DATABASDESIGN FÖR INGENJÖRER - 1DL124

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Assignment 4 - AMOS II Database Project – Molecular Geometry

1.1 Goals

The exercise consists of the development of a small *molecular geometry database application* for storing and retrieving information about molecules by implementing schema definitions and queries in AMOSQL, the query language of AMOS II. The goal of this exercise is to give a practical experience to develop a small database application using an object-relational database management system including an object-relational query language. Few commercial systems exist yet, but most large relational database vendors have started to introduce extensions from the latest SQL99 standard to their current products or new object-relational database systems. In this assignment the students will work with the AMOS II object-relational DBMS which is a a research prototype system being developed at Uppsala Database Laboratory, Uppsala University.

This exercise is preferably carried out in groups with two students in each.

1.2 Preparations

Write your solutions on paper before testing them out on the AMOS II system.

1.3 Background reading

Read through chapter 20, 21 and 22 in the course book and any material (slides) from the lectures on object-oriented and object-relational databases systems and query languages. Worked through the AMOS II tutorial that is part of the AMOS II download. AMOS II is available on the course web at http://user.it.uu.se/~udbl/amos/.

Information about molecule geometry can for example be found at:
http://www.shef.ac.uk/chemistry/vsepr/

http://www.worldofmolecules.com/.

1.4 Instructions for the assignment

Connect to the course web page and download AMOS II, install the system on your PC. The exercise consists of 2 parts:

1.) Work through the AMOS II tutorial that is part of the AMOS II archive to download.

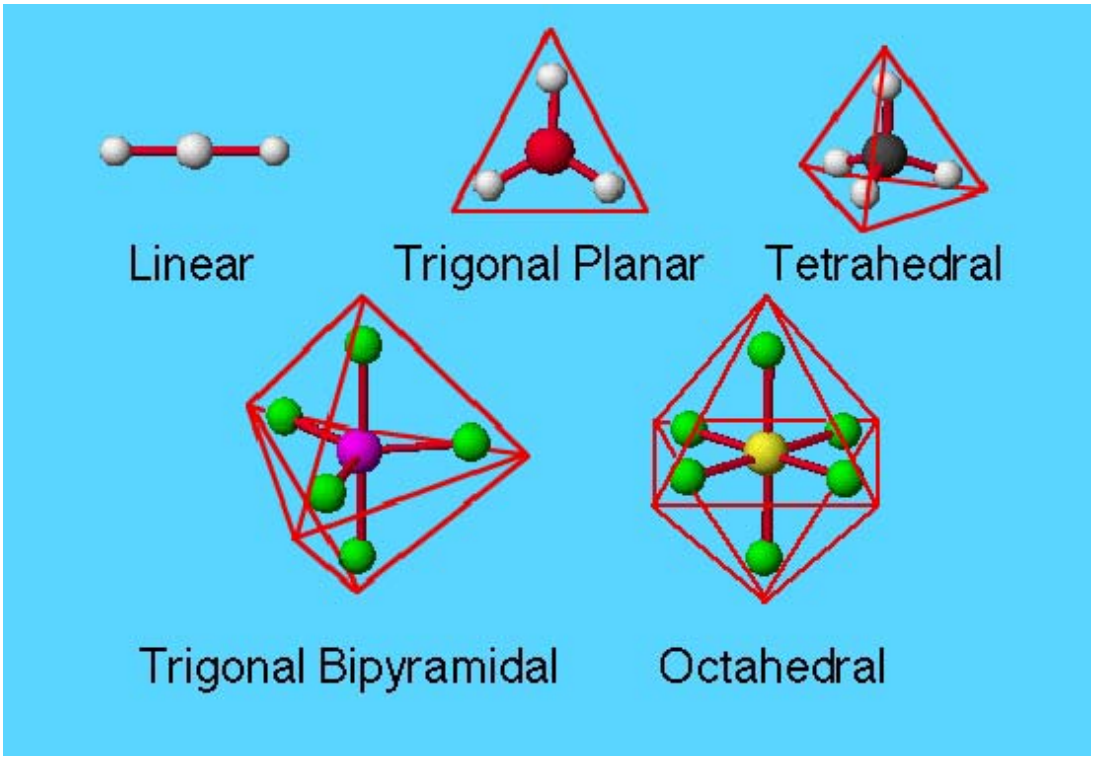

Figure 1. Molecular geometry types.

2.) Develop a molecular geometry database application to handle information regarding the structure and geometry of classes of molecules. Your test data should include at least the different molecule classes Linear, Trigonal Planar, Tetrahedral, Trigonal Bipyramidal and Octahedral. Additional molecule classes can be selected individually.

Number of electron pairs				
Total	Bonding	Nonbonding	Molecule (or ion) shape	Examples
2	2	0	linear	$HgCl_2$, $CuCl_2^-$
3	3	0	triangular planar	BF_3, $HgCl_3^-$
3	2	1	angular	$SnCl_2$, NO_2^-
4	4	0	tetrahedral	CH_4, BF_4^-
4	3	1	trigonal pyramidal angular	NH_3, PF_3
4	2	2	angular	H_2O, ICl_2^+
5	5	0	trigonal bipyramidal	PCl_5, $SnCl_5^-$
5	4	1	irregular tetrahedral	$TeCl_4$, IF_4^+
5	3	2	T-shaped	ClF_3, BrF_3
5	2	3	linear	XeF_2, ICl_2^-

6	6	0	octahedral	SF_6, PF_6^-
6	5	1	square pyramidal	IF_5, SbF_5^{2-}
6	4	2	square planar	BrF_4^-, XeF_4

Table 1. Number of electron pairs in the valence shell of the central atom and the shape of the atom or ion (from Chemistry, 6th ed, by Charles E. Mortimer, Wiley 1986).

The data collected for each molecule class should include information such as name, weight, central atom, number of valence electrons, attached groups, atoms or ions, atom (or ion) radii, number of bonding and nonbonding electrons, bonds, bond types and bond angles. Complement this information, if necessary to complete the assignment. For calculating spatial extensions of molecules, you can use an idealized model treating atoms as rigid spheres with the radius corresponding to their atomic radius.

Typical queries you should be able to answer are:

The name and type of molecules.

The weight of atoms as well as of molecules.

The angle between arbitrary atoms in the molecule.

The number of various bond types.

Which atoms are part of a certain bond.

The bounding volume (spherical) of a molecule.

Comparison of data for an unknown molecule with data stored in the database.

Matching a molecule of an unknown type with molecule types in the database.

Which molecule type does match a bounding sphere with a radius of 2,57 Å(ngström) and a molecule weight of 15u.

Which molecule type does match a bounding sphere with a radius of 2,54 Å and a molecule weight of about 18u.

Any additional and interesting queries are welcome. At least two such additional queries should be defined.

1.5 Handing in

Hand in an overview of the design, e.g. in an EER diagram, including explanations to concepts and symbols. Solutions to all the questions in the exercise as a printout of the interaction with AMOS II. This can be done by copying the results from the window where you are running AMOS II to a text file that you print out and hand-in to your assistant.