

The interaction between the reactants and bath gas Ar was modeled by the Lennard-Jones (L-J) potential [1-3]. The L-J parameters for the products formed in the backside attack reactions on EO are taken from the online database [4]. Detailed L-J values are shown in Table S1.

Table S1. Detailed L-J values for the products formed in the backside attack reactions on EO.

Species	σ	ε
C ₂ H ₅ O	5.01	267.08
CH ₃ OCH ₂	5.02	228.98
PC ₂ H ₄ OH	5.01	267.08
CH ₃ CH ₂ CH ₂ O	5.33	279.46
CH ₃ CH ₂ OCH ₂	5.34	242.28
CH ₂ CH ₂ OCH ₃	5.34	242.28
HOCH ₂ CH ₂ O	5.05	315.29
HOCH ₂ OCH ₂	5.14	279.72
C ₂ H ₄ O ₂ H	4.41	470.60

References

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- [2] Joback K, Reid R. 1987. Estimation of pure-component properties from group-contributions. *Chemical Engineering Communications* 57:233-243 doi: 10.1080/00986448708960487
- [3] Chung T, Ajlan M, Lee L, Starling KE. 1988. Generalized multiparameter correlation for nonpolar and polar fluid transport properties. *Industrial & Engineering Chemistry Research* 27:671-679 doi: 10.1021/ie00076a024
- [4] Reaction Mechanism Generator (RMG). 2024. https://rmg.mit.edu/molecule_search (accessed 16 August 2023)