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**Globally Accurate Potential Energy Surface for by using Switching Function Formalism**

**Supplemental Material (SM)**

**Y. L. Lü,1, † S.J. Chai,1, † H. Y. Ma,1 S. B. Gao,2 Y. Q. Li** **1,\***

**1***School of Physics, Liaoning University, Shenyang 110036, P. R. China.*

**2***School of Physics and Electronics, Shandong Normal University, Jinan 250014, P. R. China.*

†These authors contributed equally to this work.

\*Email addresses: [yqli@lnu.edu.cn](mailto:yqli@lnu.edu.cn) (Yongqing Li).

**Table M1**. parameters for two-body energy term of and .

|  |  |  |
| --- | --- | --- |
| parameter |  |  |
| Re/a0 | 2.6998 | 1.4010 |
| De/Eh | -0.1291 | -0.1745 |
| Rmsd/kcal mol-1 | 0.0170 | 0.0046 |
| *β*1 | 0.9150 | 2.2730 |
| *β*2 | 1.0170 | 1.1280 |
| *α*1 | 0.45164608E+02 | 0.10524396E+01 |
| *α*2 | -0.18469313E+01 | -0.58820561E-01 |
| *α*3 | -0.79210767E+02 | -0.98926826E+01 |
| *α*4 | 0.81804638E+03 | 0.76642380E+02 |
| *α*5 | -0.78738129E+04 | -0.39114782E+03 |
| *α*6 | 0.46317531E+05 | 0.13715823E+04 |
| *α*7 | -0.17143675E+06 | -0.32031633E+04 |
| *α*8 | 0.35524738E+06 | 0.44814641E+04 |
| *α*9 | -0.32382829E+06 | -0.28282034E+04 |

**Table M2**. 150 linear coefficients for three-body energy term PES.

|  |  |  |  |
| --- | --- | --- | --- |
| Coefficients |  |  |  |
|  | -2.5995126154 | -7.7797206465 | -2.5213167803 |
|  | 0.5909773396 | -1.1468724504 | 1.2116946242 |
|  | -0.3215779841 | -0.9151036498 | -0.5782501858 |
|  | 0.1623361049 | -1.5247190886 | -0.1295757204 |
|  | -0.5006588653 | 0.0944015848 | 0.1055102276 |
|  | -0.0948362037 | 0.0303807232 | 0.2551145265 |
|  | -0.1516429417 | 0.0376887206 | 0.0310570796 |
|  | 0.1027009673 | -0.0199415303 | 0.0289108504 |
|  | -0.0273406909 | 0.0390125595 | -0.0109446972 |
|  | -0.0648969511 | 0.0352080736 | 0.0173320381 |
|  | 0.0240174212 | -0.0054370773 | -0.0408323800 |
|  | -0.0062572332 | 0.0019189921 | -0.0119000230 |
|  | 0.0021848669 | -0.0093640983 | 0.0107107461 |
|  | 0.0113777796 | -0.0015661625 | 0.0041911296 |
|  | 0.0007112148 | -0.0215700950 | -0.0094579572 |
|  | -0.0015992280 | 0.0293731575 | 0.0052902292 |
|  | 0.0065272179 | -0.0071117000 | 57.3764242105 |
|  | 0.4748921973 | -1.8332749344 | 9.0943001240 |
|  | 8.3521567644 | -11.8590072721 | 4.0150679767 |
|  | 0.0431919094 | 1.3738399927 | 0.3835605674 |
|  | -0.9678560066 | -0.8497822749 | -1.2212236622 |
|  | 0.5668523079 | 0.4544948734 | 0.2207060408 |
|  | -0.2434270038 | -1.3709285983 | -0.6323859072 |
|  | -1.3273240847 | 0.2662157215 | 0.5361052676 |
|  | 0.0209551573 | 0.1311966987 | 0.1294957168 |
|  | -0.0748210985 | -0.0029666879 | -0.1205563592 |
|  | -0.1932289942 | -0.3736681827 | -0.0456195411 |
|  | -0.0384219053 | -0.0034883543 | 0.0283025919 |
|  | 0.0136580763 | 0.0039803218 | 0.0452169059 |
|  | -0.0125013659 | 0.0191442127 | -0.0010858593 |
|  | 0.0017164837 | -0.0298618338 | -0.0121341758 |
|  | -0.0180092041 | 0.0172002631 | -0.0236588596 |
|  | -0.0116914381 | -0.0092892609 | 0.0080645704 |
|  | -0.0063266326 | -11.6393434210 | -0.4598620906 |
|  | 0.0945430350 | -3.0343465449 | -2.7427420893 |
|  | 0.0123340436 | 0.1670911952 | -0.1547080129 |
|  | -0.1467170751 | -0.0617945822 | 0.0243100198 |
|  | 0.1034096128 | 0.3429361205 | -0.2791931234 |
|  | 0.0299627488 | -0.1223110290 | 0.3644257810 |
|  | 0.0188658028 | 0.0534369859 | 0.1195423368 |
|  | -0.0017145025 | -0.0448411625 | -0.0118223002 |
|  | 0.0053915711 | 0.0213142295 | 0.0125969616 |
|  | 0.0000187760 | -0.0060318904 | 0.0053045304 |
|  | 0.0250481604 | -0.0016352509 | -0.0378806027 |
|  | 0.0425728506 | -0.0027277189 | -0.0093173215 |
|  | 0.0171499288 | -0.0223799182 | -0.0187049420 |
|  | 0.0048734524 | -0.0024821835 | -0.0047780808 |
|  | -0.0001771657 | -0.0010994890 | -0.0005380563 |
|  | 0.0003717430 | -0.0073809828 | 0.0185882233 |
|  | -0.0010774915 | 0.0042150864 | 0.0005113935 |

**Table M3**. 9 nonlinear coefficients and 9 reference geometric distances

|  |  |  |  |
| --- | --- | --- | --- |
|  |  |  |  |
|  | 0.7 | 0.5 | 0.5 |
|  | 0.5 | 0.7 | 0.7 |
|  | 0.8 | 0.8 | 0.8 |
|  | 1.5 | 4.0 | 4.0 |
|  | 2.5 | 3.0 | 3.0 |
|  | 3.5 | 3.5 | 3.5 |