

Study of electronic properties and structural characteristics of polyethylene glycol oligomers

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Polyethylene glycol (PEG) is a versatile polymer widely used in various applications including drug delivery systems, cosmetics, and biomedical materials due to its biocompatibility and unique physicochemical properties.[1] This research uses computational chemistry methods to investigate the electronic and structural characteristics of PEG oligomers with different chain lengths (n=1-6). The computational analysis was conducted using Density Functional Theory (DFT) with the B3LYP functional and 6-31G(d) basis set implemented in the Gaussian software. The total energy of PEG oligomers shows a linear decrease with increasing chain length, from -189.42 Hartree for n=1 to -1136.87 Hartree for n=6. This trend indicates the increasing stability of longer PEG chains, which corresponds to their polymeric nature. First, the total energy decreases linearly with increasing chain length, demonstrating the increasing stability of longer PEG chains. The HOMO-LUMO gap systematically narrows from 8.87 eV for n=1 to 7.51 eV for n=6, indicating enhanced electron delocalization in longer oligomers. Specifically, HOMO energy levels rise from -7.56 eV to -6.56 eV, while LUMO energy levels decrease from 1.31 eV to 0.95 eV as chain length increases. Interestingly, the average CO bond length remains almost constant across all oligomers (approximately 1.42 Å), suggesting that changes in electronic structure do not significantly affect local bonding geometry. These computational results provide valuable insights into structure-property relationships in PEG oligomers. They can help guide the rational design of PEG-based materials for applications in drug delivery, tissue engineering, and biomedical devices.

References

- 1) Eldawy, H., Elrehany, M., Bekhit, A., Thabet, K. (2025). Interstitial lung disease: A review. Journal of advanced Biomedical and Pharmaceutical Sciences, 8(1), 1-6. doi: 10.21608/jabps.2024.320282.1222

Illustrations

PEG Length	Total Energy (Hartree)	HOMO (eV)	LUMO (eV)	H-L Gap (eV)	Avg. C-O Bond (Å)	Total Energy (kJ/mol)	IP	EA	χ	η
1	-189,42	-7,56	1,31	8,87	1,422	497322	7,56	-1,31	3,13	4,44
2	-378,96	-7,21	1,17	8,38	1,421	994959	7,21	-1,17	3,02	4,19
3	-568,45	-6,91	1,06	7,97	1,420	1492465	6,91	-1,06	2,93	3,99
4	-757,93	-6,72	1,01	7,73	1,420	1989945	6,72	-1,01	2,86	3,87
5	-947,39	-6,61	0,98	7,59	1,421	2487372	6,61	-0,98	2,82	3,80
6	-1136,87	-6,56	0,95	7,51	1,421	2984852	6,56	-0,95	2,81	3,76

Рис. : Table1. PEG oligomers Computational Results