Electronic Supplementary Information for

Low-Temperature Kinetics for the N + NO reaction: Experiment Guides the Way

Kevin M. Hickson,*[,1] Juan Carlos san Vicente Veliz,[2] Debasish Koner[2,3] and Markus Meuwly*[,2,4]

[1]Univ. Bordeaux, CNRS, Bordeaux INP, ISM, UMR 5255, F-33400 Talence, France

[2]Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland.

[3]Department of Chemistry, Indian Institute of Technology Hyderabad, Sangareddy, Telangana 502285, India.

[4]Department of Chemistry, Brown University, Providence, RI 02912, USA

Figures S1-S3 and Table S1

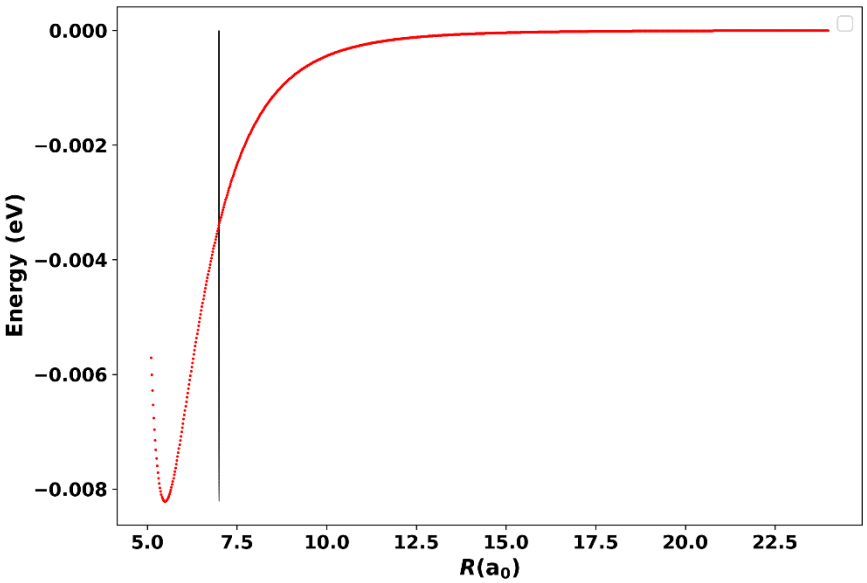

Figure S1 van der Waals NO + N long-range potential $V(R)$. Ratio between $V(R = 9)/V(R = 7)$ and $V(R = 12)/V(R = 7)$ are 0.2168 and 0.0380 respectively.

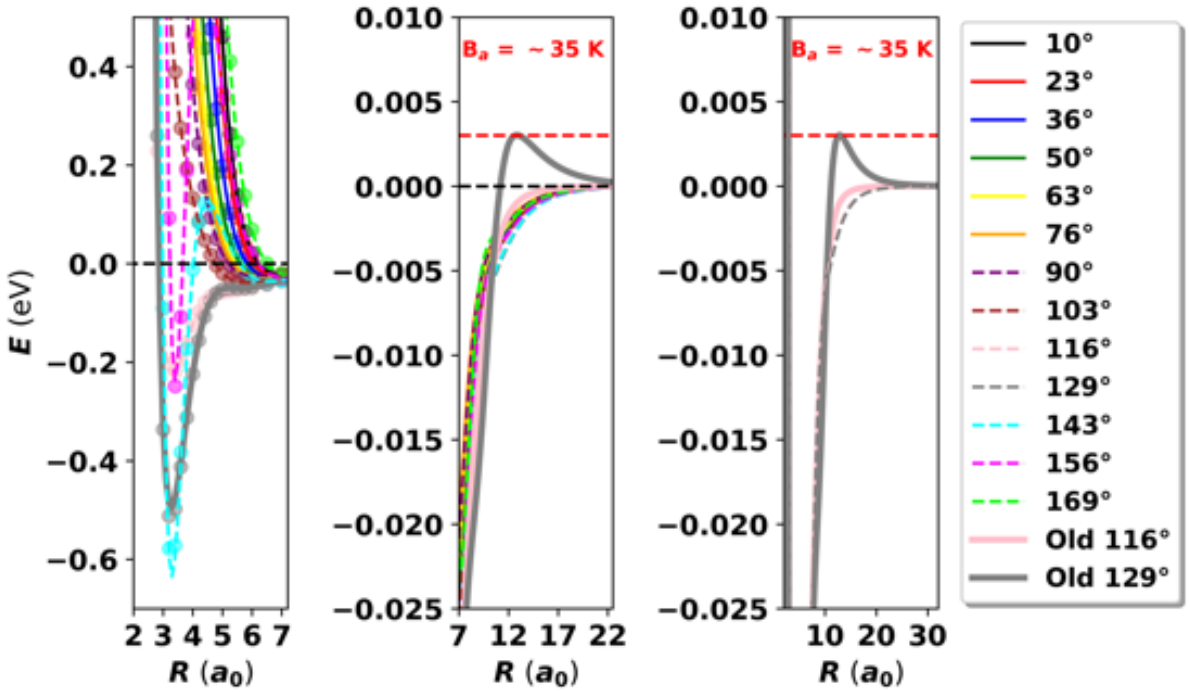

Figure S2 RKHS evaluation at different angular cuts for short (R< 7.0 a_0) and long (R>= 7.0 a_0) ranges. **Top panel:** The evaluations are at fixed r=q^- =2.100 a_0 (inner turning point)**, Middle panel:** r=r_{eq}=2.185 a_0**, Bottom Panel:** r=q^+ =2.280 a_0 (outer turning point). Points represent ab-initio reference (symbols), RKHS evaluation with PES2022-LJ1 (solid/dash lines), and RKHS evaluation with PES2020 (thick solid line) (116° and 129°)**.**

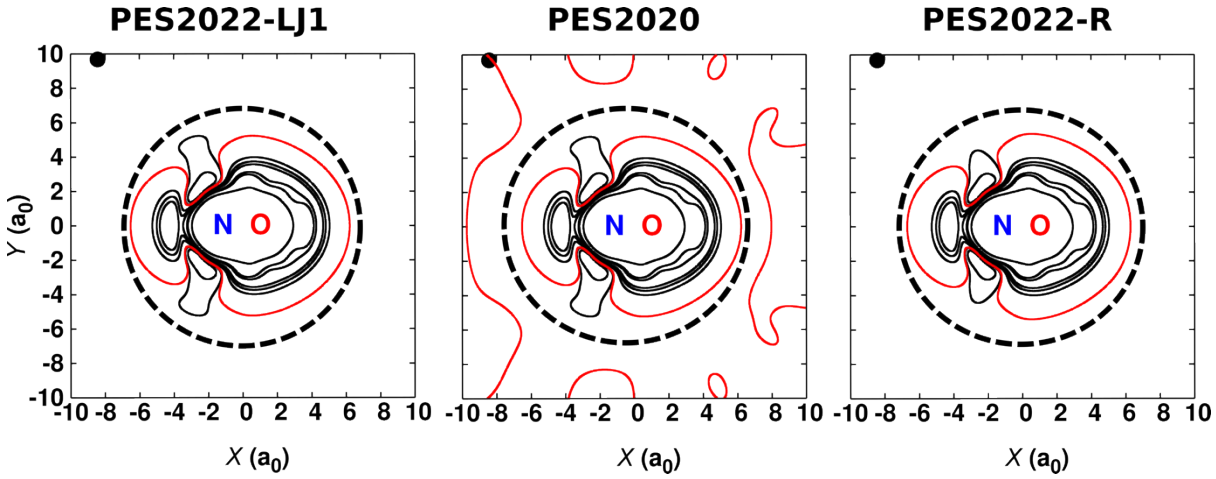

Figure S3 Contour plots of the RKHS evaluated energy surface at fixed equilibrium N-O separation of r=2.185 a_0. **Left panel:** for PES2022-LJ1, **Middle Panel:** PES2020, and **Right Panel**: PES2022-R. Contour lines are shown for energies [-0.3, -0.05, 0.45, 0.71, 0.96, 2.0, 2.5, 6.7] eV (black solid lines) and energy is reported with respect to dissociation to N + NO (r_{eq}).

To highlight the pronounced (unphysical) anisotropy present in PES2020 a selected isocontour at 0.0031 eV= 36 K (red solid line) is drawn to indicate the barrier at θ=129.0°, *R*=12.85 a_0 in the XY representation (-8.43,9.69) a_0. The solid black circle indicates a reference geometry to highlight that PES2020 contains an isocontour with positive energy at large separation *R* whereas PES2022-LJ1 and PES2022-R do not. The black dashed line is a circle with a radius of 7.0 a_0 which contains all the data we have retained from the MRCI+Q calculations.

Table S1 Experimental and calculated rate coefficients (× 10^{-11} cm^3 s^{-1}) for the N(^{4}S) + NO($X^2\Pi$) → O(^{3}P) + N_2($X^1\Sigma_g^+$) reaction.

T (K)	Expt.	PES2020 (HB)	PES2022-R (HB)	PES2022-R (GB)	PES2022-LJ1 (HB)	PES2022-LJ2 (HB)
300		3.33	2.95	3.13	3.73	3.60
296	2.81	3.41	2.98	2.92	3.75	3.62
200		3.92	3.71	3.82	4.78	4.44
177	3.50	4.19	3.93	4.21	5.17	4.75
127	4.00	4.59	4.69	4.41	6.42	5.69
100		4.88	5.37	5.41	7.42	6.35
75	5.27	5.04	6.09	6.24	8.62	7.07
50	6.64	4.83	6.80	6.54	9.97	7.64
30		4.14	6.92	6.80	10.88	7.72