

## TIG4

Energy Barrier height (kJ/mol)

QM

Interpolated Fit

OpenFF v1.3.0

slope=91.15<sup>140.52</sup><sub>41.78</sub>  
 $r^2 = 0.62^{1.07}_{0.31}$

slope=-3.04<sup>33.19</sup><sub>-39.27</sub>  
 $r^2 = 0.00^{0.01}_{-0.61}$

slope=-67.23<sup>3.61</sup><sub>-138.08</sub>  
 $r^2 = 0.30^{0.57}_{-0.25}$

Wiberg Bond Order

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