Accurate reproducing kernel-based potential energy surfaces for the triplet ground states of N; 2; O and dynamics for the N + NO ↔ O + N; 2; and N; 2; + O 2N + O reactions

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Author(s) Koner, Debasish; San Vicente Veliz, Juan Carlos; Bemish, Raymond J.; Meuwly, Markus
Author(s) at UniBasel Koner, Debasish ; San Vicente Veliz, Juan Carlos ; Meuwly, Markus ;
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Accurate potential energy surfaces (PESs) have been determined for the 3A' and 3A" states of N2O using electronic structure calculations at the multireference configuration interaction level with Davidson correction (MRCI+Q) and the augmented Dunning-type correlation consistent polarized triple zeta (aug-cc-pVTZ) basis set. More than 20 000 MRCI+Q/aug-cc-pVTZ energies are represented using a reproducing kernel Hilbert space (RKHS) scheme. The RKHS PESs successfully describe all reactant channels with high accuracy and all minima and transition states connecting them are determined. Quasiclassical trajectory (QCT) simulations are then used to determine reaction rates for N + NO and O + N2 collisions. Vibrational relaxation N2(ν = 1) N2(ν = 0) and dissociation of N2 2N for O + N2 collisions are also investigated using QCT. The agreement between results obtained from the QCT simulations and from available experiments is favourable for reaction and vibrational relaxation rates, which provides a test for the accuracy of the PESs. The PESs can be used to calculate more detailed state-to-state observables relevant for applications to hypersonic reentry.
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