Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information to:

"Development of a potential energy surface for the O_3–Ar system: Rovibrational states of the complex"

Sangeeta Sur, Ernesto Quintas-Sánchez, Steve A. Ndengué, and Richard Dawes*

Department of Chemistry, Missouri University of Science & Technology, Rolla, MO 65401, USA

E-mail: dawesr@mst.edu

Table S1: Geometric parameters—and energy—for each critical point of all considered isotopologues of ozone (MRCI O_3–Ar PESs). V_{min} represents the energy at the bottom of the well. $V_{barrier}$ represents the energy of the barrier—at the transition structure (TS)—between the two equivalent wells. All distances are in Angströms, angles in degrees, and energies in wave numbers.

	686	666	668
R_{min}	3.301	3.295	3.290
θ_{min}	110.02	110.15	110.01
ϕ_{min}	90.00	90.00	88.01
V_{min}	-229.67	-229.70	-229.57
R_{TS_1}	3.299	3.808	3.802
θ_{TS_1}	31.98	31.95	25.97
ϕ_{TS_1}	0.00	0.00	0.00
$V_{barrier1}$	-146.77 (82.90*)	-146.77 (82.93*)	-146.75 (82.82*)
R_{TS_2}	3.299	3.808	3.845
θ_{TS_2}	31.98	31.95	38.00
ϕ_{TS_2}	180.00	180.00	180.0
$V_{barrier2}$	-146.77 (82.90*)	-146.77 (82.93*)	-146.74 (82.83*)

* Energy with respect to the global minima of the PES.

Table S2: Convergence test of sbasis sets using 8 packets for J = 0.

30-60	*40-80*	*50-100*	*50-120*	*50-140*	*50-160*
-163.004	-163.004	-163.004	-163.004	-163.004	-163.004
-162.983	-162.983	-162.983	-162.983	-162.983	-162.983
-134.958	-134.958	-134.958	-134.958	-134.958	-134.958
-134.898	-134.898	-134.898	-134.898	-134.898	-134.898
-131.238	-131.238	-131.238	-131.238	-131.238	-131.238
-131.043	-131.043	-131.043	-131.043	-131.043	-131.043
-124.368	-124.368	-124.368	-124.368	-124.368	-124.368
-123.253	-123.253	-123.253	-123.253	-123.253	-123.253

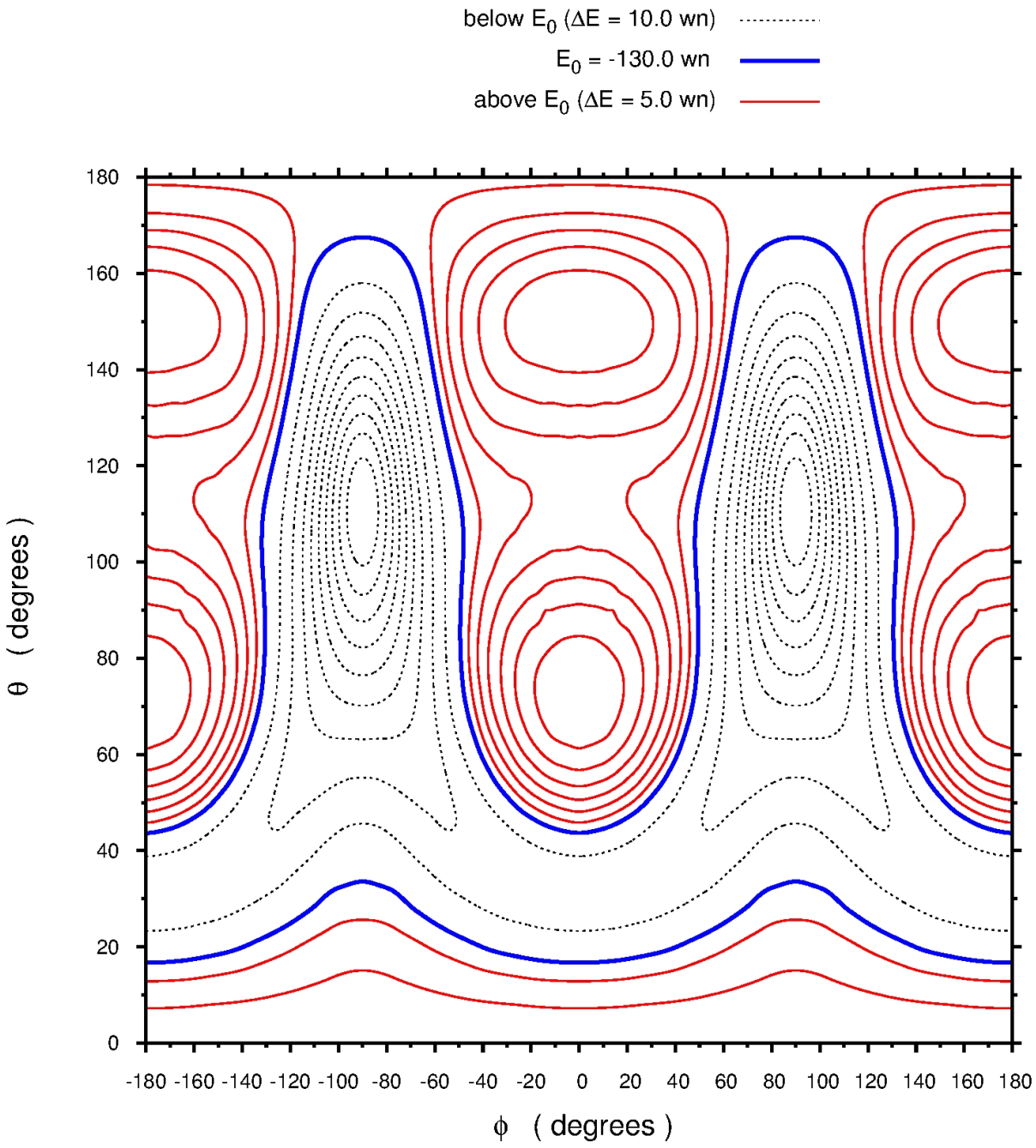

Figure S1: R-optimized plot for the 686 O_3–Ar MRCI-PES. For each pair of angles the energy is optimized with respect to the center-of-mass distance R.

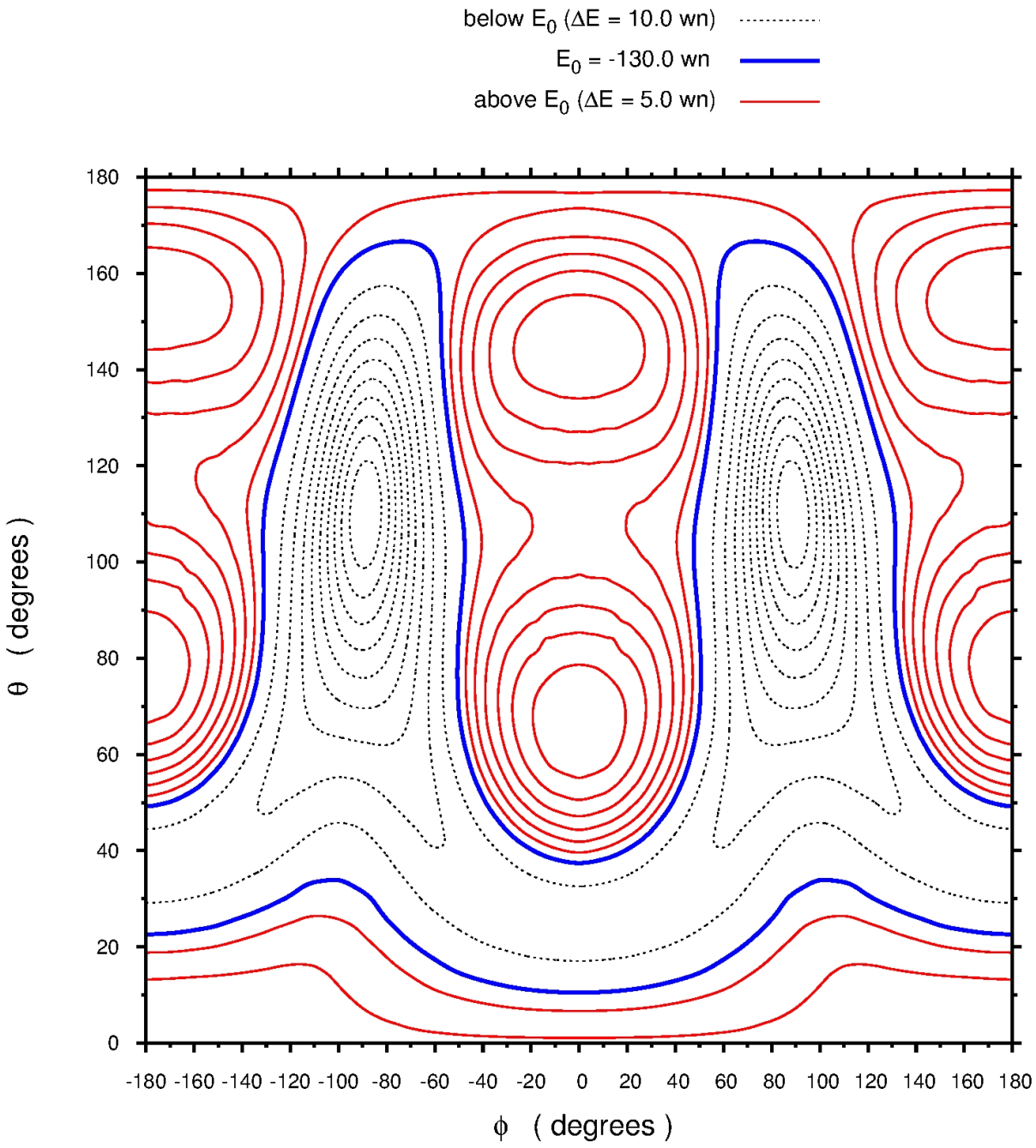

Figure S2: R-optimized plot for the 668 O_3–Ar MRCI-PES. For each pair of angles the energy is optimized with respect to the center-of-mass distance R.

Table S3: $J = 0$–6 allowed rovibrational states for the 686 O_3–Ar isotope.

$J = 0$	$J = 1$	$J = 2$	$J = 3$	$J = 4$	$J = 5$	$J = 6$
-164.693791	-164.573827	-164.334032	-163.974672	-163.496143	-162.898969	-162.183794
	-164.217910	-163.985399	-163.636737	-163.172049	-162.591497	-161.895282
	-164.210534	-163.963273	-163.592496	-163.098344	-162.481002	-161.740710
		-162.953877	-162.594270	-162.114953	-161.516059	-160.797759
		-162.953760	-162.593682	-162.113191	-161.511956	-160.789578
			-160.854948	-160.375669	-159.776577	-159.057684
			-160.854947	-160.375661	-159.776545	-159.057587
				-157.974941	-157.376668	-156.658819
				-157.974941	-157.376668	-156.658819
					-154.258114	-153.541347
					-154.258114	-153.541347
						-149.759408
						-149.759408

Table S4: $J = 0$–6 allowed rovibrational states for the 668 O_3–Ar isotope.

$J = 0$	$J = 1$	$J = 2$	$J = 3$	$J = 4$	$J = 5$	$J = 6$
-163.885582	-163.765717	-163.526146	-163.167184	-162.689305	-162.093129	-161.379419
-163.866684	-163.746812	-163.507228	-163.148245	-162.670336	-162.074120	-161.360358
	-163.443043	-163.211289	-162.863778	-162.400654	-161.822100	-161.128345
	-163.435120	-163.192422	-162.844869	-162.381693	-161.803075	-161.109241
	-163.424192	-163.187513	-162.816250	-162.321475	-161.703407	-160.962321
	-163.416281	-163.168682	-162.797413	-162.302634	-161.684562	-160.943471
		-162.219528	-161.860225	-161.381333	-160.783002	-160.065420
		-162.219385	-161.859511	-161.379192	-160.778019	-160.055496
		-162.200850	-161.841528	-161.362609	-160.764243	-160.046617
		-162.200708	-161.840816	-161.360474	-160.759274	-160.036721
			-160.227004	-159.748122	-159.149499	-158.431139
			-160.227001	-159.748111	-159.149454	-158.431006
			-160.208606	-159.729694	-159.131039	-158.412640
			-160.208601	-159.729683	-159.130994	-158.412508
				-157.461922	-156.864144	-156.146870
				-157.461922	-156.864144	-156.146869
				-157.443897	-156.846085	-156.128770
				-157.443897	-156.846085	-156.128770
					-153.924506	-153.208409
					-153.924506	-153.208409
					-153.906927	-153.190788
					-153.906927	-153.190788
						-149.615128
						-149.615128
						-149.598142
						-149.598142

Table S5: $J = 0$–6 allowed rovibrational states for the CCSD(T)-F12b PES.

$J = 0$	$J = 1$	$J = 2$	$J = 3$	$J = 4$	$J = 5$	$J = 6$
-162.689860	-162.568421	-162.325683	-161.961724	-161.477585	-160.873207	-160.149485
	-162.210708	-161.975501	-161.622553	-161.152743	-160.565501	-159.861288
	-162.203073	-161.952599	-161.576879	-161.076457	-160.451141	-159.701321
		-160.937028	-160.572851	-160.087814	-159.481594	-158.754534
		-160.936903	-160.572228	-160.085939	-159.477229	-158.745833
			-158.823123	-158.338043	-157.731586	-157.003864
			-158.823121	-158.338034	-157.731551	-157.003758
				-155.922273	-155.316681	-154.590061
				-155.922273	-155.316681	-154.590061
					-152.179047	-151.453532
					-152.179047	-151.453532
						-147.647981
						-147.647981

Table S6: $J = 0$–6 allowed rovibrational states for the scaled MRCI-PES.

$J = 0$	$J = 1$	$J = 2$	$J = 3$	$J = 4$	$J = 5$	$J = 6$
-163.661814	-163.539854	-163.296021	-162.930774	-162.444369	-161.837426	-161.110643
	-163.175496	-162.939247	-162.585165	-162.113170	-161.523503	-160.816380
	-163.167790	-162.916121	-162.538950	-162.036175	-161.408080	-160.654923
		-161.906737	-161.541235	-161.053967	-160.445152	-159.714968
		-161.906634	-161.540598	-161.052056	-160.440702	-159.706100
			-159.784307	-159.297061	-158.688007	-157.957154
			-159.784306	-159.297052	-158.687970	-157.957046
				-156.886628	-156.278459	-155.548736
				-156.886628	-156.278459	-155.548735
					-153.133392	-152.404801
					-153.133392	-152.404801
						-148.603741
						-148.603741