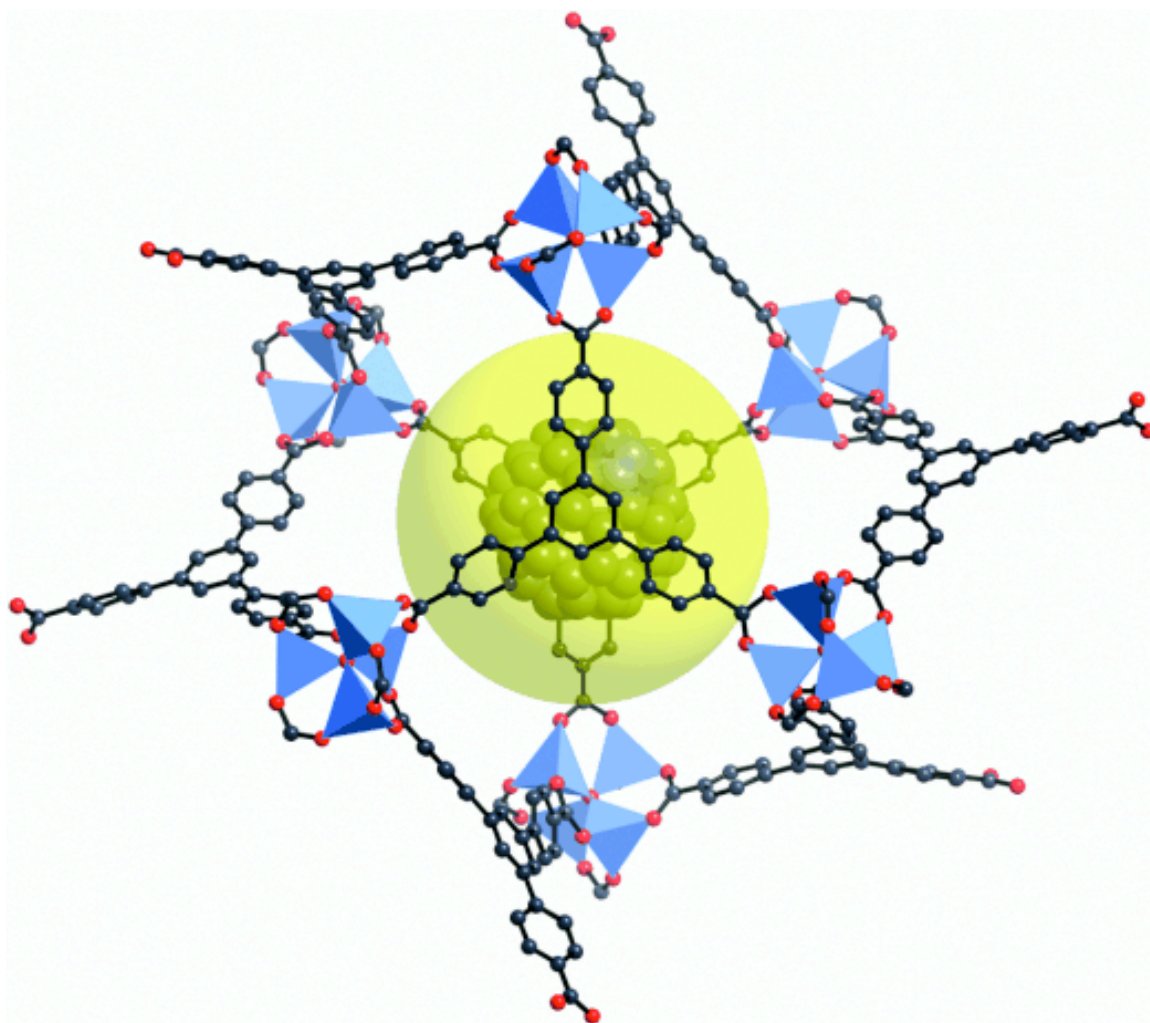


Hydrogen Storage



Suggested Reading:

[1] *Strategies for Hydrogen Storage in Metal-Organic Frameworks.* Rowsell, J. L. C.; Yaghi, O. M. *Angew. Chem. Int. Ed.* **2005**, *44* (30), 4670-4679.

Question 1. Provide brief and concise definitions for each term. State what each abbreviation stands for (spell it out) and explain what that means. For abbreviations that refer to chemicals, give the full name, the structure, and the function. (20 points)

MOF

IRMOF

MJL⁻¹

DOE

bdc, as in $Zn_4O(bdc)_3$, IRMOF-1

Question 2. It is said that “hydrogen has approximately three times the gravimetric energy density of petrol.” What does that mean? (a) Explain “gravimetric energy density,” (b) provide estimates for the gravimetric energy densities of hydrogen and petrol, and (c) explain the origin of the factor of three. (15 points)

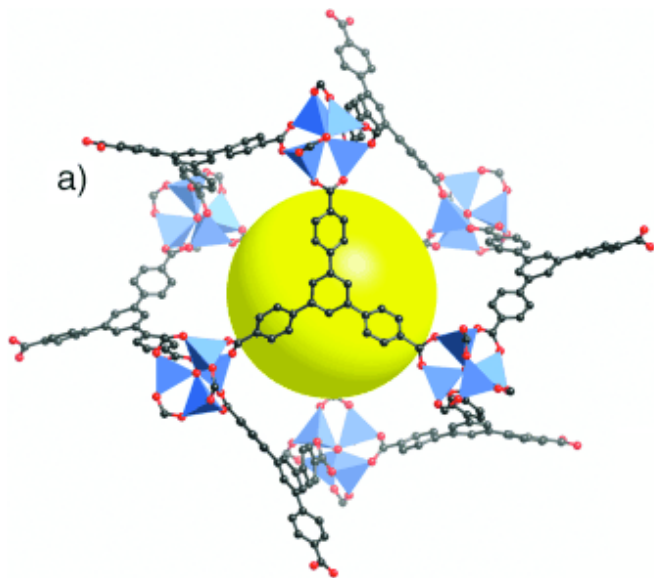
Question 3. The mass density of elemental hydrogen is **70.8 kg m⁻³** in its liquid state at 20 K and 1 atm. (a) What is the approximate mass density of water at room temperature? (b) Neglecting, T-effects on the mass density of condensed and frozen water, are there more molecules of H₂ or of H₂O in 1 m⁻³ of their respective liquids? (c) Explain your answer to (b) using your knowledge of intermolecular interactions. (15 points)

(a) Mass density of water at RT?

(b) Number of Particles?

(c) Atomistic Explanation for (b)?

Question 4. The image shows **MOF-177** as displayed in Figure 1 in the AC review. What exactly is shown? Can you translate this image into “normal structural formulas?” For the organic ligands also provide names. (16 points)



<p>Draw the structure of “one blue tetrahedron with the red edges.”</p>	<p>The organic ligand in MOF-177:</p>
<p>Draw the structure of “one organic ligand together with the two blue tetrahedral with their red corners on one side of the organic ligand.”</p>	<p>Provide the structure of another organic ligand used in other MOFs.</p>

Question 5. The gas-carrying capacity of MOF-177 is specified by two numbers in the AC review and these numbers and their units are given below. For each number, explain its meaning. (12 points)

4,500 m² g⁻¹

0.69 cm³ cm⁻³ [*sic*]

Question 6. In the AC review, the “**kinetic diameter of hydrogen molecule**” is said to be 289 pm. Any idea what this might be? Answer the basic questions in the top two rows and then argue that data relates to the “kinetic diameter.” (12 points)

What is the approximate bond length in H–H in pm?	What is the approximate van der Waals radius of hydrogen atom in pm?
What is the approximate length of H–H in pm when measured <u>along</u> the long axis?	What is the approximate length of H–H in pm when measured <u>perpendicular</u> the long axis?
Explain “kinetic diameter”	

Question 7. The image shown on the cover page is taken from Figure 3 of the AC review and was employed to explain the concept of “**impregnation**” to achieve an increased hydrogen storage. Explain the concept and explain what is displayed in the image as an application of the concept. (10 points)

