STUDI INTERAKSI ION Zr(IV) DAN Hf(IV) DENGAN ORGANOFOSFOR MENGGUNAKAN METODE DENSITY FUNCTIONAL THEORY (DFT)
FARUQ MUBAROK, Dr.rer.nat Ria Armunanto, S.Si, M.Si
Universitas Gadjah Mada, 2015 | Diunduh dari http://etd.repository.ugm.ac.id/

DAFTAR PUSTAKA

Alguacil, F.J., Delgado, A.L., Alonso, M., Sastre, A.M., 2004, The phosphine oxides Cyanex 921 and Cyanex 923 as carriers for facilitated transport of chromium (VI)-chloride aqueous solutions, *Chemosphere, 57*, 813-9.

Banda, R., Lee, H.Y., Lee, M.S., 2012, Separation of Zr from Hf in Hydrochloric Acid Solution Using Amine Based Extractants, *Ind. Eng. Chem. Res., 51*, 9652−9660.

Bhatta, B.C. and Mishra, S., 2014, Binary Mixture of Tri-Octyl Amine and Cyanex 923 as Extractant for the Extraction of Zr (IV) from Acidic Chloride Medium, *Int. J. Nonferrous Metall., 3*, 9-17.

Brathwaite, A.D. and Duncan, M.A., 2013, Infrared Photodissociation Spectroscopy of Saturated Group IV (Ti, Zr, Hf) Metal Carbonyl Cations, *J. Phys. Chem. A, 117*, 11695−11703.

Cramer, C., 2004, *Essentials of Computational Chemistry Theories and Models*, 2ed., Chichester, England: John Wiley & Son, Ltd.

Cuypers, R., Burghoff, B., Marcelis, A.T.M., Sudho¨lter, E.J.R., Haan, A.B.D., Zuilhof, H., 2008, Complexation of Phenols and Thiophenol by Phosphine Oxides and Phosphates. Extraction, Isothermal Titration Calorimetry, and ab Initio Calculations, *J. Phys. Chem. A, 112*, 11714–11723.

Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G.A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H.P., Izmaylov, A.F., Bloino, J., Zheng, G., Sonnenberg, J.L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, J.A., Peralta, J.E., Ogliaro, F., Bearpark, M., Heyd, J.J., Brothers, E., Kudin, K.N., Staroverov, V.N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J.C., Iyengar, S.S., Tomasi, T., Cossi, M., Rega, N., Millam, J.M., Klene, M., Knox, J.E., 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., Martin, R.L., Morokuma, K., Zakrzewski, V.G., Voth, G.A., Salvador, P., Dannenberg, J.J., Dapprich, S., Daniels, A.D., Farkas, O., Foresman, J.B., Ortiz, J.V., Cioslowski, J., Fox, D.J., 2009, Gaussian, Inc., Wallingford CT.

Hosseini, M.H. and Alizadeh, N., 2010, Coalescence Extraction System for Rapid Efficient and Selective Separation of Zirconium and Hafnium, *Ind. Eng. Chem. Res., 49*, 7068–7073.

UNIVERSITAS GADJAH MADA
STUDI INTERAKSI ION Zr(IV) DAN Hf(IV) DENGAN ORGANOFOSFOR MENGGUNAKAN METODE DENSITY FUNCTIONAL THEORY (DFT)
FARUQ MUBAROK, Dr.rer.nat Ria Armunanto, S.Si, M.Si
Universitas Gadjah Mada, 2015 | Diunduh dari http://etd.repository.ugm.ac.id/

Jensen, F., 2007, *Introduction to Computational Chemistry*, Chichester, England: John Wiley & Son, Ltd.

Krishna, G.G., Reddy, R.S., Raghunath, P., Bhanuprakash, K., Kantam, M.L., Choudary, B.M., 2004, A Computational Study of Ligand Interactions with Hafnium and Zirconium Metal Complexes in the Liquid-Liquid Extraction Process, *J. Phys. Chem. B, 108*, 6112-6120.

Kumar, S. and Babu B.V., 2009, Extraction of Pyridine-3-carboxylic Acid Using 1-Dioctylphosphoryloctane (TOPO) with Different Diluents: Equilibrium Studies, *J. Chem. Eng. Data, 54*, 2669–2677.

Leach, A., 2001, *Molecular Modelling Principles and Applications*, Great Britain, england: Dorset.

Mohammed, S.A. and Ahmad, H.H., 2009, Selective Extraction of Zirconium from Various Samples and Subsequent Spectrophotometric Determination with Eriochrome Cyanine R Reagent, *J. Raf. Sci., 20*, 74- 83.

Pal, D. and Keshav, A., 2014, Extraction Equilibria of Pyruvic Acid Using Tri-n-butyl Phosphate: Influence of Diluents, *J. Chem. Eng. Data, 59*, 2709−2716.

Reddy, B.R., Kumar, J.R., Reddy A.V., 2004, Solvent extraction of tetravalent hafnium from acidic chloride solutions using 2-ethyl hexyl phosphonic acid mono-2-ethyl hexyl ester (PC-88A), *Miner. Eng., 17*, 553–556.

Rosocka, M.R., Rozenblat, M., Nowaczyk, R., Wisniewski, M., 2005, Dibutylbutyl Phosphonate as an Extractant of Zinc(II) from Hydrochloric, *Physicochem. Probl. Miner. Process., 39*, 99-106.

Sahira, K., 2013, Matrix Studies on Solvent Extraction of Zirconium and Hafnium from Loaded Solvent obtained from Scrub Raffinate, *Int. j. eng. sci. Invention, 2*, 123-146.

Silanes, I., Mercero, J.M., Ugalde, J.M., 2006, Comparison of Ti, Zr, and Hf as Cations for Metallocene-Catalyzed Olefin Polymerization, *Organometallics, 25*, 4483-4490.

Taghizadeh, M., Ghanadi, M., Zolfonoun, E., 2011, Separation of zirconium and hafnium by solvent extraction using mixture of TBP and Cyanex 923, *J. Nucl. Mater., 412*, 334–337.

Toyoshima, A., Kasamatsu, Y., Tsukada, K., Asai, M., Ishii, Y., Toume, H., Nishinaka, I., Sato, T.K., Nagame, Y., Schädel, M., Haba, H., Goto, S., Kudo, H., Akiyama, K., Oura, Y., Ooe, K., Shinohara, A., Sueki, K.,

UNIVERSITAS
GADJAH MADA
STUDI INTERAKSI ION Zr(IV) DAN Hf(IV) DENGAN ORGANOFOSFOR MENGGUNAKAN METODE DENSITY FUNCTIONAL THEORY (DFT)
FARUQ MUBAROK, Dr.rer.nat Ria Armunanto, S.Si, M.Si
Universitas Gadjah Mada, 2015 | Diunduh dari http://etd.repository.ugm.ac.id/

Kratzh, J.V., 2010, Extraction Chromatographic Behavior of Rf, Zr, and Hf in HCl Solution with Styrene-divinylbenzene Copolymer Resin Modified by TOPO (trioctylphosphine oxide), *J. Nucl. Radiochem. Sci.*, *11*, 7-11.