

## Bibliography:

1. Brandrup, J.; Immergut, E.H.; Grulke, E.A. *Polymer handbook*, 4th ed.; Johyn Wiley & Sons: NY, USA, 1999.
2. Bicerano, J. *Prediction of polymer properties*, 2nd ed.; M. Dekker: USA, New York, 1996.
3. Sigma-Aldrich database, <http://www.sigmaaldrich.com/united-states> (accessed Jan 2020).
4. Refractive Index of Amorphous Polymers. <https://polymerdatabase.com/polymer-physics/refractive-index.html> (accessed Jan 2020).
5. Xu, J.; Chen, B.; Zhang, Q.; Guo, B. Prediction of refractive indices of linear polymers by a four-descriptor QSPR model. *Polym.* 2004, 45, 8651–8659, doi:10.1016/j.polymer.2004.10.057.
6. Gooch, J. W. *Encyclopedic dictionary of polymers*, 2nd ed.; Vol. 1; Springer: New York, NY, 2011.
7. Refractive Index of Polymers by Index. <https://scientificpolymer.com/technical-library/refractive-index-of-polymers-by-index/> (accessed Jan 2020).
8. Latour, M. Electrical properties of polymers. *Digest of Literature on Dielectrics Volume 40* 1976 1976, 1–64, doi:10.1109/dld.2016.7593204.
9. Whewell, W. *A History of the Inductive Sciences. History of the Inductive Sciences*, 1837, pp. 1–2.
10. Liu, J.-G.; Ueda, M. High refractive index polymers: fundamental research and practical applications. *J. Mater. Chem.* 2009, 19, 8907–8919, doi:10.1039/b909690f.
11. Takafuji, M.; Kajiwara, M.; Hano, N.; Kuwahara, Y.; Ihara, H. Preparation of High Refractive Index Composite Films Based on Titanium Oxide Nanoparticles Hybridized Hydrophilic Polymers. *Nanomater.* 2019, 9, 514, doi:10.3390/nano9040514.
12. Wei, Z.; He, L.; Chi, Z.; Ran, X.; Guo, L. Two-photon isomerization triggers two-photon-excited fluorescence of an azobenzene derivative. *Spectrochim. Acta Part A: Mol. Biomol. Spectrosc.* 2019, 206, 120–125, doi:10.1016/j.saa.2018.07.098.
13. Suwa, M.; Niwa, H.; Tomikawa, M. High Refractive Index Positive Tone Photo-sensitive Coating. *J. Photopolym. Sci. Technol.* 2006, 19, 275–276, doi:10.2494/photopolymer.19.275.
14. Walheim, S. Nanophase-Separated Polymer Films as High-Performance Antireflection Coatings. *Sci.* 1999, 283, 520–522, doi:10.1126/science.283.5401.520.
15. Nakabayashi, K.; Sobu, S.; Kosuge, Y.; Mori, H. Synthesis and nanoimprinting of high refractive index and highly transparent polythioethers based on thiol-ene click chemistry. *J. Polym. Sci. Part A: Polym. Chem.* 2018, 56, 2175–2182, doi:10.1002/pola.29181.
16. Giuri, A.; Yuan, Z.; Miao, Y.; Wang, J.; Gao, F.; Sestu, N.; Saba, M.; Bongiovanni, G.; Colella, S.; Corcione, C.E.; et al. Ultra-Bright Near-Infrared Perovskite Light-Emitting Diodes with Reduced Efficiency Roll-off. *Sci. Rep.* 2018, 8, 15496, doi:10.1038/s41598-018-33729-9.

17. Miclos, S.; Savastru, D.; Savastru, R.; Lancranjan, I. Transverse mechanical stress and optical birefringence induced into single-mode optical fibre embedded in a smart polymer composite material. *Compos. Struct.* 2019, 218, 15–26, doi:10.1016/j.compstruct.2019.03.044.
18. Cerna, J.R.; Alejandro, A.S.; Matla, M. Analysis of the influence of glycidyl methacrylate on molecular weight and refractive index in styrene-methylmethacrylate-glycidyl methacrylate copolymers through mixture design of experiments. *J. Appl. Polym. Sci.* 2009, 114, 1935–1941, doi:10.1002/app.30602.
19. Oban, R.; Matsukawa, K.; Matsumoto, A. Heat resistant and transparent organic-inorganic hybrid materials composed of N -allylmaleimide copolymer and random-type SH-modified silsesquioxane. *J. Polym. Sci. Part A: Polym. Chem.* 2018, 56, 2294–2302, doi:10.1002/pola.29202.
20. Kasarova, S.; Sultanova, N.; Ivanov, C.D.; Nikolov, I.D. Analysis of the dispersion of optical plastic materials. *Opt. Mater.* 2007, 29, 1481–1490, doi:10.1016/j.optmat.2006.07.010.
21. Bobbitt, J.M.; Mendivelso-Pérez, D.; Smith, E.A. Scanning angle Raman spectroscopy: A nondestructive method for simultaneously determining mixed polymer fractional composition and film thickness. *Polym.* 2016, 107, 82–88, doi:10.1016/j.polymer.2016.10.063.
22. Dearden, J.C. The History and Development of Quantitative Structure-Activity Relationships (QSARs). In *Oncology*; IGI Global, 2017; pp. 67–117.
23. Arodz, T.; Gálvez, J.; Dudek, A.Z. Computational Methods in Developing Quantitative Structure-Activity Relationships (QSAR): A Review. *Comb. Chem. High Throughput Screen.* 2006, 9, 213–228, doi:10.2174/138620706776055539.
24. Quintero, F.A.; Patel, S.J.; Muñoz, F.; Mannan, M.S. Review of Existing QSAR/QSPR Models Developed for Properties Used in Hazardous Chemicals Classification System. *Ind. Eng. Chem. Res.* 2012, 51, 16101–16115, doi:10.1021/ie301079r.
25. Le, T.C.; Epa, V.C.; Burden, F.R.; Winkler, D.A. Quantitative Structure–Property Relationship Modeling of Diverse Materials Properties. *Chem. Rev.* 2012, 112, 2889–2919, doi:10.1021/cr200066h.
26. Juretic, D.; Kusic, H.; Dionysiou, D.D.; Rasulev, B.; Bozic, A.L. Modeling of photooxidative degradation of aromatics in water matrix; combination of mechanistic and structural-relationship approach. *Chem. Eng. J.* 2014, 257, 229–241, doi:10.1016/j.cej.2014.07.053.
27. Chen, G.; Shen, Z.; Iyer, A.; Ghuman, U.F.; Tang, S.; Bi, J.; Chen, W.; Li, Y. Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. *Polym.* 2020, 12, 163, doi:10.3390/polym12010163.
28. Turabekova, M.; Rasulev, B.; Dzhakhangirov, F.; Leszczynska, D.; Leszczynski, J. Aconitum and Delphinium alkaloids of curare-like activity. QSAR analysis and molecular docking of alkaloids into AChBP. *Eur. J. Med. Chem.* 2010, 45, 3885–3894, doi:10.1016/j.ejmech.2010.05.042.
29. Bouteloup, R.; Mathieu, D. Improved model for the refractive index: application to potential components of ambient aerosol. *Phys. Chem. Chem. Phys.* 2018, 20, 22017–22026, doi:10.1039/c8cp02701c.

30. Toropova, A.P.; Toropov, A.A.; Rasulev, B.; Benfenati, E.; Gini, G.; Leszczynska, D.; Leszczynski, J. QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by graph of atomic orbitals and SMILES. *Struct. Chem.* 2012, 23, 1873–1878, doi:10.1007/s11224-012-9996-z.
31. Katritzky, A.R.; Sild, S.; Karelson, M. Correlation and Prediction of the Refractive Indices of Polymers by QSPR. *J. Chem. Inf. Comput. Sci.* 1998, 38, 1171–1176, doi:10.1021/ci980087w.
32. Xu, J.; Chen, B.; Zhang, Q.; Guo, B. Prediction of refractive indices of linear polymers by a four-descriptor QSPR model. *Polym.* 2004, 45, 8651–8659, doi:10.1016/j.polymer.2004.10.057.
33. Jabeen, F.; Chen, M.; Rasulev, B.; Ossowski, M.; Boudjouk, P. Refractive indices of diverse data set of polymers: A computational QSPR based study. *Comput. Mater. Sci.* 2017, 137, 215–224, doi:10.1016/j.commatsci.2017.05.022.
34. Khan, P.M.; Rasulev, B.; Roy, K. QSPR Modeling of the Refractive Index for Diverse Polymers Using 2D Descriptors. *ACS Omega* 2018, 3, 13374–13386, doi:10.1021/acsomega.8b01834.
35. Duchowicz, P.R.; Fioretti, S.E.; Bacelo, D.E.; Saavedra, L.M.; Toropova, A.P.; Toropov, A.A. QSPR studies on refractive indices of structurally heterogeneous polymers. *Chemom. Intell. Lab. Syst.* 2015, 140, 86–91, doi:10.1016/j.chemolab.2014.11.008.
36. ChemDraw Professional, Version 16.0.0.82 (68); Perkin Elmer Informatics, Inc.: Cambridge, MA, 2019; (accessed Apr 2020).
37. HyperChem<sup>Tm</sup>, Version 8.0.10 for Windows; Hypercube, Inc.: Gainesville, FL, 2019.
38. R. Toddeschini, V. Consonni, A. Mauri, M. Pavan, Dragon software for the calculation of molecular descriptors, version 6 for Windows, Talte SRL: Milan, Italy, 2014.
39. Gramatica, P.; Chirico, N.; Papa, E.; Cassani, S.; Kovarich, S. QSARINS: A new software for the development, analysis, and validation of QSAR MLR models. *J. Comput. Chem.* 2013, 34, 2121–2132, doi:10.1002/jcc.23361.
40. Gramatica, P. Principles of QSAR models validation: internal and external. *QSAR Comb. Sci.* 2007, 26, 694–701, doi:10.1002/qsar.200610151.
41. Chirico, N.; Gramatica, P. Real External Predictivity of QSAR Models: How To Evaluate It? Comparison of Different Validation Criteria and Proposal of Using the Concordance Correlation Coefficient. *J. Chem. Inf. Model.* 2011, 51, 2320–2335, doi:10.1021/ci200211n.
42. Koopmans, T. Über die Zuordnung von Wellenfunktionen und Eigenwerten zu den Einzelnen Elektronen Eines Atoms. *Phys.* 1934, 1, 104–113, doi:10.1016/s0031-8914(34)90011-2.
43. Reddy, R.; Ahammed, Y.N.; Gopal, K.R.; Azeem, P.A.; Rao, T. Physico-chemical parameters of alkali halides using optical electronegativity. *Infrared Phys. Technol.* 2001, 42, 49–54, doi:10.1016/s1350-4495(00)00053-0.
44. Lorenz, L. Ueber die Refractionsconstante. *Ann. der Phys.* 1880, 247, 70–103, doi:10.1002/andp.18802470905.

45. Lorentz, H.A. Nachtrag zu der Abhandlung: Ueber die Anwendung des Satzes vom Virial in der kinetischen Theorie der Gase. *Ann. der Phys.* 1881, 248, 660–661, doi:10.1002/andp.18812480414.
46. Gilman, J.J. Chemical and physical “hardness.” *Mater. Res. Innov.* 1997, 1, 71–76, doi:10.1007/s100190050023.
47. Bender, G.W.; Legrand, D.G.; Gaines, G.L. Molecular Weight Dependence of Surface Tension and Refractive Index for Some Poly(ethylene oxide) Derivatives. *Macromol.* 1969, 2, 681–682, doi:10.1021/ma60012a024.
48. Askadskii, A.; Kovriga, O. Effect of branching on the physical characteristics of polymers. *Polym. Sci. U.S.S.R.* 1991, 33, 1821–1831, doi:10.1016/0032-3950(91)90019-m.