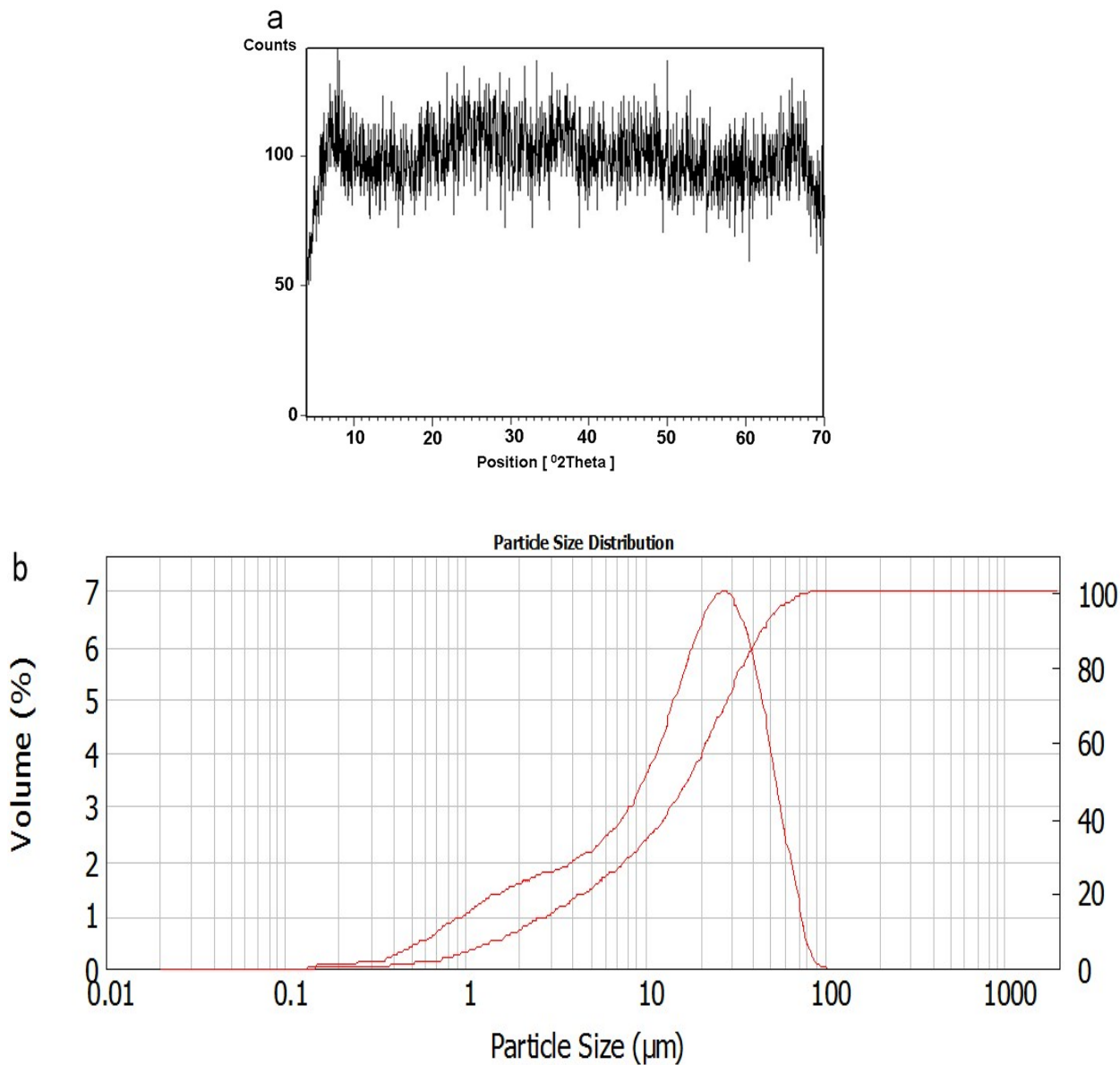


Fig. S1. Physical characterisation of ATM: (a) XRD diffraction pattern, (b) particle size distribution

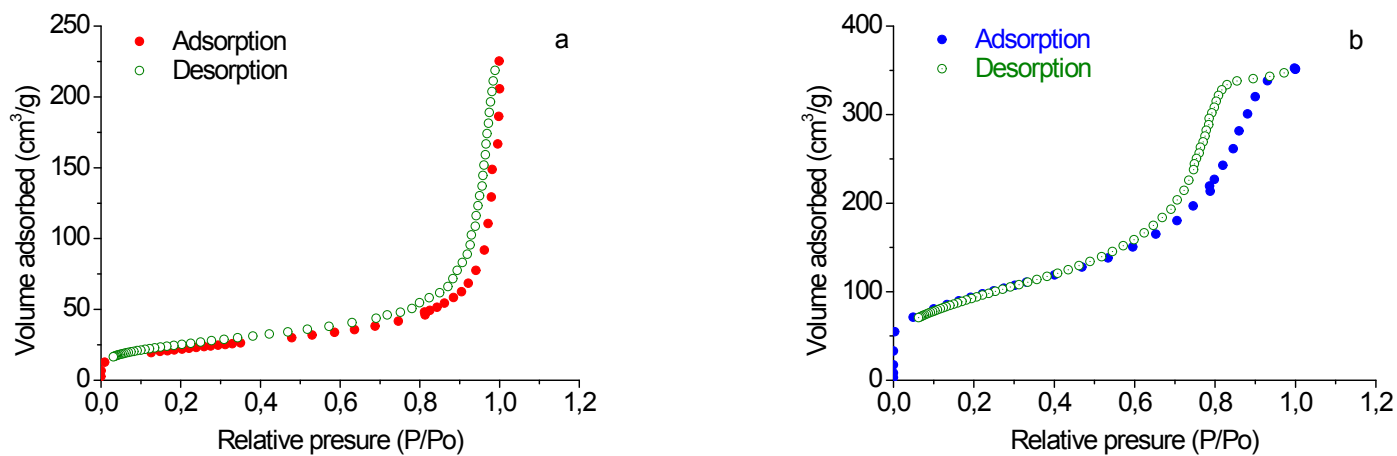


Fig. S2. Nitrogen adsorption-desorption isotherm of ATM (a) and TM (b).

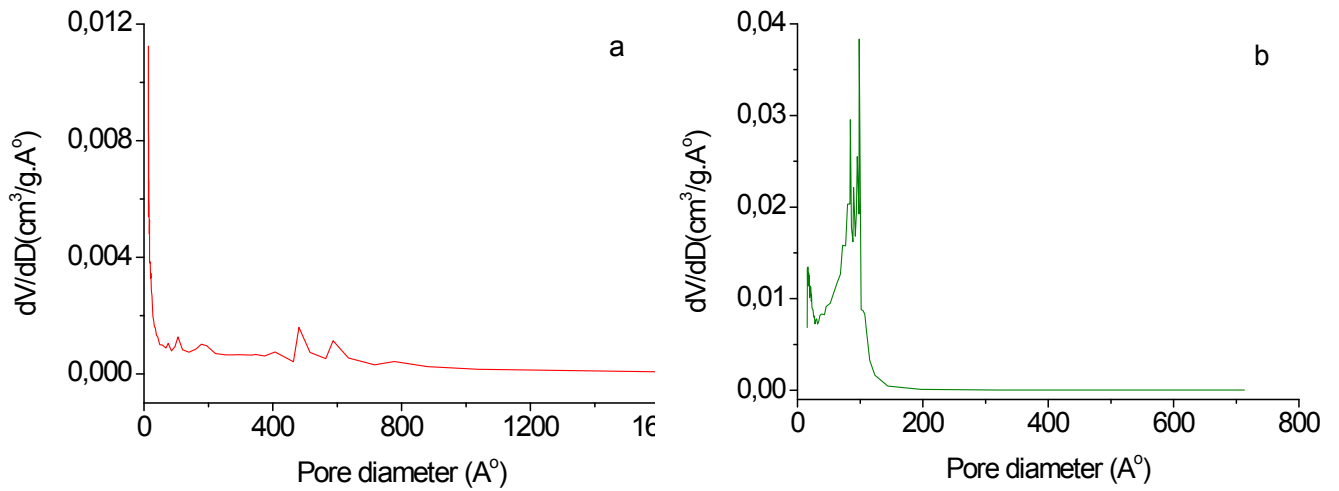


Fig. S3. Pore size distribution of ATM (a) and TM (b).

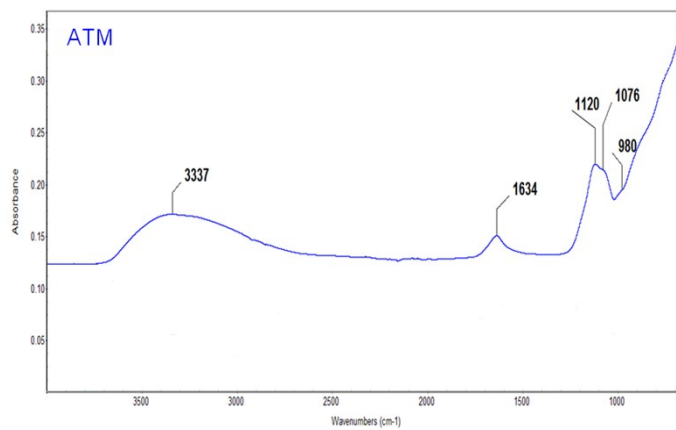


Fig. S4. FTIR spectra of the ATM in the range of 400 – 4000  $\text{cm}^{-1}$

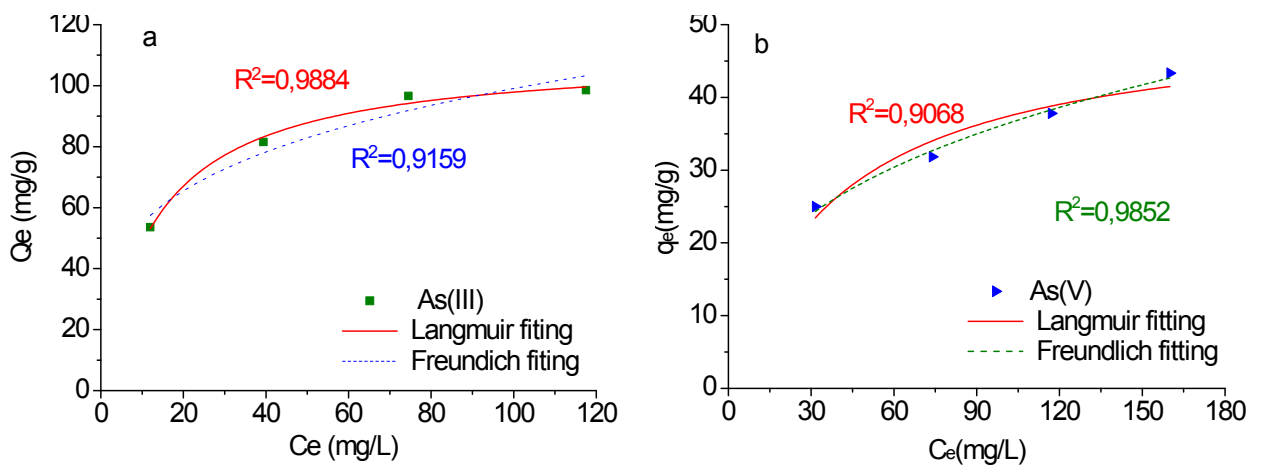


Fig. S5. Adsorption isotherms for (a) As(III) and (b) As(V) by TM at pH 7 and  $T = 25 \pm 1$  °C; (—) Langmuir model fitting and (----) Freundlich model fitting.

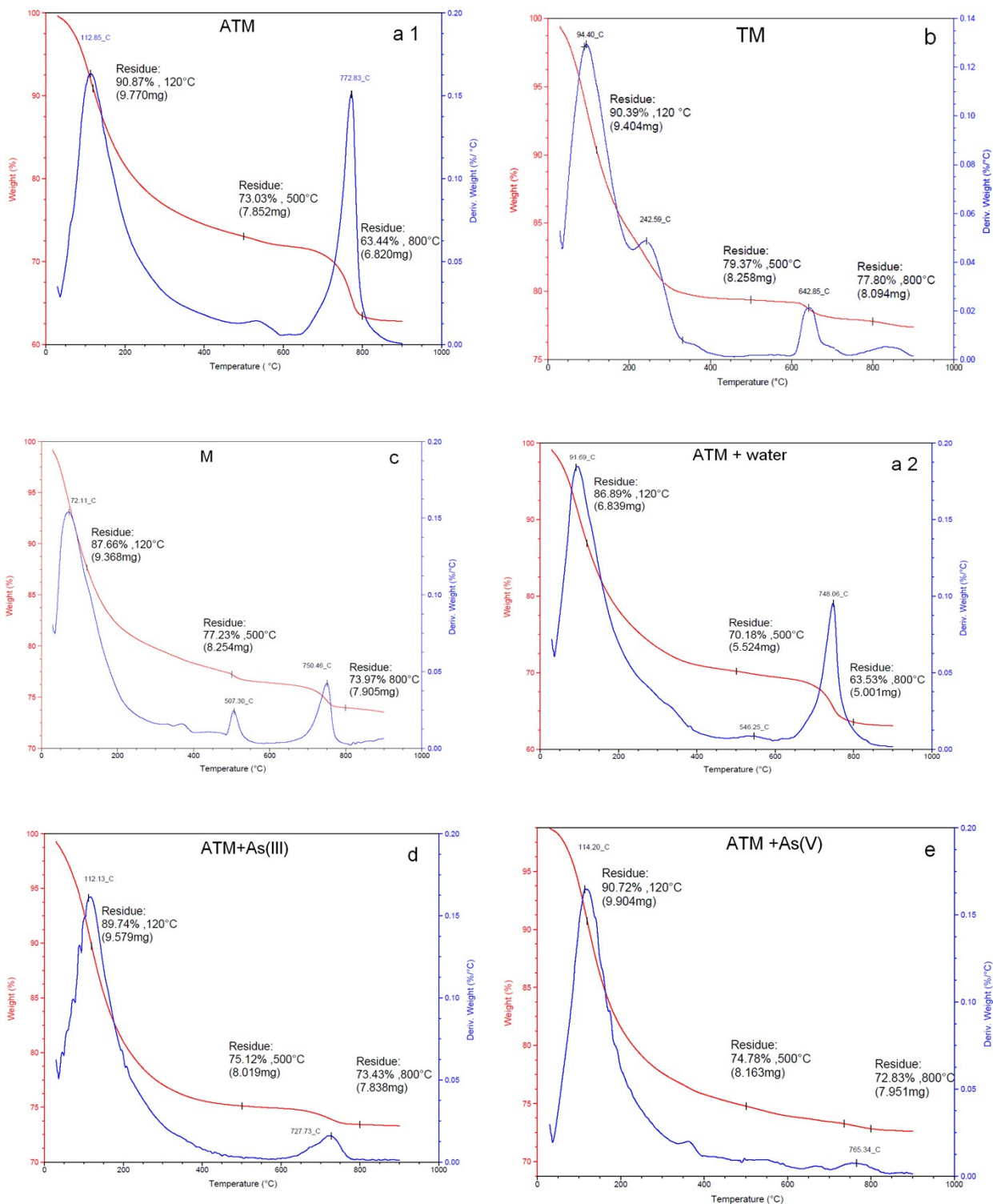


Fig. S6. The TGA–DTA curves of (a1) ATM, b) Ti-Mn binary hydrous oxide (TM), c) Mn hydrous oxide (M), a2) Al-Ti-Mn trimetal hydrous oxide after sharking in water (ATM+water), d) ATM after adsorption As(III) and e) after adsorption As(V).

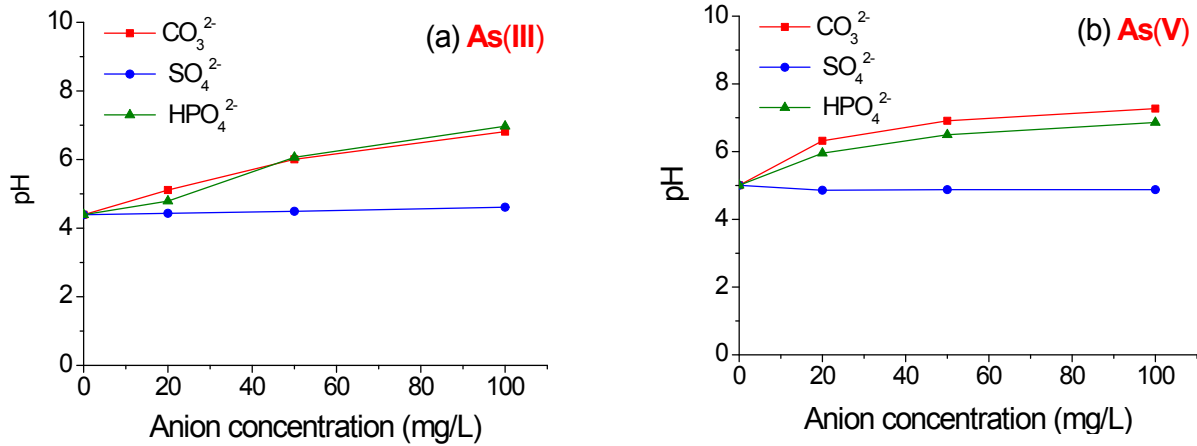


Fig. S7. The change of pH at different anions concentration

- [1] R. Mueller, H.K. Kammler, K. Wegner, S.E. Pratsinis, Langmuir 19 (2002) 160-165.
- [2] R.A. Lidin, L.L. Andreyeva, V.A. Molochko, Constants of Inorganic Substances: A Handbook, Begell House, 1995.