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Combined Theoretical and Computational Study of the Belousov–Zhabotinsky Chaotic Reaction and Curtius Rearrangement for Synthesis of Mechlorethamine, Cisplatin, Streptozotocin, Cyclophosphamide, Melphalan, Busulphan and BCNU as Anti–Cancer Drugs

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Belousov-Zhabotinsky is a chaotic reaction with a special period for synthesis of some anti-cancer drugs such as Mechlorethamine, Cisplatin, Streptozotocin, Cyclophosphamide, Melphalan, Busulphan and BCNU **(Figure 1).** Mathematical modeling of this reaction yields three non-linear differential equations which do not have analytical solutions. By numerical simulation (solving the equations numerically) of this reaction, the qualitative behavior of the reaction is specified, which clearly shows the oscillation of reaction [1-17]. On the other hand, Mechlorethamine, Cisplatin, Streptozotocin, Cyclophosphamide, Melphalan, Busulphan and BCNU **(Figure 1)** can be converted to the other new anti-cancer drugs. The reactions were happen by Curtius rearrangement. Using *ab initio* and density functional theory (DFT) computational methods and also different basis sets, some structural, thermodynamic and spectroscopic parameters such as electronic energy, polarizability, hardness and electrophilicity values are calculated for the reactants and products of the above mentioned rearrangements. It should be noted that all calculations are carried out by Gaussian 09. Geometry optimization for each molecule are be fulfilled at HF, PM3, MM2, MM3, AM1, MP2, MP3, MP4, CCSD, CCSD(T), LDA, BVWN, BLYP and B3LYP computational methods with 31G, 6-31G*, 6-31+G*, 6-31G(3df, 3pd), 6-311G, 6-311G* and 6-311+G* basis sets, respectively. The change of the hardness, polarizability and electrophilicity index during these reactions are calculated. It is shown that the maximum hardness, minimum polarizability and minimum electrophilicity principle are valid in all reactions. These results show the validation of this new principle in Curtius rearrangement [18-29].

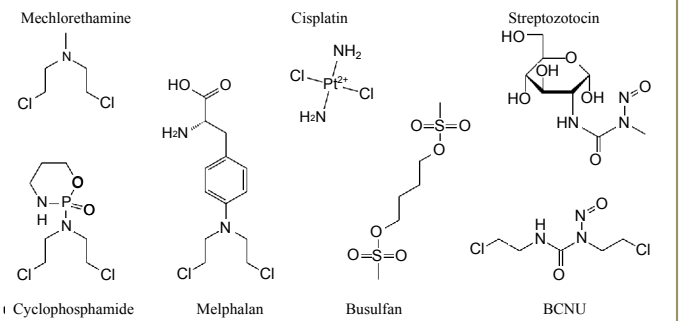

Figure 1 Molecular structure of Mechlorethamine, Cisplatin, Streptozotocin, Cyclophosphamide, Melphalan, Busulphan and BCNU as anti–cancer drugs.

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