

An intramolecular vibrationally excited intermolecular potential energy surfaces and predicted 2OH overtone spectroscopy of $\text{H}_2\text{O-Kr}$

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Table SI. Calculated rovibrational energy levels (in cm^{-1}) of the $\text{H}_2\text{O}-^{84}\text{Kr}$ complex from the vibrationally averaged V_{MLR} PESs at the $|00^+\rangle$ state.

$J = 5$	$J = 6$	$J = 7$	$J = 8$	$J = 9$	$J = 10$
$k=\text{even}, (-1)^{J+P}=\text{even}$					
-116.850	115.908	-114.810	113.555	-112.145	-110.580
-87.489	-86.576	-85.511	-84.294	-82.927	-81.409
-79.968	-79.050	-77.980	-76.759	-75.389	-73.870
-75.426	-74.497	-73.413	-72.174	-70.780	-69.229
-57.215	-56.370	-55.385	-54.261	-52.998	-51.596
-53.328	-52.623	-51.763	-50.749	-49.581	-48.258
-50.862	-49.717	-48.421	-46.974	-45.379	-43.637
-44.662	-43.896	-42.996	-41.963	-40.793	-39.487
-41.959	-41.029	-39.949	-38.721	-37.345	-35.823
-38.695	-37.718	-36.580	-35.281	-33.821	-32.202
$k=\text{even}, (-1)^{J+P}=\text{odd}$					
-79.911	78.967	77.868	-76.611	-75.199	-73.631
-52.227	-51.299	-50.217	-48.982	-47.593	-46.050
-42.178	-41.324	-40.327	-39.186	-37.902	-36.474
-38.698	-37.724	-36.590	-35.297	-33.845	-32.236
-23.104	-22.296	-21.343	-20.245	-19.001	-17.611
-21.937	-20.971	-19.854	-18.588	-17.174	-15.613
-17.968	-17.227	-16.330	-15.276	-14.066	-12.701
-15.804	-14.679	-13.408	-11.994	-10.442	-8.759
-10.781	-9.939	-8.951	-7.815	-6.525	-5.075
$k=\text{odd}, (-1)^{J+P}=\text{even}$					
-100.688	-99.764	98.685	-97.454	96.069	-94.531
-88.413	-87.460	-86.348	-85.079	-83.652	-82.069
-79.519	-78.560	-77.440	-76.162	-74.724	-73.126
-67.187	-66.303	-65.272	-64.095	-62.772	-61.303
-54.963	-54.072	-53.034	-51.849	-50.518	-49.040
-44.970	-44.077	-43.036	-41.848	-40.514	-39.037
-44.138	-43.344	-42.414	-41.344	-40.133	-38.777
-38.588	-37.624	-36.508	-35.245	-33.836	-32.287
-33.803	-32.929	-31.909	-30.740	-29.423	-27.957
$k=\text{odd}, (-1)^{J+P}=\text{odd}$					
-88.471	-87.541	-86.456	-85.218	-83.825	82.280
-79.559	-78.615	-77.514	-76.256	-74.842	-73.271
-62.267	-61.317	-60.210	-58.945	-57.524	-55.945
-55.014	-54.144	-53.129	-51.971	-50.669	-49.225
-45.004	-44.125	-43.099	-41.928	-40.612	-39.150
-38.768	-37.864	-36.808	-35.603	-34.247	-32.741
-30.462	-29.585	-28.563	-27.396	-26.086	-24.632
-29.486	-28.525	-27.405	-26.129	-24.699	-23.117
-26.996	-26.193	-25.257	-24.186	-22.979	-21.634
-16.732	-15.926	-14.985	-13.911	-12.705	-11.366

Table SII. Calculated rovibrational energy levels (in cm^{-1}) of the $\text{H}_2\text{O}-^{84}\text{Kr}$ complex from the vibrationally averaged V_{MLR} PESs at the $|02^- \rangle$ state.

$J = 0$	$J = 1$	$J = 2$	$J = 3$	$J = 4$
		$k=\text{even}, (-1)^{J+P}=\text{even}$		
-123.273	-123.116	-122.803	-122.332	-121.705
-95.760	-95.608	-95.302	-94.844	-94.234
	-88.732	-88.418	-87.947	-87.319
-81.113	-80.964	-80.664	-80.215	-79.616
-64.799	-64.659	-64.377	-63.954	-63.390
	-61.701	-61.473	-61.118	-60.630
-60.131	-59.931	-59.536	-58.956	-58.200
-50.009	-49.924	-49.729	-49.410	-48.957
	-49.359	-48.993	-48.472	-47.804
-37.775	-37.644	-45.807	-45.318	-44.668
		$k=\text{even}, (-1)^{J+P}=\text{odd}$		
	-88.732	-88.418	-87.946	-87.318
	-61.657	-61.347	-60.882	-60.262
	-49.412	-49.129	-48.703	-48.136
		-45.807	-45.319	-44.669
		-32.043	-31.665	-31.148
	-31.642	-31.293	-30.781	-30.110
	-26.660	-26.494	-26.192	-25.741
	-25.783	-25.317	-24.671	-23.860
	-18.010	-17.737	-17.328	-16.782
		-11.781	-11.333	-10.738
		$k=\text{odd}, (-1)^{J+P}=\text{even}$		
-108.269	108.114	-107.806	-107.343	-106.727
	-94.868	-94.552	-94.078	-93.447
	-88.393	-88.073	-87.592	-86.951
-75.564	-75.415	-75.117	-74.670	-74.075
	-61.568	-61.270	-60.822	-60.225
	-53.450	-53.150	-52.701	-52.102
-52.357	-52.228	-51.969	-51.579	-51.058
	-47.179	-46.852	-46.364	-45.716
-41.493	-41.347	-41.055	-40.617	-40.034
		-38.626	-38.142	-37.498
		$k=\text{odd}, (-1)^{J+P}=\text{odd}$		
	-94.872	-94.563	-94.099	-93.482
	-88.396	-88.080	-87.607	-86.976
	-70.196	-69.879	-69.404	-68.771
	-61.571	-61.279	-60.841	-60.257
	-53.452	-53.157	-52.714	-52.124
	-47.193	-46.896	-46.450	-45.855
	-37.980	-38.626	-38.143	-37.498
		-37.685	-37.244	-36.656
	-32.478	-32.209	-31.806	-31.268
	-24.553	-24.280	-23.872	-23.328

Table SII. Calculated rovibrational energy levels (in cm^{-1}) of the $\text{H}_2\text{O}-^{84}\text{Kr}$ complex from the vibrationally averaged V_{MLR} PESs at the $|02^- \rangle$ state.

$J = 5$	$J = 6$	$J = 7$	$J = 8$	$J = 9$	$J = 10$
$k=\text{even}, (-1)^{J+P}=\text{even}$					
-120.922	-119.982	118.886	-117.635	-116.228	-114.666
-93.471	-92.555	-91.488	-90.268	-88.897	-87.374
-86.535	-85.596	-84.501	-83.251	-81.848	-80.292
-78.867	-77.968	-76.920	-75.722	-74.375	-72.878
-62.685	-61.838	-60.850	-59.719	-58.446	-57.029
-60.001	-59.228	-58.309	-57.242	-56.027	-54.663
-57.274	-56.184	-54.934	-53.526	-51.963	-50.246
-48.368	-47.643	-46.780	-45.779	-44.641	-43.366
-46.993	-46.039	-44.943	-43.705	-42.325	-40.804
-43.855	-42.881	-41.746	-40.450	-38.995	-37.382
$k=\text{even}, (-1)^{J+P}=\text{odd}$					
-86.533	85.592	-84.494	-83.240	81.830	-80.265
-59.487	-58.558	-57.475	-56.237	-54.846	-53.301
-47.427	-46.574	-45.579	-44.441	-43.160	-41.736
-43.858	-42.887	-41.757	-40.467	-39.020	-37.416
-30.490	-29.686	-28.738	-27.643	-26.401	-25.012
-29.285	-28.307	-27.178	-25.898	-24.469	-22.891
-25.138	-24.382	-23.471	-22.406	-21.186	-19.813
-22.887	-21.756	-20.471	-19.032	-17.444	-15.709
-16.098	-15.276	-14.315	-13.214	-11.971	-10.584
-9.993	-9.102	-8.063	-6.878	-5.547	-4.072
$k=\text{odd}, (-1)^{J+P}=\text{even}$					
-105.956	-105.032	-103.954	-102.723	-101.339	-99.802
-92.658	-91.712	-90.610	-89.351	-87.937	-86.368
-86.150	-85.189	-84.068	-82.786	-81.345	-79.744
-73.331	-72.439	-71.399	-70.211	-68.875	-67.393
-59.479	-58.586	-57.544	-56.355	-55.020	-53.538
-51.354	-50.457	-49.411	-48.216	-46.875	-45.390
-50.403	-49.614	-48.689	-47.625	-46.422	-45.075
-44.910	-43.948	-42.832	-41.565	-40.149	-38.587
-39.305	-38.429	-37.409	-36.242	-34.929	-33.471
$k=\text{odd}, (-1)^{J+P}=\text{odd}$					
-92.711	-91.786	-90.708	-89.477	-88.094	-86.559
-86.187	-85.241	-84.136	-82.875	-81.456	-79.879
-67.979	-67.030	-65.923	-64.659	-63.238	-61.661
-59.527	-58.652	-57.632	-56.468	-55.161	-53.710
-51.386	-50.502	-49.470	-48.292	-46.967	-45.496
-45.112	-44.220	-43.179	-41.990	-40.652	-39.166
-36.694	-35.730	-34.606	-33.324	-31.883	-30.287
-35.921	-35.040	-34.013	-32.840	-31.522	-30.058
-30.597	-29.793	-28.855	-27.784	-26.582	-25.247
-22.648	-21.833	-20.883	-19.798	-18.579	-17.226

Table SIII. Calculated rovibrational energy levels (in cm^{-1}) of the $\text{H}_2\text{O}-^{84}\text{Kr}$ complex from the vibrationally averaged V_{MLR} PESs at the $|02^+\rangle$ state.

$J = 0$	$J = 1$	$J = 2$	$J = 3$	$J = 4$
		$k=\text{even}, (-1)^{J+P}=\text{even}$		
-120.686	-120.529	-120.215	-119.744	-119.116
-92.625	-92.473	-92.168	-91.711	-91.101
	-85.629	-85.316	-84.847	-84.222
-79.330	-79.179	-78.876	-78.423	-77.818
-61.999	-61.859	-61.578	-61.157	-60.596
	-58.726	-58.557	-58.261	-57.823
-57.885	-57.642	-57.188	-56.551	-55.746
-48.388	-48.277	-48.051	-47.704	-47.230
	-47.214	-46.879	-46.385	-45.738
		-44.188	-43.696	-43.041
		$k=\text{even}, (-1)^{J+P}=\text{odd}$		
	-85.628	85.314	-84.842	-84.213
	-58.639	-58.329	-57.864	-57.245
	-47.242	-46.960	-46.537	-45.971
		-44.189	-43.697	-43.043
		-29.560	-29.164	-28.632
	-28.834	-28.505	-28.014	-27.364
	-24.248	-24.087	-23.785	-23.334
	-23.468	-22.995	-22.347	-21.535
	-16.085	-15.813	-15.406	-14.862
		-10.466	-10.017	-9.418
		$k=\text{odd}, (-1)^{J+P}=\text{even}$		
-105.374	-105.219	-104.911	-104.449	-103.833
	-92.651	-92.333	-91.855	-91.218
	-85.383	-85.064	-84.586	-83.948
-72.450	-72.302	-72.005	-71.561	-70.968
	-59.342	-59.043	-58.595	-57.997
	-50.668	-50.370	-49.923	-49.327
-49.785	-49.658	-49.403	-49.018	-48.503
	-45.041	-44.707	-44.207	-43.545
-39.108	-38.964	-38.675	-38.243	-37.665
	-30.857	-36.246	-35.762	-35.117
		$k=\text{odd}, (-1)^{J+P}=\text{odd}$		
	92.655	-92.344	-91.878	-91.256
	-85.386	-85.072	-84.601	-83.973
	-67.911	-67.594	-67.119	-66.485
	-59.345	-59.053	-58.615	-58.031
	-50.670	-50.377	-49.936	-49.350
	-45.059	-44.759	-44.310	-43.712
	-35.868	-36.246	-35.762	-35.117
		-35.574	-35.133	-34.546
	-30.861	-30.593	-30.192	-29.656
	-22.116	-21.846	-21.440	-20.900

Table SI III. Calculated rovibrational energy levels (in cm^{-1}) of the $\text{H}_2\text{O}-^{84}\text{Kr}$ complex from the vibrationally averaged V_{MLR} PESs at the $|02^+\rangle$ state.

$J = 5$	$J = 6$	$J = 7$	$J = 8$	$J = 9$	$J = 10$
$k=\text{even}, (-1)^{J+P}=\text{even}$					
-118.331	-117.389	-116.292	-115.038	-113.629	-112.064
-90.339	-89.425	-88.359	-87.141	-85.772	-84.251
-83.441	-82.505	-81.415	-80.171	-78.775	-77.227
-77.062	-76.155	-75.096	-73.887	-72.525	-71.012
-59.893	-59.050	-58.066	-56.941	-55.675	-54.267
-57.237	-56.501	-55.614	-54.575	-53.384	-52.042
-54.779	-53.654	-52.374	-50.941	-49.355	-47.619
-46.626	-45.887	-45.014	-44.005	-42.858	-41.575
-44.941	-43.998	-42.909	-41.677	-40.300	-38.781
-42.223	-41.242	-40.099	-38.795	-37.331	-35.708
$k=\text{even}, (-1)^{J+P}=\text{odd}$					
-83.427	-82.485	-81.386	-80.131	-78.720	-77.153
-56.472	-55.543	-54.461	-53.225	-51.835	-50.292
-45.264	-44.414	-43.421	-42.284	-41.004	-39.581
-42.227	-41.250	-40.113	-38.817	-37.362	-35.750
-27.960	-27.147	-26.192	-25.092	-23.848	-22.458
-26.558	-25.596	-24.481	-23.213	-21.793	-20.223
-22.729	-21.970	-21.057	-19.990	-18.770	-17.397
-20.562	-19.432	-18.147	-16.710	-15.123	-13.391
-14.180	-13.361	-12.403	-11.305	-10.064	-8.678
-8.670	-7.774	-6.731	-5.540	-4.203	-2.721
$k=\text{odd}, (-1)^{J+P}=\text{even}$					
-103.063	-102.139	-101.061	-99.831	-98.447	-96.911
-90.423	-89.470	-88.358	-87.089	-85.664	-84.081
-83.150	-82.193	-81.077	-79.802	-78.368	-76.774
-70.227	-69.339	-68.304	-67.122	-65.792	-64.317
-57.251	-56.356	-55.313	-54.123	-52.786	-51.303
-48.583	-47.690	-46.650	-45.463	-44.133	-42.676
-47.856	-47.074	-46.155	-45.096	-43.894	-42.530
-42.723	-41.742	-40.607	-39.320	-37.885	-36.304
-36.944	-36.078	-35.068	-33.913	-32.613	-31.167
-34.310	-33.342	-32.214	-30.926	-29.478	-27.872
$k=\text{odd}, (-1)^{J+P}=\text{odd}$					
-90.480	-89.549	-88.464	-87.225	85.832	-84.286
-83.189	-82.247	-81.149	-79.894	-78.483	-76.915
-65.693	-64.743	-63.635	-62.370	-60.948	-59.370
-57.302	-56.427	-55.408	-54.244	-52.936	-51.486
-48.616	-47.737	-46.711	-45.540	-44.223	-42.761
-42.964	-42.066	-41.019	-39.822	-38.476	-36.981
-34.312	-33.346	-32.221	-30.937	-29.499	-27.973
-33.813	-32.933	-31.907	-30.736	-29.415	-27.881
-28.988	-28.186	-27.252	-26.185	-24.986	-23.656
-20.225	-19.416	-18.472	-17.395	-16.185	-14.842

Table SIV. Calculated infrared $|02^-\rangle \leftarrow |00^+\rangle$ transition energies (in cm^{-1}) of $\text{H}_2\text{O}-^{84}\text{Kr}$ with the intensity at 18K.

Transiton	Cal.	Line strength	Int.(18K)
$\Sigma^e(1_{01}) \leftarrow \Sigma^e(0_{00})$			
R(0)	7260.911	0.432	0.153
R(1)	7261.062	0.879	0.307
R(2)	7261.210	1.342	0.456
R(3)	7261.355	1.819	0.596
R(4)	7261.497	2.312	0.720
R(5)	7261.636	2.818	0.824
R(6)	7261.772	3.339	0.906
R(7)	7261.905	3.873	0.962
R(8)	7262.034	4.420	0.993
R(9)	7262.161	4.980	1.000
P(1)	7260.599	0.416	0.145
P(2)	7260.439	0.817	0.278
P(3)	7260.276	1.202	0.393
P(4)	7260.110	1.570	0.489
P(5)	7259.941	1.923	0.563
P(6)	7259.770	2.260	0.613
P(7)	7259.596	2.582	0.641
P(8)	7259.419	2.887	0.649
P(9)	7259.240	3.177	0.638
P(10)	7259.059	3.452	0.612
$\Sigma^e(2_{02}) \leftarrow \Pi^{e/f}(1_{01})$			
Q(1)	7280.532	0.180	0.146
Q(2)	7280.616	0.295	0.234
Q(3)	7280.730	0.407	0.311
Q(4)	7280.866	0.518	0.376
Q(5)	7281.015	0.629	0.429
Q(6)	7281.175	0.740	0.469
Q(7)	7281.340	0.853	0.495
Q(8)	7281.510	0.967	0.509
Q(9)	7281.681	1.083	0.510
Q(10)	7281.852	1.199	0.499
P(2)	7280.210	0.352	0.278
P(3)	7280.127	0.574	0.437
P(4)	7280.071	0.826	0.598
P(5)	7280.031	1.092	0.742
P(6)	7280.003	1.363	0.858
P(7)	7279.982	1.633	0.940
P(8)	7279.963	1.898	0.987
P(9)	7279.945	2.154	1.000
P(10)	7279.925	2.400	0.982

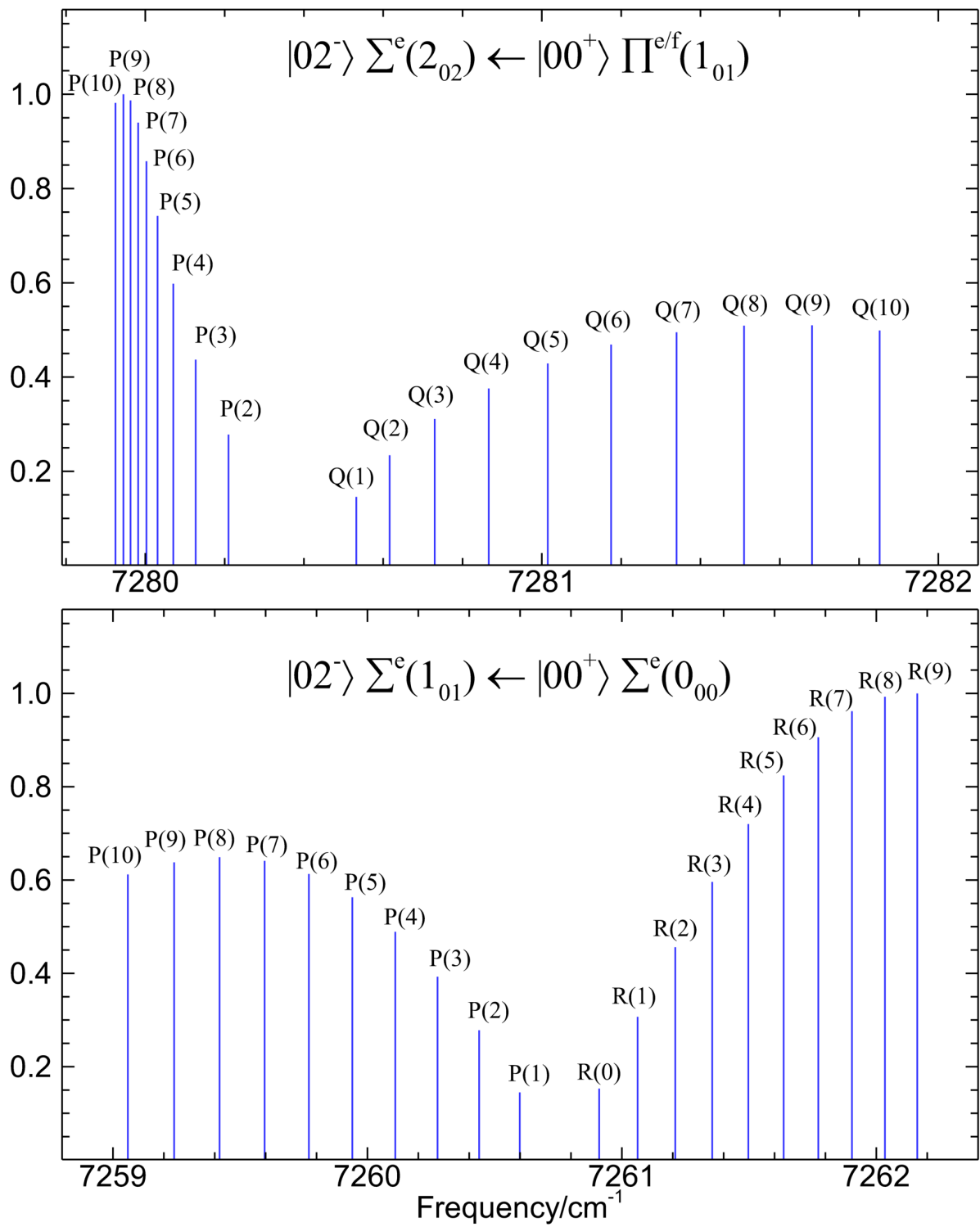


Figure S1. Simulated IR spectra of $|02^- \rangle \leftarrow |00^+ \rangle$ in the 7259 – 7282 cm⁻¹ region for H₂O-Kr at 18K.