

Supplementary Material for

**Quasi-classical Trajectory Studies on the Full-dimensional  
Accurate Potential Energy Surface for the  $\text{OH} + \text{H}_2\text{O} = \text{H}_2\text{O} +$   
 $\text{OH}$  Reaction**

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This file contains two parts:

- 1) The PIP-NN PES parameters, including the NN structure, the precondition factors, and the weights, are given;
- 2) The PES-II parameter, biases, are then followed.

*The PES program can be obtained from the corresponding author (JL).*

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## 1) Weights

\*\*\*\*\*weights\*\*\*\*\*

138 2 1 !ninput, nhidden, noutput

10 80 !number of nodes in the hidden layers

1 2351 !transfer function type, in this work, hyperbolic tangent function is used, and the latter is the total number of parameters, including weights and biases

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## 2) Biases

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