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热力学

多氯联苯热力学性质的构效关系

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摘要 通过计算二噁英类化合物多氯联苯（PCBs）217种分子的定位指数和基团对应指数，以这些分子的热力学性质的文献值为建模样本，运用多元线性回归方法建立了多氯联苯的标准熵（S0）、标准焓（H0）、标准自由能（G0）、分子总能量（ET）、热能校正值（Eth）、零点振动能（Ezpv）及恒容热容（Cv0）等热力学性质的定量结构-性质相关方程，相关系数均在0.99以上。这些模型能较好地解释多氯联苯热力学性质的递变规律，而且相关系数高，稳定性好，预测能力强。采用留一法对模型稳健性进行了检验，得到的预测模型对另外一些多氯联苯分子的热力学性质进行预测，预测结果和文献值基本吻合。

关键词

定位指数 基团对应指数 多氯联苯 热力学性质 定量结构-性质相关

分类号

QSPR research of thermodynamic properties of polychlorinated biphenyl

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Abstract

The orientation indices and group corresponding indices of 210 molecular structures of polychlorinated biphenyls （PCBs）and biphenyl were calculated By combining these indices with seven thermodynamic properties reported in literature of such PCBs， including standard entropy （ S_0）， standard enthalpy （ H_0）， standard free energy （ G_0）， total energy （ E_T）， thermal energy correction （ E_{th} ）， zero point vibration energy （ E_{zpv} ） and constant volume molar heat capacity （ C^0_V ）， a series of quantitative structure property relationship (QSPR) equations were built up by the multiple regression method All the correlation coefficients were larger than 0 99 These models could better explain the change of thermodynamic properties for the PCBs，and the QSPR models had high correlation coefficients，good stability and good predictability A modified leave one out procedure test was performed to validate model robustness，and predict the S_0，H_0，G_0，E_T， E_{th} ， E_{zpv} ， $C0_V$ of other PCBs molecules by the regression equation，and the error analysis were discussed The results showed better agreement between the values predicted by the model developed and the observed values of the thermodynamic properties.

Key words

orientation index group corresponding index PCBs thermodynamic properties QSPR

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