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Online Resources in Biophysical Chemistry

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Online Resources in Biophysical Chemistry

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Biophysical chemistry is an interdisciplinary field that focuses on the physical and chemical principles governing biological systems. Biophysical chemists seek to understand the molecular basis of interactions involving biological macromolecules and biological processes. This discipline employs spectroscopy and other physical methods to study biological molecules and processes. In academia, the interdisciplinary nature of this field is reflected in its alliance with a variety of traditional academic departments: Biochemistry, Chemistry, Molecular and Cell Biology, Physics, and Physiology. The Elsevier journal *Biophysical Chemistry* aptly applies a descriptive subtitle: "... devoted to the physics and chemistry of biological phenomena" (http://www.elsevier.com/locate/inca/522499, accessed 10/8/05).

Many of the sites listed below also appear on the "Biophysical Chemistry Web Site" (http://chemistry.library.wisc.edu/biophysics/biophysicshome.htm) developed by Dr. Silvia Cavagnero and Emily Wixson at the University of Wisconsin-Madison Chemistry Department. This site was originally developed for Dr. Cavagnero's course Chemistry 565/665 "Biophysical Chemistry". Emily Wixson maintains the site as a resource for the biophysical chemistry community at UW-Madison.

I. Sites of General Interest

- CMS Molecular Biology Resource. http://restools.sdsc.edu/ (accessed 10/8/05).
- IMB Jena Image Library of Biological Macromolecules. http://www.imb-jena.de/IMAGE.html (accessed 10/8/05).
- ExPASy Proteomics Server. http://us.expasy.org/ (accessed 10/8/05).
- National Center for Biotechnology Information (NCBI) ENTREZ Databases. http://www.ncbi.nlm.nih.gov/Database/ (accessed 10/8/05).

II. Structure of Biomolecules

- Entrez Structure. http://www.ncbi.nlm.nih.gov/entrez/query.fcgi?db=Structure (accessed 10/8/05). Molecular Modeling Database contains 3-D macromolecular structures (subset of PDB).
- Enzyme Structures Database. http://www.ebi.ac.uk/thornton-srv/databases/enzymes/ (accessed 10/8/05). Enzyme structures deposited in the PDB.
- Macromolecular Structure Database. EMBL-EBI. http://www.ebi.ac.uk/Databases/ (accessed 10/8/05).
- Nucleic Acids Database. http://ndbserver.rutgers.edu/ (accessed 10/8/05). Repository of three-dimensional structural information.
- PIR-NRL3D. http://pir.georgetown.edu/pirwww/dbinfo/nrl3d.html (accessed 10/8/05). Permits similarity searching of Protein Data Bank sequences; cross-references other PIR Protein Sequence Databases.
- Protein Data Bank ("PDB"). http://www.rcsb.org/pdb/ (accessed 10/8/05). Worldwide repository for 3-D biological macromolecular structure data.
- SCOP: Structural Classification of Proteins. http://scop.berkeley.edu/ (accessed 10/7/05).
- VIPER (VIrus Particle ExploreR). http://viperdb.scripps.edu/ (accessed 10/7/05). Descriptions of icosahedral virus structures in the PDB.

III. Function, Physical Properties, and Prediction

- Bioinformatics Center. RNA & DNA Folding Applications. http://www.bioinfo.rpi.edu/applications/mfold/ (accessed 10/7/05).
- BRENDA. http://www.brenda.uni-koeln.de/ (accessed 10/7/05). Enzyme Information System available free of charge for academic, non-profit users via the internet and as an in-house database for commercial users.
- Catalytic Site Atlas. EMBL-EBI. http://www.ebi.ac.uk/thornton-srv/databases/CSA/ (accessed 10/7/05)
- Database of Macromolecular Movements. http://molmovdb.mbb.yale.edu/. (accessed 10/7/05)

- PSA Protein Structure Prediction Server. http://bmerc-www.bu.edu/psa/ (accessed 10/7/05).
- PRINTS. http://bioinf.man.ac.uk/dbbrowser/PRINTS/ (accessed 10/7/05). Groups of conserved motifs used to characterize protein families.

IV. Visualization Tools

- Chime, MDL (plug-in). http://www.mdl.com/products/framework/chime/ (accessed 10/7/05).
- Cn3D, NCBI (plug-in). http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml (accessed 10/7/05).
- GRASP. Graphical Representation and Analysis of Structural Properties. http://trantor.bioc.columbia.edu/grasp/ (accessed 10/7/05).
- MolMol http://www.mol.biol.ethz.ch/groups/wuthrich_group/software (accessed 10/7/05). Molecular analysis and display. Also other tools from Institute for Molecular Biology and Biophysics. Zurich.
- Protein Explorer, University of Massachusetts (Java). http://www.umass.edu/microbio/chime/pe/protexpl/frntdoor.htm (accessed 10/7/05).
- RasMol, University of Massachusetts (plug-in). http://www.umass.edu/microbio/rasmol/index2.htm (accessed 10/7/05).
- Richardsons' 3D Protein Structure Laboratory, Duke University (plug-ins). http://kinemage.biochem.duke.edu/ (accessed 10/7/05).
- Deep View Swiss-Pdb Viewer, GlaxoSmithKline R&D Geneva. http://us.expasy.org/spdbv/ (accessed 10/7/05).
- WebMol, EMBL-Heidelberg (Java). http://www.cmpharm.ucsf.edu/cgi-bin/webmol.pl (accessed 10/7/05).

V. Techniques for the Study of Biomolecules

- Biophysical Techniques. http://www.biophysics.org/education/techniques.htm (accessed 10/7/05)
- spectroscopyNOW.com. http://www.spectroscopynow.com (accessed 10/7/05). Includes ezine, news, education and links for Atomic, IR, MRI, MS< NMR< Raman, UV, X-ray, Chemometrics, and Proteomics spectroscopy.
- Understanding Chemistry: Instrumental Analysis. http://www.chemguide.co.uk/analysismenu.html (accessed 10/7/05).
- The Basics of NMR. http://www.cis.rit.edu/htbooks/nmr/ (accessed 10/7/05).
- Crystallography Online. http://www.iucr.org/cww-top/crystal.index.html (accessed 10/7/05).
- Interactive Course on Symmetry and Analysis of Crystal Structure by Diffraction. http://marie.epfl.ch/x-ray/ (accessed 10/7/05).
- Interactive Tutorial about Diffraction. http://www.uni-wuerzburg.de/mineralogie/crystal/teaching/teaching.html (accessed 10/7/05).Guide to crystal structures and their Fourier transforms
- Mass Spectrometry On-line Tutorial. http://www.public.iastate.edu/%7Ekamel/mstutorial.html (accessed 10/7/05).
- NMR Information Server. http://spincore.com/nmrinfo/ (accessed 10/7/05).
- Structure Determination of Proteins with NMR Spectroscopy. http://www.cryst.bbk.ac.uk/PPS2/projects/schirra/html/home.htm (accessed 10/7/05).
- WebSpectra. http://www.chem.ucla.edu/%7Ewebspectra/ (accessed 10/7/05). NMR and IR study problems.

VI. Organizations

- Biophysical Society (BPS). http://www.biophysics.org/ (accessed 10/7/05).
- Bioelectrochemical Society (BES). http://www.bes-online.usf.edu/ (accessed 10/7/05).
- Biophysical Society of Canada (BSC). http://www.uqtr.ca/bsc/(accessed 10/7/05).
- European Biophysical Societies Association. http://www.ebsa.org/(accessed 10/7/05).
- International Union for Pure and Applied Biophysics.http://www.iupab.org/ (accessed 10/7/05).

- The Protein Society. http://www.proteinsociety.org/(accessed 10/7/05).

For background reading, see:

1. Bloomfield, Victor A., Donald M. Crothers, and Ignacio Tinoco, Jr. *Nucleic Acids: Structures, Properties, and Functions*. University Science Books: Sausalito, Calif., 2000.
2. Cantor, Charles R. and Paul R. Schimmel. *Biophysical Chemistry*. W. H. Freeman: San Francisco, 1980.
3. Creighton, Thomas E. P*roteins: Structures and Molecular Properties*, 2nd ed. W.H. Freeman: New York, 1993.
4. Eisenberg, David and Donald Crothers. *Physical Chemistry with Applications to the Life Sciences*. Benjamin/Cummings: Menlo Park, Calif., 1979.
5. Hammes, Gordon G. *Thermodynamics and Kinetics for the Biological Sciences*. Wiley-Interscience: New York, 2000.
6. Tinoco, Jr., Ignacio et al. *Physical Chemistry: Principles and Applications in Biological Sciences*, 4th ed. Prentice Hall: Upper Saddle River, N.J., 2002.❖

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pH properly Help: Thermodynamics

Linda Shackle

The Four Horsemen of Thermodynamics:
Entropy
Free Energy
Heat Capacity
Heat of Formation

Thermodynamics is the study of energy and equilibrium at a macro, rather than molecular, level. Normally three laws of thermodynamics are given although sometimes a fourth is presented as the "Zeroth Law," a precursor to the First Law. The laws of thermodynamics can be applied in almost all areas of science and engineering. For a practical example, the recent hurricanes[1] that struck the southern United States owe their existence in part to the thermodynamics forces at work in the atmosphere.

Energy, unless restricted, has a tendency to disperse; this tendency is called entropy. S is the symbol for entropy and has units of energy (joule, calorie, British thermal unit) per temperature (Kelvin, Celsius, Fahrenheit, Rankine) hence J $^{\circ}C^{-1}$, Btu $^{\circ}R^{-1}$, etc.

Free energy, as its name implies, is the amount of energy available to the system under study. There are two types of free energy, Gibbs, named after Professor Josiah Willard Gibbs (1839-1903) of Yale University, and Helmholtz, named after Hermann von Helmholtz (1821-1894) a German physicist and physician. Gibbs free energy uses the symbol G and Helmholtz uses A (Arbeitfunktion = work function), however both may sometimes be designated as F. You are more likely to see Gibbs free energy in chemical reference sources and Helmholtz in physics resources.

Heat capacity is defined as the amount of energy needed to change a system's temperature by one unit. The symbol for heat capacity is C; the units are the same as for entropy. Sometimes specific heat capacity is given in thermodynamics tables; specific heat capacity is the amount of energy needed to raise one unit of a substance one degree in termperature. The symbol for specific heat capacity is Cp and the units are the same as for heat capacity except for the addition of the substance unit (ex. J $kg^{-1} K^{-1}$).

Heat of formation is the heat released or absorbed during the formation of a substance. Sometimes the term "enthalpy" is used instead