Metal−Organic Scandium Framework: Useful Material for Hydrogen Storage and Catalysis

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The 3D polymeric terephthalate of scandium has been synthesized and its structure solved by single-crystal XRD. It was obtained as a single phase and characterized and tested as a hydrogen and nitrogen adsorbent and heterogeneous catalyst as a redox agent in the oxidation of sulfides. The compound shows a BET area of 721 $m^2 g^{-1}$ with a high $C_{BET} = 7000$. The high chemical and thermal stability and excellent hydrogen sorption properties make this compound a useful material for hydrogen storage.

Introduction

Hydrogen would be ideal as a synthetic fuel because it is lightweight and highly abundant and its oxidation product (water) is environmentally benign, but storage remains a problem. The major obstacle for the commercial use of hydrogen-based fuel-cell vehicles is on-board hydrogen storage. Different approaches are used to overcome difficulties in storing and using gaseous hydrogen in high-pressure vessels appropriate for stationary or mobile applications. Among the materials under investigation, complex hydrides, carbon and nongraphitic nanotubes, and finally metal−organic frameworks[1] are found, the last being the less studied yet.

It is a well-known fact that rare-earth-containing compounds can be used as strong and effective catalysts. However, despite the rich chemistry of rare-earth open frameworks, it is remarkable that there are only a few works[2−4] dedicated to the research of their catalytic activity.

Sulfoxides are important intermediates of many natural products.[5] Their synthesis has been achieved by means of a wide range of oxidizing systems, starting from the corresponding sulfides. Aqueous hydrogen peroxide is a particularly attractive oxidant, since it is cheap, environmentally friendly, and easy to handle and produces only water as a byproduct, which reduces purification requirements. The catalysts, often used to enhance the efficiency of the oxidation, are mostly metal salts (chlorides, oxides, peroxides, acetates, and acetyl acetonates of Ti, V, Mo, W, Re, and Mn). They play a very important role as catalytic activators of hydrogen peroxide: the resulting metal−peroxo derivatives are such powerful catalysts that usually give rise to overoxidized byproducts. Lanthanides have scarcely been explored in the oxidation of thioethers, yet these elements are receiving increasing attention in the literature.[6]

Three-dimensional coordination polymers of rare earths and transition metals have received significant attention in the past few years because of their potential useful attributes, such as magnetism, zeolite-like catalytic activity, and optical properties.[7] Among the available ligands to form these compounds, the dicarboxylic acids present interesting complexing behavior due to the diverse modes of coordination: in particular, terephthalate anion (1,4-benzenedicarboxylate) can bridge either in a bidentate or a monodentate fashion and may be completely or partially deprotonated. The dicarboxylic acids have many possibilities in coordinative behavior, even with large coordination numbers of the metallic center. The resulting coordination polymers are materials in which the properties of individual components are combined.[8] Terephthalic acid has been successfully used to build coordination architectures with metal ions of diverse sizes and shapes, adopting different coordination fashions.[9]

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(1) Rossi, N. L.; Eckert, J.; Eddaoudi, M.; Vodak, D. T.; Kim, J.; O'Keeffe, M.; Yaghi, O. M. *Science* **2003**, *300*, 1127.

(2) Perles, J.; Iglesias, M.; Ruiz-Valero, C.; Snejko, N. *Chem. Commun.* **2003**, *3*, 346.

(3) Perles, J.; Iglesias, M.; Ruiz-Valero, C.; Snejko, N. *J. Mater. Chem.* **2004**, *14*, 2683.

(4) Snejko, N.; Cascales, C.; Gómez-Lor, B.; Gutiérrez-Puebla, E.; Iglesias, M.; Ruiz-Valero, C.; Monge, A. *Chem. Commun.* **2002**, *13*, 1366−1367.

(5) Prilezhaeva, E. *Russ. Chem. Rev.* **2002**, *4*, 715.

(6) Kagan, B. *Chem. Rev.* **2002**, *102*, 1805.

(7) (a) Robson, R. *Comprehensive Supramolecular Chemistry*; Pergamon: New York, 1996; Vol. 6, p 733. (b) Eddaoudi, M.; O'Keeffe, M.; Yaghi, O. M. *Nature* **1999**, *402*, 276. (c) Moulton, B.; Zaworotko, M. *Chem. Rev.* **2001**, *101*, 1629. (d) Braga, D.; Grepioni, F.; Desiraju, G. R. *Chem. Rev.* **1998**, *98*, 1375.

(8) (a) Hoskins, B. F.; Robson, R. *J. Am. Chem. Soc.* **1990**, *112*, 1546. (b) Hagrman, D.; Zubieta, C.; Haushalter, R. C.; Zubieta, J. *Angew. Chem., Int. Ed.* **1997**, *36*, 873. (c) Miller, J. S. *Adv. Mater.* **2001**, *13*, 525. (d) Choudhury, A.; Natarajan, S.; Rao, C. N. R. *J. Solid State Chem.* **2000**, *155*, 62.

(9) (a) Thirumurugan, A.; Natarajan, S. *Eur. J. Inorg. Chem.* **2004**, 762. (b) Pan, L.; Zheng, N.; Wu, Y.; Han, S.; Yang, R.; Huang, X.; Li, J. *Inorg. Chem.* **2001**, *40*, 828. (c) Reineke, T. M.; Eddaoudi, M.; Fehr, M.; Kelley, D.; Yaghi, O. M. *J. Am. Chem. Soc.* **1999**, *121*, 1651. (d) Li, H.; Eddaoudi, M.; Groy, T. L.; Yaghi, O. M. *J. Am Chem Soc.* **1998**, *120*, 8571. (e) Millange, F.; Serre, C.; Férey, G. *Chem. Commun.* **2002**, 822. (f) Barthelet, K.; Marrot, J.; Riou, D.; Férey, G. *Angew. Chem., Int. Ed.* **2002**, 41. (g) Chen, W.; Wang, J.-Y.; Chen, C.; Yue, Q.; Yuan, H.-M.; Chen, J.-S.; Wang, S.-N. *Inorg. Chem.* **2003**, *42*, 944. (h) Barthelet, K.; Marrot, J.; Riou, D.; Férey, G. *Chem. Commun.* **2004**, 520. (i) Serre, C.; Millange, F.; Thouvenot, C.; Nouges, M.; Marsolier, G.; Louer, D.; Férey, G. *J. Am. Chem Soc.* **2002**, *124*, 13519. (j) Férey, G.; Latroche, M.; Serre, C.; Millange, F.; Percheron-Guégan, A. *Chem. Comm.* **2003**, 2355.

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Extending our previous work on rare-earth carboxylates[2,3] in the search for innovative materials, we have synthesized the scandium terephthalate $[Sc_2(C_8H_4O_4)_3]$, characterized the compound, and tested its sorption capacities and catalytic ability.

Experimental Section

Synthesis. The scandium terephthalate $[Sc_2(C_8H_4O_4)_3]$ was synthesized under hydrothermal conditions by the reaction of Sc^{3+} ions with a mixture of terephthalic acid and disodium terephthalate in a 2:2.25:1.5 ratio. In a container, 0.554 g (2 mmol) of scandium acetate hydrate, 0.375 g (2.25 mmol) of terephthalic acid, and 0.31 g (1. 5 mmol) of disodium terephthalate were mixed in 10 mL of distilled water. After addition of *o*-phenanthroline (*o*-Phen) (0.360 g), the reaction mixture was stirred to homogeneity in a 25 mL PTFE bottle and sealed in a stainless steel autoclave (PARR). The reaction was carried out at 180 °C for 4 days under autogenous pressure and afterward cooled slowly at a rate of 10 °C h^{-1}. The compound was obtained in good yield (>80%) as a single phase of transparent prismatic crystals without any traces of amorphous impurities. The crystals were filtered off, washed thoroughly with distilled water, ethanol, and acetone, and finally dried at room temperature.

Structural Determination. A transparent prismatic crystal of $[Sc_2(C_8H_4O_4)_3]$ was mounted on a Bruker-Siemens Smart CCD diffractometer equipped with a normal focus, 2.4 kW sealed tube X-ray source (Mo Kα radiation, $\lambda = 0.71073$ Å) operating at 40 kV and 20 mA. Data were collected over a quadrant of reciprocal space by a combination of three sets of exposures. Each set had a different φ angle for the crystal, and each exposure of 20 s covered 0.3° in ω. Unit cell dimensions were determined by a least-squares fit of 40 reflections with $I > 20\sigma(I)$. The first 30 frames of data were recollected at the end of the data collection to monitor crystal decay. The intensities were corrected for Lorentz and polarization effects. Scattering factors for neutral atoms and anomalous dispersion corrections for Sc were taken from the *International Tables for Crystallography*.[10] The structure was solved by Multan and Fourier methods. Full-matrix least-squares refinement with anisotropic thermal parameters for all non-hydrogen atoms was carried out. A summary of the conditions for data collection is given in Table 1. All calculations were performed using SMART software for data collection, SAINT[11] for data reduction, SHELXTL[12] to resolve and refine the structure and to prepare material for publication, and ATOMS[13] for molecular graphics.

Characterization. Thermogravimetric and differential thermal analyses (TGA/DTA) of the compound were carried out under a N_2 gas flow (50 mL min^{-1}) at a heating rate of 5 °C min^{-1} in the range 25−900 °C in an Exstar 6000 (TGA/DTA 6300, Seiko Instruments, Inc.). The IR spectrum was recorded on an FTIR Nicolet Magna-550 spectrophotometer with samples as KBr pellets in the 4000−400 cm^{-1} region. Gas chromatography was performed in a Hewlett-Packard 5890 II chromatograph equipped with a flame ionization detector in a cross-linked methyl silicone column.

Table 1. Crystal Data and Structure Refinement for $[Sc_2(C_8H_4O_4)_3]$

empirical formula	$C_{12}H_6O_6Sc$
fw	291.13
temp	275(2) K
wavelength	0.71073 Å
cryst syst	orthorhombic
space group	*Fddd*
unit cell dimensions	$a = 8.7433(5)$ Å $b = 20.7448(11)$ Å $c = 34.3664(18)$ Å
vol, *Z*	6233.3(6) Å^3, 16
density(calcd)	1.241 Mg/m^3
abs coeff	0.487 mm^{-1}
F(000)	2352
cryst size	0.30 × 0.30 × 0.30 mm^3
θ range for data collection	2.29−28.99°
index ranges	$-11 \leq h \leq +10, -19 \leq k \leq +23, -46 \leq l \leq +18$
no. of reflns collected	7608
no. of independent reflns	1778 [R(int) = 0.0219]
completeness to $\theta = 28.99°$	85.6%
abs correction	semiempirical
max and min transm	0.8677 and 0.8677
refinement method	full-matrix least-squares on F^2
no. of data/restraints/params	1778/0/101
GOF on F^2	1.092
final *R* indices [$I > 2\sigma(I)$]	R1 = 0.0306, wR2 = 0.0773
R indices (all data)	R1 = 0.0370, wR2 = 0.0793
largest diff peak and hole	0.277 and −0.279 e·Å−3

Gas Sorption. The textural properties and hydrogen sorption of the solid were measured in a Coulter Omnisorp 100 apparatus by adsorption−desorption of N_2 or H_2 at 77 K. The sample was outgassed for 16 h at 350 °C to remove any loosely held adsorbed species, and the isotherms obtained are included in Figures 6 and 7. The apparent specific surface area (S_{BET}) was obtained by the BET method assuming an area of 0.162 nm^2 for the nitrogen molecule, and the external area (S_{ext}) and micropore volume (V_{mic}) were calculated by applying the *t*-plot method[14] to the experimental data. The total pore volume was calculated from the amount adsorbed at relative pressure $p/p° = 0.96$, on the desorption branch, equivalent to the filling of all pores below 50 nm in diameter. The micropore size distribution was analyzed by assuming cylindrical pores according to Horvath−Kawazoe's calculations.[15]

Catalytic Reactions. *Acetalization of Aldehydes*. A solution of the carbonyl compound (1.0 mmol) and trimethyl orthoformate (TMOF) (10 mmol) in tetrachloromethane (5 mL) was added to a suspension of the catalyst (0.001 mmol), and the resulting mixture was magnetically stirred at reflux temperature. Samples were taken at intervals, and the reaction products were analyzed by gas chromatography (GC).

Oxidation of Sulfides. The reactions were carried out in a 25 mL flask equipped with a magnetic stirrer and charged with 5 mL of a suspension of the catalyst (0.0025 mmol) in acetonitrile and a solution of the corresponding thioether (methyl phenyl sulfide or 2-ethylbutyl phenyl sulfide, 2.52 mmol). The oxidant H_2O_2 (30%, 1.5 or 1.1 mmol) was added dropwise, while the overall suspension was heated at 50 °C. Samples were taken every hour and analyzed after filtration. The chemical yields of the sulfoxides and sulfones were measured by GC with a chiral glass capillary column of a 15:85 mixture of methyl silicone (OV-1701) and methyl silicone−heptakis[2,3-dipentyl-6-(*tert*-butyldimethylsilyl)]-β-cyclodextrin as stationary phase.[16]

Results and Discussion

Upon determination of the crystal structure, the composition of the compound was found to be $[Sc_2(C_8H_4O_4)_3]$. It

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(10) *International Tables for Crystallography*; Kynoch Press: Birmingham, U.K., 1974; Vol. 4, p 72.

(11) Siemens. *SAINT. Data collection and procedure software for the SMART system*; Siemens Analytical X-ray Instruments, Inc.: Madison, WI, 1995.

(12) Siemens. *SHELXTL^{TL}*, version 5.0; Siemens Analytical X-ray Instruments, Inc.: Madison, WI, 1995.

(13) Dowty, E. *ATOMS for Windows 3.1, a computer program for displaying atomic structure*; Kingsport, TN, 1995.

(14) (a) Lippens, B. C.; de Boer, J. H. *J. Catal.* **1965**, *4*, 319. (b) Rouquerol, F.; Rouquerol, J.; Sing, K. *Adsorption by powders and porous solids*−*principles, methodology and applications*; Academic Press: London, 1999.

(15) Horvath, G.; Kawazoe, K. *J. Chem. Eng. Jpn.* **1983**, *16*, 470.

(16) Miranda, E.; Sánchez, F.; Sanz, J.; Jiménez, M. I.; Martínez Castro, I. *J. High. Resolut. Chromatogr.* **1998**, *21*, 225.

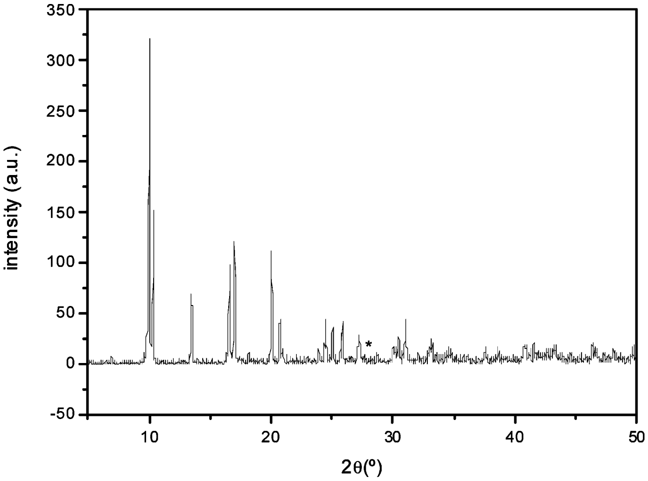

Figure 1. Powder X-ray pattern of the synthesized material. The asterisk shows the 2θ position where the terephthalic acid strongest peak would appear if any.

has to be noticed that the synthesis method is of very high importance from the point of view of the further application of the material. In this sense, the materials obtained by hydrothermal synthesis have some advantages in stability compared with the materials obtained by conventional methods of synthesis.[1,7b,9c,d] It is also important to note that, in our case, the use of a mixture of the organic acid and its sodium salt yields the compound as a single phase while the use of just the acid or a salt of the acid gives rise to a mixture of crystals of terephthalic acid and [$Sc_2(C_8H_4O_4)_3$], which can only be purified by a calcination of the organic ligand (when the terephthalic acid is present in the sample, a strong peak in the X-ray diffraction diagram appears always at 2θ = 28.1°; this peak is absent in the X-ray diffractogram of the sample synthesized from the acid−salt mixture (Figure 1)). It is worth pointing out, too, that though *o*-Phen has not been found in the structure of the material, it is a necessary component of the starting reaction mixture due, probably, to its pH-adjusting ability (the starting pH value of the reaction mixture was ~5). In the absence of *o*-Phen the reaction yield and crystal quality are very poor.

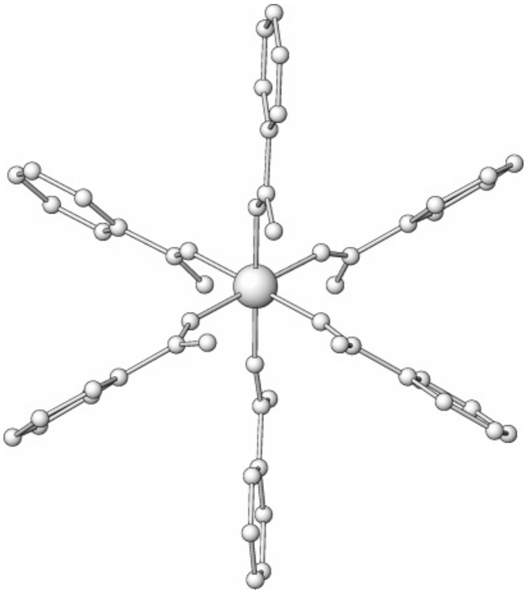

Figure 2. View of the scandium environment with the metal center coordinated to six different ligands (hydrogen atoms and the second carboxylate group in the terephthalate ligands have been omitted for clarity).

Table 2. Bond Distances (Å) and Angles (deg) for [$Sc_2(C_8H_4O_4)_3$]

Sc(1)−O(1)	2.068(1) × 2	Sc(1)−O(3)	2.093(1) × 2
Sc(1)−O(2)	2.048(1) × 2	Sc(1)−Sc(1)	4.433
O(1)−Sc(1)−O(2)	87.48(6) × 2	O(3)−Sc(1)−O(3)[a]	88.04 (7) × 1
O(1)−Sc(1)−O(3)	88.13(5) × 2	O(1)−Sc(1)−O(2)[a]	92.01 (6) × 2
O(2)−Sc(1)−O(3)	92.30(5) × 2	O(1)−Sc(1)−O(3)[a]	92.37 (6) × 2
O(1)−Sc(1)−O(1)[a]	179.29 (9) × 1	O(2)−Sc(1)−O(3)[a]	179.4 (3) × 2
O(2)−Sc(1)−O(2)[a]	87.35(8) × 1		

[a] Symmetry transformations used to generate equivalent atoms: 1 − x + 3/4, −y + 7/4.

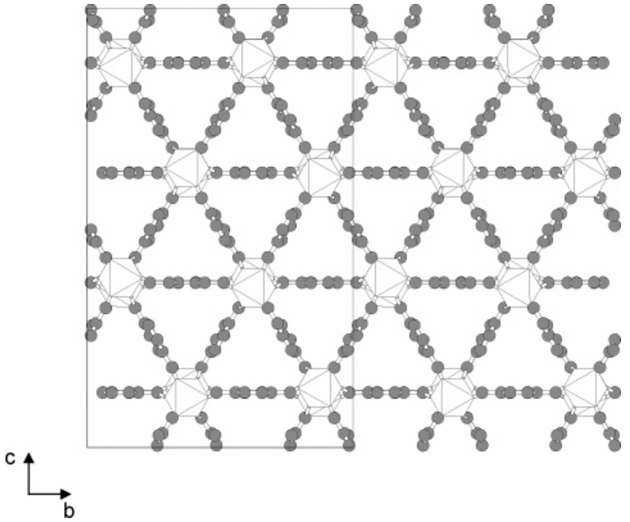

Figure 3. View of the 3D structure with the triangular channels parallel to the *a* axis.

The crystals of [$Sc_2(C_8H_4O_4)_3$] belong to the orthorhombic *Fddd* group. The structure consists of a polymeric 3D framework with each scandium atom octahedrically coordinated to six carboxylic oxygen atoms of six different terephthalate anions (Figure 2). Consequently, the asymmetric unit comprises one scandium atom, which is situated on an inversion center, and three oxygen and seven carbon atoms, belonging to two different terephthalate ions. Carboxylic groups connect metal atoms by forming ScO_6 octahedra through two types of bridges: one of them, Sc−O−C−O−Sc, keeps the scandium polyhedra quite close (Sc−Sc distance 4.433 Å) in a row parallel to the *a* axis, while the other, which involves the full length of the terephthalate anion, connects the scandium atoms at 10.399 Å. The Sc−O length range [2.048(1)−2.093(1) Å] is usual for oxygen-coordinated scandium[17] compounds with carboxylic acids (Table 2) Although there are two crystallographically independent terephthalate anions situated along the [010] and [101] directions, both are chemically equivalent, acting as μ^4-bridging ligands to four different scandium atoms and delimiting the empty channels that run along the *a* direction. These channels have the shape of an equilateral triangle with 10.4 Å edges, as shown in Figure 3. The effective space inside these channels is approximately 5.4 Å; other channels of 5 × 2 Å run along the [110] direction (van der Waals radii taken into account in both cases) (Figure 4).

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(17) Cotton, S. A. *Polyhedron* **1999**, *18*, 1691.

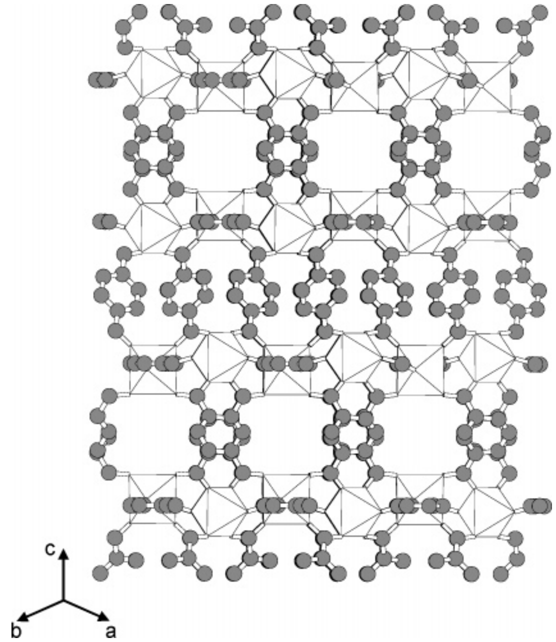


Figure 4. View of the 3D structure with the rectangular channels in the [110] direction.

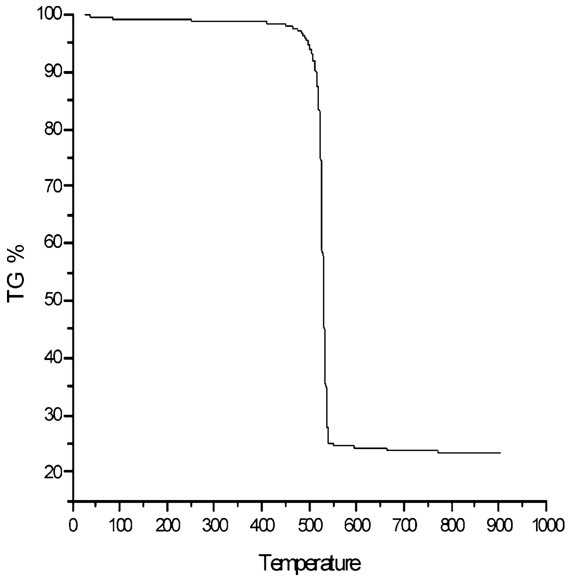


Figure 5. Thermogravimetry of the scandium terephthalate (*T* in °C).

The IR spectrum shows the antisymmetric ν_{asym}(C=O) vibrations in the range 1570−1500 cm^{-1} and the symmetric ν_{sym}(C=O) vibrations at 1410 cm^{-1}. The difference between the bands $\nu_{asym}(COO^-) = 1566$ cm^{-1} and $\nu_{sym}(COO^-) = 1410$ cm^{-1} ($\Delta\nu = 156$ cm^{-1}) confirms the bridging mode of the carboxylate groups in this compound. TGA/DTA (Figure 5) shows the stability of the material up to ~520 °C and the nonexistence of intermediate steps indicative of the presence of occluded terephthalic acid molecules (theoretical weight loss 76.3%, observed 76.4%).

Gas Sorption. Nitrogen adsorption on the sample leads to a type I isotherm (Figure 6) with a practically nonexistent hysteresis loop as corresponds to its microporous and quasi-non-mesoporous nature, and due to this characteristic, the apparent specific surface area was determined by the BET method in the relative pressure range of $p/p° = 0.02-0.12$. This sample gave a BET area of 721 m^2 g^{-1} with a high $C_{BET} = 7000$, as expected for microporous solids. However, it should be pointed out that this surface area result is only apparent, because at very low relative pressures the adsorption in micropores (ca. 90% of the total) is a volume-filling effect. A high total pore volume of 0.332 cm^3 g^{-1} (equivalent to the pore volume in all pores of diameter less than 50 nm) is found, and applying a *t*-plot analysis of the isotherm with the equation of Harkins−Jura, a micropore volume of 0.293 cm^3 g^{-1} and an external area of 28 m^2 g^{-1} (i.e., the area not involved in the volume filling of the micropores) are obtained. The micropore size distribution according to Horvath−Kawazoe's calculation is included in Figure 8, and as can be seen, the sample is constructed by a narrow pore size distribution with main pore diameters of ca. 0.55 nm.

It is a known fact the energy of the interaction of hydrogen with adsorbent surfaces is low;[18] however, the interaction potential can be enhanced in pores with sizes close to that of the hydrogen molecule[19] (ca. 0.3 nm), due to the overlap of the potential fields from the pore walls. The high amount of hydrogen sorbed by the sample, indicated in Figure 7, and the isotherm being of type I, as corresponds to its microporous nature, agree with the analysis of the pore size distribution from the nitrogen sorption data of the sample, which indicates a main pore size corresponding to 0.5−0.6 nm, this value corresponding to the crystallographic one. The results obtained here are on the same order as those of Zhao et al.[18a] and Panella et al.,[18b] both finding ca. 1% weight storage for MOF-M and MOF-5. It is worth pointing out that the micropore volumes are 0.277 and 0.293 cm^3 g^{-1} for Panella's and our samples, respectively, revealing thus the

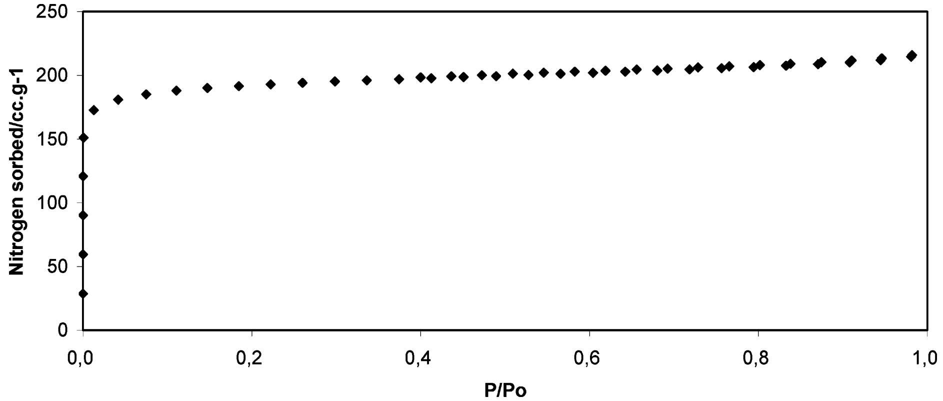


Figure 6. Nitrogen sorption curve at 77 K.

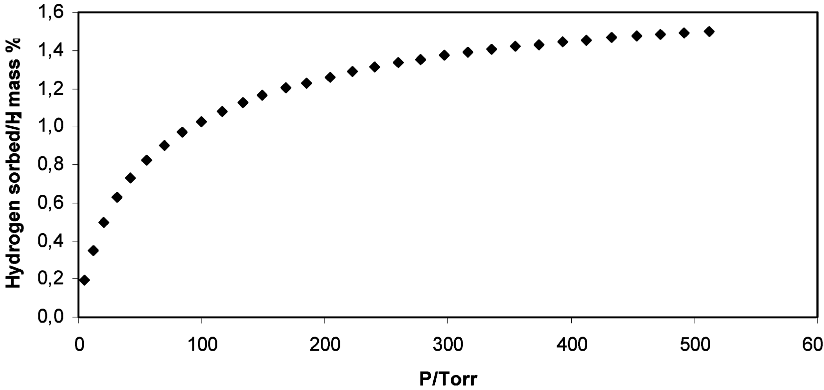


Figure 7. Hydrogen sorption curve at 77 K.

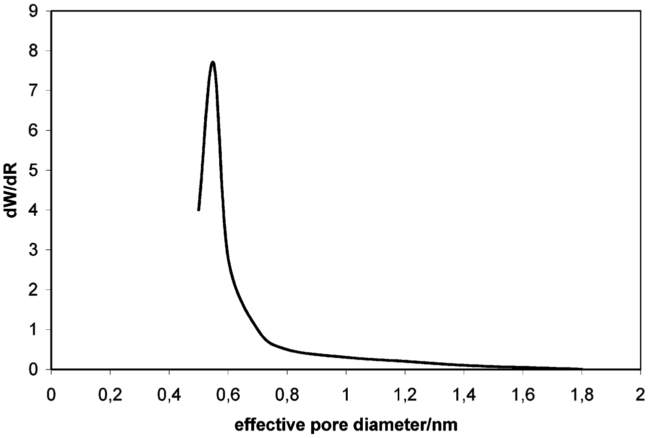


Figure 8. Micropore size distribution.

correlation between microporous volume and the hydrogen sorption amounts.

The high thermal stability, sorption capability, and narrow pore size distribution, with pores of sizes close to 1−2 hydrogen molecules, make this sample an interesting candidate for hydrogen storage purposes (patent registry no. P200501671).

Catalytic Activity. The compound was tested for catalytic properties with two reactions: acetalization of aldehydes, to test its ability as a Lewis acid catalyst, and oxidation of sulfides, to prove its effect in redox reactions. To compare the activity of this scandium derivative with those of other compounds previously tested,[3] we used Sc_2O_3 and $Sc_2(C_4H_4O_4)_{2.5}(OH)$ in the same reaction conditions. The results of these tests are shown in Figures 9 and 10.

In the acetalization of aldehydes, the scandium terephthalate showed no activity. However, in the oxidation of sulfides (Scheme 1), this compound showed good activity and selectivity. The kinetic profiles (Figure 9) indicate that the two organic−inorganic 3D compounds are better catalysts than pure Sc_2O_3, which is a logical consequence of the greater availability of the scandium centers in the porous compounds. The comparative data of the two polymeric carboxylates prove that the terephthalate makes the reaction proceed faster than the succinate, and the selectivity toward the sulfoxide is also better (Figure 10).

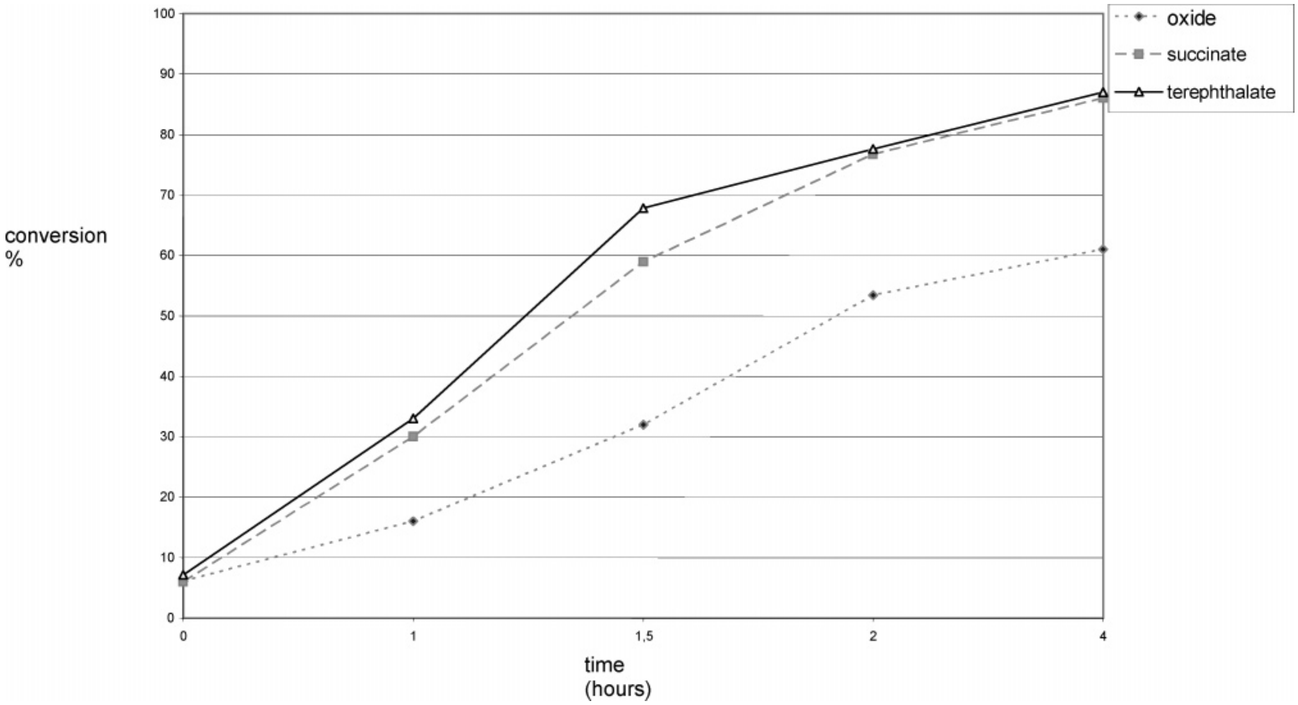


Figure 9. Kinetic profile of the oxidation of methyl phenyl sulfide with scandium terephthalate as catalyst.

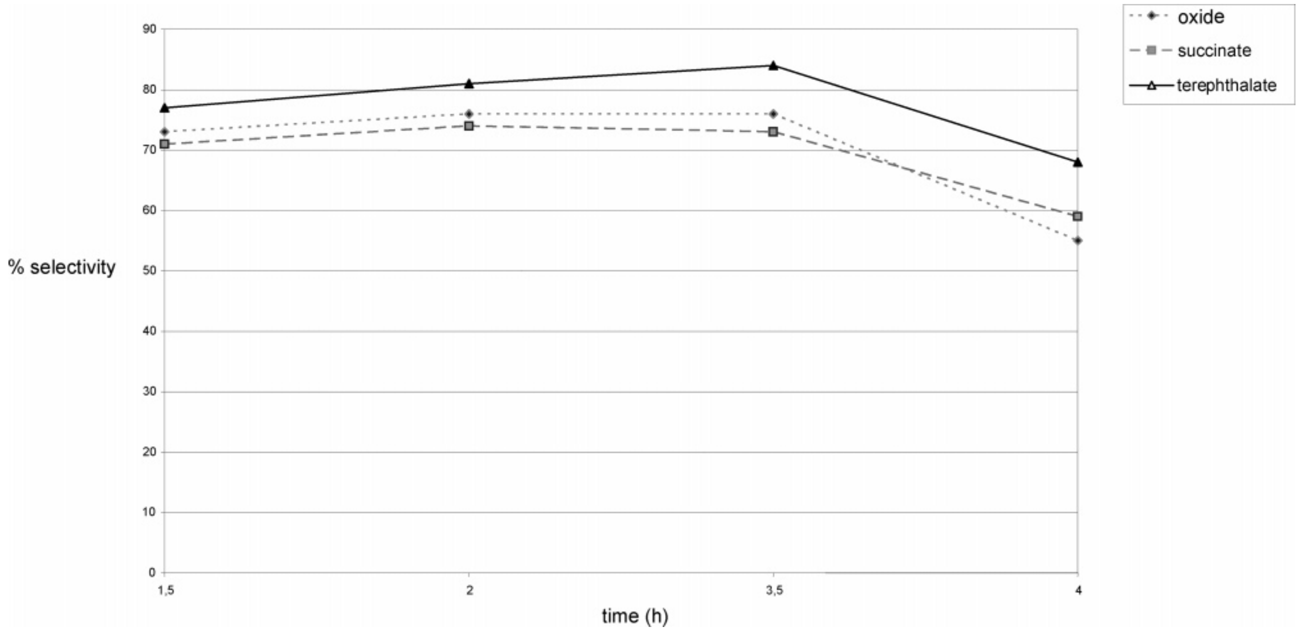
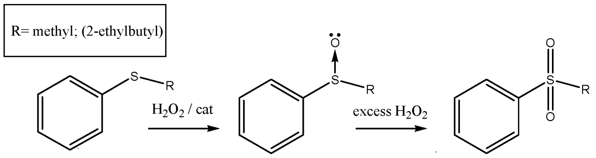


Figure 10. Selectivity to sulfoxide of scandium terephthalate.

Scheme 1. Oxidation of Alkyl Phenyl Sulfides



The behavior of the terephthalate as a heterogeneous catalyst contributes to enhance its interest as a catalyst, due to the ease of recovery and recycling of the catalyst and the simpler working procedure, which allows the removal of the catalysts from the reaction media through a simple filtration. The lifetime of this catalyst was examined by using it in several reaction cycles. To recover the catalyst, the solid was separated from the reaction medium by filtration and washed with a suitable solvent.

The scandium terephthalate could be reused at least four times with loss of neither activity nor selectivity with a catalyst loading as low as 1 mol %. The slight decrease in the rate observed for the consecutive runs is due to the small amount of catalytic material loss by filtration. While the oxidation of the sulfide continued as the catalyst was present, there was no further significant conversion when the catalyst was removed from the reaction medium.

During the process of evaluation of this paper, an advanced paper by P. A. Wright et al. appeared on the *Chem. Commun.* Web site reporting this same solid.[20] One difference with the present paper is the lower specific surface area for P. A. Wright's solid (due to the method of synthesis used, their solid has some amount of terephthalic acid inside the channels, which is not so easy to eliminate from the framework); in our paper, apart from the data presented,[20] some new results are reported: a synthesis approach to obtain the pure scandium material (which is very important for successful applications), study of hydrogen adsorption, and catalytic comparative properties of scandium compounds.

Conclusions

The new material $[Sc_2(C_8H_4O_4)_3]$, a scandium metal–organic framework, shows a high thermal stability and interesting sorption and catalytic properties. In particular, the high quantity of sorbed hydrogen makes this compound a potentially interesting material for hydrogen storage applications; further studies on the adsorption properties of this and other scandium compounds[2] are in progress. Catalytic activity in sulfide oxidation as a heterogeneous catalyst is another useful property this new compound possesses.

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Supporting Information Available: CIF file for $C_{12}H_6O_6Sc$. This material is available free of charge via the Internet at http://pubs.acs.org.

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(18) (a) Zhao, X.; Xiao, B.; Fletcher, A. J.; Thomas, K. M.; Bradshaw, D.; Rosseinsky, M. J. *Science* **2004**, *306*, 1012. (b) Panella, B.; Hirscher, M. *Adv. Mater*. **2005**, *17*, 538.

(19) Breck, D. W. *Zeolite molecular sieves*: John Wiley and Sons: New York, 1974.

(20) Miller, S. R.; Wright, P. A.; Serre, C.; Loiseau, T.; Marrot, J.; Ferey, G. *Chem. Commun*. **2005**, 3850.