Theoretical study of Optimum conditions of intrinsic viscosity of polyethylene oxide solution using QSPR model

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Abstract

Quantitative Structure–Property Relationship (QSPR) models method have been used for the prediction intrinsic viscosity of (poly ethylene oxide) in solution. Several models for the prediction of intrinsic viscosity have been drawn up by using the multiple regression technique. Penta models with R^2 ranges from 0.87-0.99 by using MLR based on descriptors calculated from molecular structure have been developed present in this study. The results show excellent model with high correlation coefficient, minimum standard of error by using five parameters, which indicate that these parameters Total Energy T.E, capacity heat of organic solvent Cp(s), Van Der Waals Area V.W.AREA, The energy of Highest Occupied Molecular Orbital HOMO and The energy of Lowest Unoccupied Molecular Orbital LUMO, play an important role in effect on intrinsic viscosity of polymer in these solvents .

Keywords*. *Intrinsic Viscosity, Organic Solvents, Redesign QSPR Model.

الخلاصة

العلاقة التركيبية الخصائصية الكمية استخدمت للتنبأ باللزوجة الجوهرية ل(بولي اثليين اوكسيد) في المحلول. عدة موديلات للتنبأ باللزوجة الجوهرية وضعت بأستخدام تحليل MLR . خمسة موديلات تملك معامل احصائي ضمن المدى R=0.87–0.99 باستعمال   MLR اعتمادا على الموصوفات المحسوبه من التركيب الجزيئي . النتائج اظهرت أن أفضل موديل ممتاز والتي لها أفضل الوسائط الاحصائية (اعلى قيمه لمعامل الارتباط واقل خطأ) باستخدام خمس متغيرات ,   HOMO, LUMO, T.E, Cp(s) and V.W.AREA   والتي اكدت بأن هذه المتغيرات تلعب دورا مهما في التأثير على اللزوجة الجوهرية [η] لمحلول بولي أثلين اوكسيد في المذيبات المختارة .

Introduction

Intrinsic viscosity [η] is the ratio of a solution's specific viscosity to the concentration of the solute, extrapolated to zero concentration. Intrinsic viscosity reflects the capability of a polymer in solution to enhance the viscosity of the solution. The intrinsic viscosity number is defined as the limiting value of the specific viscosity/concentration ratio at zero concentration. Intrinsic viscosity is dependent on the salinity of the solvent, temperature, molecular weight and the percentage of polymer hydrolysis [1-2]. The variation of the viscosity number with concentration depends on the type of molecule as well as the solvent. In general, the