

DAFTAR PUSTAKA

- Allen , M.P., Tildesley, D.J., 1991, *Computer Simulation of Liquids*, Oxford University Press, New York.
- Allen , M.P., 2004, *Introduction to Molecular Dynamics Simulation*, Centre for Scientific Computing and Department of Physics, University of Warwick United Kingdom.
- Aberg, M., 1977. An X-Ray Investigation of Some Aqueous Zirconium(IV) Halide a Hafnium(IV) Chloride, and Some Zirconium(IV) Perchlorate Solutions. *Acta Chem. Scand., Ser. B.*, 31, 171.
- Armunanto, R., Schwenk, C. F., Randolph, B.R., dan Rode, B. M., 2004, Ag(I) ion in liquid ammonia, *Chem. Phys. Lett.*, 388, 395-399.
- Armunanto, R., Schwenk, C. F., dan Rode, B. M., 2003, Structure and dynamics of hydrated Ag (I): Ab initio quantum mechanical-molecular mechanical molecular dynamics simulation, *J. Phys. Chem. A*, 107, 3132–3138.
- Armunanto, R., Schwenk, C. F., Setiaji, A.H.B., dan Rode, B. M., 2003, Classical and QM/MM molecular dynamics simulations of Co^{2+} in water, *Chem. Phys.*, 295, 63–70.
- Armunanto, R., Schwenk, C.F., Tran, H.T., dan Rode, B.M., 2004, Structure and Dynamics of Au^+ Ion in Aqueous Solution: Ab Initio QM/MM MD Simulations, *J. Am. Chem. Soc.*, 126, 2582-2587.
- Armunanto, R., Schwenk, C. F., dan Rode, B. M., 2005, Ab initio QM/MM simulation of Ag^+ in 18.6% aqueous ammonia solution: Structure and dynamics investigations. *J. Phys. Chem. A*, 109, 4437–4441.
- Armunanto, R., Schwenk, C.F., dan Rode, B.M., 2004, Gold(I) in Liquid Ammonia: Ab Initio QM/MM Molecular Dynamics Simulation, *J. Am. Chem. Soc.*, 126, 9934-9935.
- Armunanto, R., Schwenk, C.F., Randolph, B.R., dan Rode, B.M., 2004, Structure and dynamics of Co^{2+} in liquid ammonia: ab initio QM/MM molecular dynamics simulation, *Chem. Phys.*, 305, 135-140.
- Ahlich, R. M. Br, Horn, H., Hser, M., dan Klmel, C., 1989, Turbomole, *Chem. Phys.Lett.* 162, 165.

- Azam, S.S., Hofer, T.S., Randolph, B.R., dan Rode, B.M., 2009, Hydration of Sodium(I) and Potassium(I) Revisited: A Comparative QM/MM and QMCF MD Simulation Study of Weakly Hydrated Ions, *J. Phys. Chem. A*, 113, 1827–1834.
- Berthod, H. dan Pullman, A., 1980, On the Affinities of Ammonia and Water for Li^+ , Na^+ and K^+ , *Chem. Phys. Lett.*, 70, 434-437.
- Blauth, C.M., Pribil, A.B., Randolph, B.R., Rode, B.M., dan Hofer, T.S., 2010, Structure and dynamics of hydrated Ag^+ : An ab initio quantum mechanical/charge field simulation, *Chem. Phys. Lett.*, 500, 251-255.
- Blumenthal, W. B., 1958, *The chemical behavior of zirconium*, Van Nostrand.
- Brancato, G., Rega, N., dan Barone, V., 2008, Microsolvation of the Zn(II) ion in aqueous solution: A hybrid QM/MM MD approach using non-periodic boundary conditions, *Chem. Phys. Lett.*, 451, 53–57.
- Brendle, J.M., Khouchaf, L., Baron, Le Dred, J.R., dan Tuilier, M.H., 1997, Zr-exchanged and pillared beidellite: preparation and characterization by chemical analysis, XRD and Zr K EXAFS, *Microporous Materials*, 11, 171–183.
- Cox, P.J., 1982. Molecular Mechanics: Illustrations of its application, *J. Chem. Educ.*, 59,4, 274-277.
- Cramer, C. J., 2004, *Essentials of Computational Chemistry: Theories and Models*, John Wiley & Sons, England.
- Dennington, R., Keith, T., Millam, J. GaussView, Version 5, *Semichem Inc.*, Shawnee Mission, KS, 2009.
- Durdagi, S., Hofer, T.S., Randolph, B.R., Rode, B.M., 2005, Structural and dynamical properties of Bi^{3+} in water, *Chem. Phys. Lett.*, 406, 20–23.
- Eklund, L., 2014, *Hydration of Oxo Anions: A Combined Computational and Experimental Structure and Dynamics Study in Aqueous Solutions*, Uppsala, Swedia.
- Fatmi, M.Q., Hofer, T.S., Randolph, B.R. dan Rode, B.M., 2005, An extended ab initio QM/MM MD approach to structure and dynamics of Zn(II) in aqueous solution., *J. Chem. Phys.* 123, 054514.
- Fatmi, M.Q., 2007, *Molecular dynamics simulations of industrially and biologically relevant ions*. Leopold-Franzens-Universität Innsbruck, Austria.

- Fatmi, M.Q., Hofer, T.S., Randolph, B.R. dan Rode, B.M, 2006, Temperature Effects on the Structural and Dynamical Properties of the Zn(II)-Water Complex in Aqueous Solution: A QM/MM Molecular Dynamics Study, *J. Phys. Chem. B*, 110, 616-621.
- Fatmi, M.Q., Hofer, T.S., Randolph, B.R. dan Rode, B.M, 2006, Structure and dynamics of the $[Zn(NH_3)(H_2O)_5]^{2+}$ complex in aqueous solution obtained by an ab initio QM/MM molecular dynamics study, *Phys. Chem. Chem. Phys.*, 8, 1675–1681.
- Fatmi, M.Q., Hofer, T.S., Randolph, B.R. dan Rode, B.M., 2007, Stability of Different Zinc(II)-Diamine Complexes in Aqueous Solution with Respect to Structure and Dynamics: A QM/MM MD Study, *J. Phys. Chem. B*, 111, 151-158.
- Frick, R.J., Pribil, A.B., Hofer, T.S., Randolph, B.R., Bhattacharjee, A., dan Rode, B.M., 2009, Structure and Dynamics of the U^{4+} Ion in Aqueous Solution: An ab Initio Quantum Mechanical Charge Field Molecular Dynamics Study, *Inorg. Chem*, 3993-4002.
- Favre-Réguillon, A., Fiaty, K., Laurent, P., Poriel, L., Pellet-Rostaing, S. dan Lemaire, M., 2007, Solid/Liquid Extraction of Zirconium and Hafnium in Hydrochloric Acid Aqueous Solution with Anion Exchange Resin-Kinetic Study and Equilibrium Analyses, *Ind. Eng. Chem. Res.*, 46, 1286–1291.
- Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Montgomery, Jr., J. A., Vreven, T., Kudin, K. N., Burant, J. C., Millam, J. M., Iyengar, S. S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G. A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J. E., Hratchian, H. P., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Ayala, P. Y., Morokuma, K., Voth, G. A., Salvador, P., Dannenberg, J. J., Zakrzewski, V. G., Dapprich, S., Daniels, A. D., Strain, M. C., Farkas, O., Malick, D. K., Rabuck, A. D., Raghavachari, K., Foresman, J. B., Ortiz, J. V., Cui, Q., Baboul, A. G., Clifford, S., Cioslowski, J., Stefanov, B. B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Martin, R. L., Fox, D. J., Keith, T., Al-Laham, M. A., Peng, C. Y., Nanayakkara, A., Challacombe, M., Gill, P. M. W., Johnson, B., Chen, W., Wong, M. W., Gonzalez, C. dan Pople, J. A., 2004, Gaussian 03, Revision E.01, Wallingford CT, Gaussian, Inc.
- Glusker, J.P., Amy K. Katz, A.K dan Bock, C.W., 1999, Metal Ions In Biological Systems, *The Rigaku Journal*, 16, 8-15.

- Hagfeldt, C., Kessler, V., dan Persson, I., 2004, Structure of the hydrated, hydrolysed and solvated zirconium(IV) and hafnium(IV) ions in water and aprotic oxygen donor solvents. A crystallographic, EXAFS spectroscopic and large angle X-ray scattering study, *Dalton Trans.*, 14, 2142.
- Hannongbua, S. V., Ishida, T., Spohr, E. dan Heizinger, K. Z., 1988, Molecular Dynamics Study of a Lithium Ion in Ammonia, *Naturforsch*, 43a, 572–582.
- Harris, D.J., Brodholt, J.P., dan Sherman, D.M., 2003, Hydration of Sr^{2+} in Hydrothermal Solutions from ab Initio Molecular Dynamics, *J. Phys. Chem. B*, 107, 9056-9058.
- Hebre, W. J., 2003, *A Guide to Molecular Mechanics and Quantum Chemical Calculations*, Wavefunction, Inc, Irvine.
- Hedman, F., 2006, Algorithms for Molecular Dynamics Simulations, *Thesis*, Stockholms Universitet, Stockholm, 2006.
- Himanen, L., 2015, Hybrid Quantum Mechanical and Molecular Mechanical Modeling in Ion-Water Solutions, *Thesis*, Aalto University, Espoo
- Hofer, T. S., Pribil, A. B., Randolph, B. R. dan Rode, B. M., 2005, Structure and dynamics of solvated Sn(II) in aqueous solution: An ab initio QM/MM MD approach, *J. Am. Chem. Soc.*, 127, 14231–14238.
- Hofer, T. S., Scharnagl, H., Randolph, B. R., dan Rode, B. M., 2006, Structure and dynamics of La(III) in aqueous solution—An ab initio QM/MM MD approach, *Chemical physics*, 327, 31–42.
- Hofer, T. S., Tran, H. T., Schwenk, C. F., dan Rode, B. M., 2003, Characterization of dynamics and reactivities of solvated ions by ab initio simulations. *Journal of computational chemistry*, 25, 211–217.
- Hofer, T. S., Randolph, B. R., dan Rode, B. M., 2006, Sr(II) in Water: A Labile Hydrate with a Highly Mobile Structure, *J. Phys. Chem. B*, 110, 20409-20417.
- Hofer, T. S., Randolph, B. R., dan Rode, B. M., 2006, The influence of quantum forces on molecular dynamics simulation results for hydrated aluminium(III), *Chem. Phys. Lett.*, 422, 492–495
- Hofer, T.S., Rode, B.M., dan Randolph, B.R., 2005, Structure and dynamics of solvated Ba(II) in dilute aqueous solution – an ab initio QM/MM MD approach, *Chem. Phys.*, 312, 81–88.

- Huheey, J.E., Keiter, E.A., dan Keiter, R.L., 1993, *Inorganic Chemistry: Principles of Structure and Reactivity*, HarperCollins College Publisher, New York.
- Humphrey, W., Dalke, A. dan Schulten, K., 1996, VMD-Visual Molecular Dynamics, *J. Molec. Graphics*, 14, 33-38.
- Inada, Y., Loeffler, H. H., dan Rode, B. M., 2002, Librational, vibrational, and exchange motions of water molecules in aqueous Ni(II) solution: classical and QM/MM molecular dynamics simulations, *Chem. Phys. Lett.*, 358, 449-458.
- Inada, Y., Mohammed, A.M., Loeffler, H.H., and Rode, B.M., 2002, Hydration Structure and Water Exchange Reaction of Nickel(II) Ion: Classical and QM/MM Simulations, *J. Phys. Chem. A*, 106, 6783-6791.
- Jursic, B.S., 1999, Complete basis set, Gaussian, and hybrid density functional theory evaluation of the proton affinities of water and ammonia, *Theochem*, 190, 1-6.
- Kerdcharoen, T., Rode, B.M., 2000, What Is the Solvation Number of Na^+ in Ammonia? An Ab Initio QM/MM Molecular Dynamics Study, *J. Phys. Chem. A*, 104, 7077.
- Kerdcharoen, T., Liedl, K. R., dan Rode, B. M., 1996, A QM/MM simulation method applied to the solution of Li^+ in liquid ammonia, *Chem. Phys.*, 211, 313-323.
- Koehl, P., Orland, H., dan Delarue, M., 2009, Solvation of Ion Pairs: The Poisson-Langevin Model, *International Conference*, 917-923.
- Kraus, F., Baer, S. A. dan Fichtl, M. B., 2009, The Reactions of Silver, Zirconium, and Hafnium Fluorides with Liquid Ammonia: Syntheses and Crystal Structures of $Ag(NH_3)_2 F \cdot 2NH_3$, $[M(NH_3)_4 F_4] \cdot NH_3$ (M= Zr, Hf), and $(N_2H_7) F$. *Eur. J. Inorg. Chem.*, 2009, 441-447.
- Kritayakornpong, C., Plankensteiner, K. dan Rode, B.M, 2003, Structure and Dynamics of the Cd^{2+} Ion in Aqueous Solution: Ab Initio QM/MM Molecular Dynamics Simulation, *J. Phys. Chem. A*, 107, 10330-10334.
- Kritayakornpong, C., Yagüe, J.I. dan Rode, B. M., 2002, Molecular Dynamics Simulations of the Hydrated Trivalent Transition Metal Ions Ti^{3+} , Cr^{3+} , and Co^{3+} , *J. Phys. Chem. A*, 106, 10584-10589.
- Kritayakornpong, C. dan Hannongbua, S., 2007, Structure and dynamics of high-spin Ru^{2+} in aqueous solution: Ab initio QM/MM molecular dynamics simulation, *Chem. Phys.*, 332, 95-101.

- Kritayakornupong, C., Plankensteiner, K. dan Rode, B.M, 2003, Dynamics in the hydration shell of Hg²⁺ ion: classical and ab initio QM/MM molecular dynamics simulations, *Chem. Phys. Lett.*, 371, 438–444.
- Kropman, M. F., dan Bakker, H. J., 2001, Dynamics of Water Molecules in Aqueous Solvation Shells, *Science*, 291, 2118–2120.
- Leach, A.R., 2001, *Molecular Modelling Principles and Applications*, Prentice Hall, London.
- Lev, B.B, Salahub, D.R. dan Noskov, S.Y., 2010, Na⁺, K⁺ and TI⁺ Hydration from QM/MM Computations and MD Simulations with a Polarizable Force Field, *Interdiscip Sci Comput Life Sci*, 2, 12–20.
- Lutz, O.M.D., Hofer, T.S., Randolf, B.R., Weiss, A.K.H., dan Rode, B.M., 2012, A QMCF-MD Investigation of the Structure and Dynamics of Ce⁴⁺ in Aqueous Solution, *Inorg. Chem.*, 51, 6746–6752.
- Lindqvist-Reis, P., 2000, Structure of solvated metal ions: Solution and crystal structure of Ga³⁺, In³⁺, Sc³⁺, Y³⁺, La³⁺ and Ca²⁺ ions with water and non-aqueous oxygen donor solvents, *Thesis*, Department of Chemistry, Royal Institute of Technology, Stockholm.
- Li, X., 2011, Applications of Molecular Dynamics in Atmospheric and Solution Chemistry, *Thesis*, Department of Theoretical Chemistry and Biology, Royal Institute of Technology, Stockholm.
- Loeffler, H.H., Yague, J.I. dan Rode, B.M., 2002, QM/MM–MD simulation of hydrated vanadium(II) ion, *Chem. Phys. Lett.*, 363, 367–371.
- Loeffler, H. H., 2003, Many-body effects on structure and dynamics of aqueous ionic solutions, *Journal of computational chemistry*, 24, 1232–1239.
- Mahler, J. dan Persson, I., 2011, A Study of the Hydration of the Alkali Metal Ions in Aqueous Solution, *Inorg. Chem*, 51, 425–438.
- Marini, G.W., Liedl, K.R. dan Rode, B.M., 1999, Investigation of Cu²⁺ Hydration and the Jahn-Teller Effect in Solution by QM/MM Monte Carlo Simulations, *J. Phys. Chem. A.*, 103, 11387-11393.
- Mark, T. C. W., 1968, Refinement of the crystal structure of zirconyl chloride octahydrate, *Can. J. Chem.*, 46, 3491-3497.
- Meier, W., Bopp, P., Probst, Spohr, E. dan Lin, J., 1990, Molecular dynamics studies of lanthanum chloride solutions, *Phys. Chem*, 94, 4672.

- Messner, C.B., Hofer, T.S., Randolph, B.R. dan Rode, B.M., 2011, Structure and dynamics of the Zr^{4+} ion in water, *Phys. Chem. Chem. Phys.*, 13, 224–229.
- Messner, C.B., Hofer, T.S., Randolph, B.R. dan Rode, B.M., 2011, Computational study of the hafnium(IV) ion in aqueous solution, *Chem. Phys. Lett.*, 501, 292–295.
- Miehe´-Brendle´, J., Khouchaf, L., Baron, J., Dred, R.L. dan Tuilier, M.H., 1997, Zr-exchanged and pillared beidellite: preparation and characterization by chemical analysis, XRD and Zr K EXAFS, *Microporous Materials*, 11, 171–183
- Miessler, G. L., Tarr, D. A., 2003, *Inorganic Chemistry*, Minnesota, Pearson Prentice Hall
- Mohammed, A.M., 2003, Hydration Structure of Ti(III) and Cr(III): Monte Carlo Simulation Including Three-Body Corrections, *Bull. Chem. Soc. Ethiop.*, 17, 199-210.
- Ogbonna, N., 2004, *Molecular Dynamics Simulation*, African Institute for Mathematical Sciences, South Africa.
- Ohtaki, H., Radnai, R., 1993, Structure and Dynamics of Hydrated Ions, *Chem. Rev.*, 93, 1157-1204.
- Orabi, E.A., dan Lamoureux, G., 2013, Molecular Dynamics Investigation of Alkali Metal Ions in Liquid and Aqueous Ammonia, *J. Chem. Theory Comput.*, 9, 2324–2338.
- Owen, S.M. dan Brooker, A.T., 1991, *A Guide to Modern Inorganic Chemistry*, Singapore, Longman Singapore Publishers Pte Ltd.
- Plitzko, C., Strecker, M. dan Meyer, G., 1997, Synthesis and Crystal Structure of the Fluoride-Ammine Complexes $Zr(NH_3)F_4$ and $Hf(NH_3)F_4$, *Zeitschrift für anorganische und allgemeine Chemie*, 623, 79–83.
- Pranowo, H.D., Mudasir, Kusumawardani, C. dan Purtadi, S., 2006, The structure of Co^{2+} in liquid ammonia: Monte Carlo simulation including three-body correction, *Chem. Phys.*, 324, 573–578.
- Pranowo, H.D. dan Rode, B.M., 2001, Preferential Cu^{2+} solvation in aqueous ammonia solution of various concentrations, *Chem. Phys.*, 263, 1-6.
- Pranowo, H.D. dan Rode, B.M., 1999, Solvation of Cu^{2+} in Liquid Ammonia: Monte Carlo Simulation Including Three-Body Corrections, *J. Phys. Chem. A*, 103, 4298-4302.

- Pranowo, H.D., Setiaji, A. H. B. dan Rode, B.M., 1999, Cu^+ in Liquid Ammonia and in Water: Intermolecular Potential Function and Monte Carlo Simulation, *J. Phys. Chem. A*, 103, 11115-11120.
- Ramachandran, K. I., Deepa, G. dan Namboori, K., 2008, *Computational Chemistry and Molecular Modeling: Principles and Applications*. Springer.
- Rao, N., Holerca, M.N., Klein, M.L., dan Pophristic, V., 2007, Computational Study of the Zr^{4+} Tetranuclear Polymer, $[Zr_4(OH)_8(H_2O)_{16}]^{8+}$, *J. Phys. Chem. A*, 111, 11395- 11399
- Rasaiah, J.C dan Lynden-Bell, R.M., 2001, Computer simulation studies of the structure and dynamics of ions and non-polar solutes in water, *Phil. Trans. R. Soc. Lond. A*, 359, 1545-1574.
- Remsungnen, T. dan Rode, B. M., 2003, QM/MM Molecular Dynamics Simulation of the Structure of Hydrated Fe(II) and Fe(III) Ions, *J. Phys. Chem. A*, 107, 2324-2328.
- Remsungnen, T. dan Rode, B. M., 2004, Molecular dynamics simulation of the hydration of transition metal ions: the role of non-additive effects in the hydration shells of Fe^{2+} and Fe^{3+} ions. *Chem. Phys. Lett.*, 385, 491–497.
- Rybicki, M., Hawlicka, E., 2012, Solvation of Mg^{2+} ions in methanol–water mixtures: Molecular dynamics simulation, *Chem. Phys.*, 400, 79–85.
- Rode, B. M., dan Hofer, T. S., 2006, How to access structure and dynamics of solutions: The capabilities of computational methods. *Pure and applied chemistry*, 78, 525.
- Rode, B.M., Schwenk, C.F. dan Tongraar, A., 2004, Structure and dynamics of hydrated ions—new insights through quantum mechanical simulations, *Journal of Molecular Liquids*, 110, 105–122.
- Rode, B.M., Schwenk, C.F., , Hofer, T.S. dan Randolph, B.R., 2005, Coordination and ligand exchange dynamics of solvated metal ions, *Coordination Chemistry Reviews*, 249, 2993–3006.
- Stillinger, F. H.; Rahman, A., 1978, Revised central force potentials for water. *J. Chem. Phys.*, 68, 666–670.
- Schwenk, C. F., Loferer, M. J. dan Rode, B. M., 2003, Ultrafast ligand exchange rates determined by ab initio QM/MM molecular dynamics. *Chem. Phys. Lett.*, 382 (3), 460–465.

- Schwenk, C. F., Loferer, M. J., dan Rode, B. M., 2003, Structure and Dynamics of Metal Ions in Solution: QM/MM Molecular Dynamics Simulations of Mn^{2+} and V^{2+} , *J. Am. Chem. Soc.*, 125, 1618-1624.
- Schwenk, C. F.; Rode, B. M., 2003, Influence of heteroligands on structural and dynamical properties of hydrated Cu^{2+} : QM/MM MD simulations, *Phys. Chem. Chem. Phys.*, 5, 3418–3427.
- Shah, S. A.A., Thomas S. Hofer, T.S., M. Qaiser Fatmi, M.Q., Randolph, B.R. dan Rode, B.M., 2006, A QM/MM MD simulation study of hydrated Pd^{2+} , *Chem. Phys. Lett.*, 426, 301–305.
- Spangberg, D., 2003, Cation solvation in water and acetonitrile from theoretical calculations, *Thesis*, Uppsala University.
- Tongraar, A., Liedl, K. R., dan Rode, B. M., 1997, Solvation of Ca^{2+} in water studied by Born-Oppenheimer ab initio QM/MM dynamics, *J. Phys. Chem. A*, 101, 6299–6309.
- Tongraar, A., Hannongbua, S., dan Rode, B.M., 1997, Molecular dynamics simulations of a potassium ion and an iodide ion in liquid ammonia, *Chem. Phys.*, 219, 279-290.
- Tongraar, A., Liedl, K.R. dan Rode, B.M., 1998, The Hydration Shell Structure of Li^+ Investigated By Born-Oppenheimer Ab Initio QM/MM Dynamics, *Chem. Phys. Lett.*, 286, 56–64.
- Tongraar, A., Liedl, K.R., Rode, B.M., 1998, Born–Oppenheimer ab Initio QM/MM Dynamics Simulations of Na^+ and K^+ in Water: From Structure Making to Structure Breaking Effects, *J. Phys. Chem. A*, 102, 10340–10347.
- Tongraar, A. dan Rode, B.M., 2001, A Born Oppenheimer Ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation on Preferential Solvation of Na^+ in Aqueous Ammonia Solution, *J. Phys. Chem. A*, 105, 506 510.
- Tongraar, A., Sagarik, K. dan Rode, B.M., 2001, Effects of Many-Body Interactions on the Preferential Solvation of Mg^{2+} in Aqueous Ammonia Solution: A Born Oppenheimer ab Initio QM/MM Dynamics Study, *J. Phys. Chem. B*, 105, 10559-10564.
- M.S. Valli, Matsuo, H. Wakita, T. Yamaguchi, M. Nomura, 1996, Solvation of Copper(II) Ions in Liquid Ammonia, *Inorg. Chem*, 35, 5642.

- Vizioso S. dan Rode, B.M., 1995, Na^+ in liquid hydroxylamine: pair potential function from ab initio calculations and Monte Carlo computer simulation of a 0.36 M NaCl solution (2 NaCl 200 NH_2OH). *Chem. Phys.*, 199, 129–144.
- Xenides, D., Randolph, B.R. dan Rode, B.M., 2006, Hydrogen bonding in liquid water: An ab initio QM/MM MD simulation study, *Journal of Molecular Liquids*, 123, 61 – 67.
- Yagüe, J. I., Mohammed, A. M., Loeffler, H.H. dan Rode, B. M., 2001, Classical and mixed quantum mechanical/molecular mechanical simulation of hydrated manganous ion. *J. Phys. Chem. A*, 105, 7646–7650.
- Yagüe, J.I., Mohammed, A.M., Loeffler, H.H. dan Rode, B.M., 2003, MD and MC simulations of hydrated manganous ion including three-body effects, *Journal of Molecular Structure: Theochem*, 620, 15–20.
- Zauliczny, M., Grubba, R., Ponikiewski, T. dan Pikies, J., 2013, Bis(diethylamido-N)(diethylamine-N)-bis(2,6-diisopropylphenylamido-N)-zirconium(IV), *Acta Cryst.*, E69, m72.
- Zhong, W., Parkinson, J.A., Parsons, S., Oswald, I.D.H., Coxall, R.A. dan Sadler, P.J., 2004, Structure and Dynamics of Dinuclear Zirconium(IV) Complexes, *Inorg. Chem*, 43, 3561-3572.