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Supporting Information

Spectra of CO₂-Kr in the 4.3 μm region: Intermolecular Bend and Symmetry Breaking of the Intramolecular CO₂ Bend

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Table A-1. Molecular parameters for CO₂-Kr, microwave and fundamental band (in cm⁻¹).

See also Table 2 of the paper. Note the distortion parameters were constrained to be equal in the ground and excited states except for Δ_{JK} .

	CO ₂ - ⁸⁰ Kr	CO ₂ - ⁸² Kr	CO ₂ - ⁸³ Kr	CO ₂ - ⁸⁴ Kr	CO ₂ - ⁸⁶ Kr
ν_0	2348.2586	2348.2586	2348.2586	2348.2585	2348.2585
A'	0.393209	0.393209	0.393209	0.393209	0.393209
B'	0.0454486	0.0450552	0.0448666	0.0446832	0.0443284
C'	0.0404971	0.0401827	0.0400323	0.0398858	0.0396023
$10^6 \times \Delta_{JK}'$	5.94	5.89	5.86	5.84	5.79
A''	0.396347	0.396347	0.396347	0.396347	0.396347
B''	0.0454453	0.0450547	0.0448662	0.0446828	0.0443280
C''	0.0405311	0.0402196	0.0400690	0.0399224	0.0396386
$10^6 \times \Delta_K$	-5.3	-5.3	-5.3	-5.3	-5.3
$10^6 \times \Delta_{JK}''$	5.273	5.227	5.205	5.184	5.142
$10^7 \times \Delta_J$	2.559	2.515	2.494	2.473	2.434
$10^6 \times \delta_K$	3.32	3.32	3.32	3.32	3.32
$10^8 \times \delta_J$	2.65	2.61	2.58	2.56	2.52

Table A-2. Molecular parameters for CO₂-Xe, combination band (in cm⁻¹). See also Table 2 of the paper.

	CO ₂ - ⁸⁰ Kr	CO ₂ - ⁸² Kr	CO ₂ - ⁸³ Kr	CO ₂ - ⁸⁴ Kr	CO ₂ - ⁸⁶ Kr
ν_0	2377.6963	2377.6919	2377.6897	2377.6875	2377.6831
A'	0.408780	0.408780	0.408780	0.408780	0.408780
B'	0.043894	0.043514	0.043332	0.043155	0.042812
C'	0.038892	0.038590	0.038445	0.038304	0.038032
$10^6 \times \Delta_{JK}$	47.1	46.7	46.5	46.3	46.0
$10^7 \times \Delta_J$	2.66	2.62	2.60	2.57	2.53

Table A-3. Observed and fitted fundamental band transitions of CO₂-Kr (cm⁻¹).

Isotope	J'	Ka'	Kc'	J''	Ka''	Kc''	Observed	Calculated	Obs - Calc
CO2-84Kr	5	1	5	6	2	4	2346.6467	2346.6468	-0.0001
CO2-84Kr	6	1	5	7	2	6	2346.6511	2346.6516	
CO2-86Kr	5	1	5	6	2	4	2346.6511	2346.6502	
							Blend	2346.6512	-0.0001
CO2-84Kr	5	1	4	6	2	5	2346.7214	2346.7218	-0.0004
CO2-84Kr	4	1	4	5	2	3	2346.7448	2346.7449	-0.0001
CO2-84Kr	4	1	3	5	2	4	2346.7943	2346.7944	0.0000
CO2-84Kr	3	1	3	4	2	2	2346.8398	2346.8399	-0.0001
CO2-84Kr	3	1	2	4	2	3	2346.8693	2346.8693	0.0000
CO2-86Kr	2	1	2	3	2	1	2346.9319	2346.9331	
CO2-84Kr	2	1	2	3	2	1	2346.9319	2346.9321	
							Blend	2346.9323	-0.0004
CO2-84Kr	2	1	1	3	2	2	2346.9466	2346.9467	
CO2-86Kr	2	1	1	3	2	2	2346.9466	2346.9475	
							Blend	2346.9469	-0.0003
CO2-86Kr	1	1	1	2	2	0	2347.0215	2347.0219	
CO2-84Kr	1	1	1	2	2	0	2347.0215	2347.0216	
							Blend	2347.0217	-0.0002
CO2-84Kr	1	1	0	2	2	1	2347.0264	2347.0265	
CO2-86Kr	1	1	0	2	2	1	2347.0264	2347.0267	
							Blend	2347.0265	-0.0001
CO2-84Kr	9	1	9	9	2	8	2347.0839	2347.0840	
CO2-86Kr	9	1	9	9	2	8	2347.0839	2347.0846	
							Blend	2347.0841	-0.0002
CO2-84Kr	8	1	8	8	2	7	2347.1059	2347.1060	
CO2-86Kr	8	1	8	8	2	7	2347.1059	2347.1063	
							Blend	2347.1061	-0.0002
CO2-84Kr	7	1	7	7	2	6	2347.1254	2347.1255	
CO2-86Kr	7	1	7	7	2	6	2347.1254	2347.1255	
							Blend	2347.1255	-0.0001
CO2-84Kr	6	1	6	6	2	5	2347.1424	2347.1425	
CO2-86Kr	6	1	6	6	2	5	2347.1424	2347.1423	
							Blend	2347.1425	0.0000
CO2-86Kr	5	1	5	5	2	4	2347.1571	2347.1566	
CO2-84Kr	5	1	5	5	2	4	2347.1571	2347.1570	
							Blend	2347.1569	0.0002
CO2-84Kr	4	1	4	4	2	3	2347.1692	2347.1691	
CO2-86Kr	4	1	4	4	2	3	2347.1692	2347.1685	
							Blend	2347.1690	0.0002
CO2-86Kr	3	1	3	3	2	2	2347.1788	2347.1780	
CO2-84Kr	3	1	3	3	2	2	2347.1788	2347.1788	
							Blend	2347.1786	0.0002

CO2-84Kr	2	1	2	2	2	1	2347.1861	2347.1860	
CO2-86Kr	2	1	2	2	2	1	2347.1861	2347.1851	
							Blend	2347.1858	0.0003
CO2-86Kr	2	1	1	2	2	0	2347.2004	2347.1992	
CO2-84Kr	2	1	1	2	2	0	2347.2004	2347.2003	
							Blend	2347.2000	0.0004
CO2-84Kr	3	1	2	3	2	1	2347.2074	2347.2072	
CO2-86Kr	3	1	2	3	2	1	2347.2074	2347.2060	
							Blend	2347.2070	0.0004
CO2-84Kr	4	1	3	4	2	2	2347.2163	2347.2162	
CO2-86Kr	4	1	3	4	2	2	2347.2163	2347.2149	
							Blend	2347.2159	0.0004
CO2-84Kr	5	1	4	5	2	3	2347.2272	2347.2271	0.0001
CO2-84Kr	6	1	5	6	2	4	2347.2397	2347.2395	0.0001
CO2-84Kr	7	1	6	7	2	5	2347.2533	2347.2533	0.0000
CO2-84Kr	8	1	7	8	2	6	2347.2680	2347.2679	0.0001
CO2-84Kr	9	1	8	9	2	7	2347.2832	2347.2831	0.0001
CO2-84Kr	10	1	9	10	2	8	2347.2984	2347.2984	0.0000
CO2-84Kr	4	1	3	3	2	2	2347.5551	2347.5551	0.0000
CO2-86Kr	5	1	4	4	2	3	2347.6478	2347.6466	
CO2-84Kr	6	1	6	5	2	3	2347.6478	2347.6478	
							Blend	2347.6475	0.0003
CO2-84Kr	5	1	4	4	2	3	2347.6510	2347.6513	-0.0003
CO2-82Kr	9	1	9	10	0	10	2347.6663	2347.6663	0.0000
CO2-83Kr	9	1	9	10	0	10	2347.6705	2347.6704	0.0001
CO2-84Kr	9	1	9	10	0	10	2347.6743	2347.6744	-0.0001
CO2-86Kr	9	1	9	10	0	10	2347.6821	2347.6820	0.0001
CO2-84Kr	7	1	7	6	2	4	2347.7136	2347.7134	0.0002
CO2-84Kr	6	1	5	5	2	4	2347.7495	2347.7498	-0.0003
CO2-82Kr	8	1	8	9	0	9	2347.7669	2347.7670	-0.0002
CO2-83Kr	8	1	8	9	0	9	2347.7714	2347.7707	
CO2-86Kr	8	1	8	7	2	5	2347.7714	2347.7709	
							Blend	2347.7708	0.0007
CO2-84Kr	8	1	8	9	0	9	2347.7742	2347.7743	-0.0001
CO2-86Kr	8	1	8	9	0	9	2347.7812	2347.7812	0.0000
CO2-82Kr	7	1	7	8	0	8	2347.8672	2347.8671	0.0001
CO2-83Kr	7	1	7	8	0	8	2347.8704	2347.8703	0.0001
CO2-84Kr	7	1	7	8	0	8	2347.8735	2347.8735	0.0000
CO2-84Kr	8	1	7	7	2	6	2347.9532	2347.9533	-0.0001
CO2-82Kr	6	1	6	7	0	7	2347.9663	2347.9660	0.0002
CO2-84Kr	6	1	6	7	0	7	2347.9716	2347.9716	0.0000
CO2-86Kr	6	1	6	7	0	7	2347.9767	2347.9769	-0.0002
CO2-84Kr	9	1	8	8	2	7	2348.0581	2348.0581	-0.0001
CO2-84Kr	5	1	5	6	0	6	2348.0684	2348.0684	-0.0001
CO2-86Kr	5	1	5	6	0	6	2348.0730	2348.0730	0.0000
CO2-84Kr	4	1	4	5	0	5	2348.1637	2348.1637	0.0000
CO2-86Kr	4	1	4	5	0	5	2348.1674	2348.1675	-0.0001
CO2-84Kr	3	1	3	4	0	4	2348.2571	2348.2571	0.0000

CO2-84Kr	2	1	2	3	0	3	2348.3484	2348.3486	-0.0002
CO2-84Kr	1	1	1	2	0	2	2348.4377	2348.4379	-0.0001
CO2-84Kr	1	1	0	1	0	1	2348.6117	2348.6118	-0.0001
CO2-84Kr	2	1	1	2	0	2	2348.6165	2348.6165	
CO2-86Kr	2	1	1	2	0	2	2348.6165	2348.6167	
							Blend	2348.6166	-0.0001
CO2-84Kr	3	1	2	3	0	3	2348.6236	2348.6237	
CO2-86Kr	3	1	2	3	0	3	2348.6236	2348.6238	
							Blend	2348.6237	-0.0001
CO2-84Kr	4	1	3	4	0	4	2348.6334	2348.6335	
CO2-86Kr	4	1	3	4	0	4	2348.6334	2348.6334	
							Blend	2348.6334	0.0000
CO2-84Kr	5	1	4	5	0	5	2348.6458	2348.6459	
CO2-86Kr	5	1	4	5	0	5	2348.6458	2348.6456	
							Blend	2348.6458	0.0000
CO2-84Kr	6	1	5	6	0	6	2348.6611	2348.6612	
CO2-86Kr	6	1	5	6	0	6	2348.6611	2348.6607	
							Blend	2348.6611	0.0000
CO2-84Kr	7	1	6	7	0	7	2348.6794	2348.6796	
CO2-86Kr	7	1	6	7	0	7	2348.6794	2348.6787	
							Blend	2348.6794	0.0000
CO2-84Kr	1	1	1	0	0	0	2348.6916	2348.6916	
CO2-86Kr	1	1	1	0	0	0	2348.6916	2348.6913	
							Blend	2348.6915	0.0001
CO2-84Kr	8	1	7	8	0	8	2348.7009	2348.7012	
CO2-86Kr	8	1	7	8	0	8	2348.7009	2348.7000	
							Blend	2348.7009	-0.0001
CO2-84Kr	9	1	8	9	0	9	2348.7262	2348.7264	
CO2-86Kr	9	1	8	9	0	9	2348.7262	2348.7247	
							Blend	2348.7260	0.0002
CO2-84Kr	2	1	2	1	0	1	2348.7714	2348.7713	
CO2-86Kr	2	1	2	1	0	1	2348.7714	2348.7704	
							Blend	2348.7711	0.0003
CO2-84Kr	3	1	3	2	0	2	2348.8488	2348.8486	0.0002
CO2-84Kr	4	1	4	3	0	3	2348.9237	2348.9235	0.0001
CO2-84Kr	5	1	5	4	0	4	2348.9963	2348.9962	0.0001
CO2-86Kr	6	1	6	5	0	5	2349.0636	2349.0638	-0.0002
CO2-84Kr	6	1	6	5	0	5	2349.0667	2349.0666	0.0000
CO2-86Kr	7	1	7	6	0	6	2349.1318	2349.1319	-0.0001
CO2-84Kr	7	1	7	6	0	6	2349.1351	2349.1351	0.0000
CO2-86Kr	8	1	8	7	0	7	2349.1981	2349.1982	-0.0001
CO2-84Kr	8	1	8	7	0	7	2349.2019	2349.2018	0.0000
CO2-86Kr	9	1	9	8	0	8	2349.2627	2349.2629	-0.0002
CO2-84Kr	9	1	9	8	0	8	2349.2670	2349.2669	0.0000
CO2-86Kr	10	1	10	9	0	9	2349.3262	2349.3263	-0.0001
CO2-84Kr	10	1	10	9	0	9	2349.3308	2349.3308	0.0001
CO2-82Kr	10	1	10	9	0	9	2349.3354	2349.3354	0.0000
CO2-86Kr	11	1	11	10	0	10	2349.3887	2349.3888	0.0000

CO2-84Kr	11	1	11	10	0	10	2349.3937	2349.3936	0.0001
CO2-82Kr	11	1	11	10	0	10	2349.3984	2349.3987	-0.0002
CO2-86Kr	12	1	12	11	0	11	2349.4506	2349.4505	0.0001
CO2-84Kr	12	1	12	11	0	11	2349.4559	2349.4557	0.0002
CO2-82Kr	12	1	12	11	0	11	2349.4613	2349.4612	0.0001
CO2-86Kr	13	1	13	12	0	12	2349.5115	2349.5117	-0.0002
CO2-84Kr	13	1	13	12	0	12	2349.5174	2349.5174	-0.0001
CO2-82Kr	13	1	13	12	0	12	2349.5232	2349.5234	-0.0002
CO2-86Kr	15	1	15	14	0	14	2349.6339	2349.6341	-0.0002
CO2-84Kr	15	1	15	14	0	14	2349.6407	2349.6407	0.0000
CO2-82Kr	3	3	0	4	2	3	2349.6573	2349.6580	
CO2-82Kr	3	3	1	4	2	2	2349.6573	2349.6573	
							Blend	2349.6576	-0.0003
CO2-84Kr	3	3	0	4	2	3	2349.6617	2349.6623	
CO2-84Kr	3	3	1	4	2	2	2349.6617	2349.6616	
							Blend	2349.6619	-0.0002
CO2-86Kr	3	3	0	4	2	3	2349.6660	2349.6664	
CO2-86Kr	3	3	1	4	2	2	2349.6660	2349.6657	
							Blend	2349.6660	-0.0001
CO2-86Kr	16	1	16	15	0	15	2349.6964	2349.6957	0.0008
CO2-84Kr	16	1	16	15	0	15	2349.7023	2349.7028	-0.0005
CO2-83Kr	16	1	16	15	0	15	2349.7062	2349.7065	-0.0003
CO2-82Kr	16	1	16	15	0	15	2349.7107	2349.7103	0.0004
CO2-84Kr	5	3	3	5	2	4	2349.9997	2349.9999	
CO2-84Kr	5	3	2	5	2	3	2349.9997	2349.9983	
CO2-84Kr	4	3	2	4	2	3	2349.9997	2350.0002	
CO2-84Kr	4	3	1	4	2	2	2349.9997	2349.9995	
CO2-84Kr	6	3	4	6	2	5	2349.9997	2349.9998	
CO2-84Kr	7	3	5	7	2	6	2349.9997	2349.9999	
CO2-84Kr	3	3	1	3	2	2	2349.9997	2350.0005	
CO2-84Kr	3	3	0	3	2	1	2349.9997	2350.0002	
CO2-84Kr	8	3	6	8	2	7	2349.9997	2350.0002	
CO2-84Kr	9	3	7	9	2	8	2349.9997	2350.0009	
							Blend	2349.9998	-0.0001
CO2-84Kr	3	3	0	2	2	1	2350.2541	2350.2541	
CO2-84Kr	3	3	1	2	2	0	2350.2541	2350.2541	
CO2-86Kr	3	3	0	2	2	1	2350.2541	2350.2537	
CO2-86Kr	3	3	1	2	2	0	2350.2541	2350.2537	
							Blend	2350.2540	0.0001
CO2-84Kr	4	3	1	3	2	2	2350.3381	2350.3383	
CO2-84Kr	4	3	2	3	2	1	2350.3381	2350.3381	
CO2-86Kr	4	3	1	3	2	2	2350.3381	2350.3373	
CO2-86Kr	4	3	2	3	2	1	2350.3381	2350.3371	
							Blend	2350.3380	0.0001
CO2-84Kr	5	3	2	4	2	3	2350.4222	2350.4226	
CO2-84Kr	5	3	3	4	2	2	2350.4222	2350.4218	
CO2-86Kr	5	3	2	4	2	3	2350.4222	2350.4209	
							Blend	2350.4220	0.0002

CO2-84Kr	6	3	3	5	2	4	2350.5062	2350.5068	
CO2-84Kr	6	3	4	5	2	3	2350.5062	2350.5051	
							Blend	2350.5060	0.0002
CO2-84Kr	7	3	5	6	2	4	2350.5879	2350.5878	
CO2-86Kr	7	3	4	6	2	5	2350.5879	2350.5882	
							Blend	2350.5879	0.0000
CO2-84Kr	7	3	4	6	2	5	2350.5910	2350.5912	-0.0002
CO2-86Kr	8	3	6	7	2	5	2350.6662	2350.6663	-0.0001
CO2-84Kr	8	3	6	7	2	5	2350.6700	2350.6697	0.0003
CO2-84Kr	8	3	5	7	2	6	2350.6758	2350.6758	0.0000
							Blend	2347.2070	0.0004

Table A-4. Observed and fitted combination band transitions of CO₂-Kr (cm⁻¹).

Isotope	J'	Ka'	Kc'	J''	Ka''	Kc''	Observed	Calculated	Obs - Calc
CO2-84Kr	10	0	10	11	0	11	2376.5936	2376.5944	-0.0009
CO2-86Kr	10	0	10	11	0	11	2376.5975	2376.5981	-0.0006
CO2-84Kr	10	2	8	11	2	9	2376.6150	2376.6152	-0.0002
CO2-84Kr	10	2	9	11	2	10	2376.6248	2376.6246	0.0001
CO2-84Kr	9	0	9	10	0	10	2376.7077	2376.7081	-0.0004
CO2-86Kr	9	0	9	10	0	10	2376.7109	2376.7109	0.0001
CO2-84Kr	9	2	7	10	2	8	2376.7360	2376.7361	-0.0001
CO2-84Kr	9	2	8	10	2	9	2376.7433	2376.7433	-0.0001
CO2-84Kr	8	0	8	9	0	9	2376.8190	2376.8189	0.0001
CO2-84Kr	8	2	6	9	2	7	2376.8532	2376.8533	-0.0002
CO2-84Kr	8	2	7	9	2	8	2376.8586	2376.8587	-0.0001
CO2-86Kr	7	0	7	8	0	8	2376.9273	2376.9282	
CO2-84Kr	7	0	7	8	0	8	2376.9273	2376.9269	
							Blend	2376.9272	0.0001
CO2-84Kr	7	2	5	8	2	6	2376.9670	2376.9668	0.0002
CO2-84Kr	7	2	6	8	2	7	2376.9706	2376.9706	0.0000
CO2-84Kr	6	0	6	7	0	7	2377.0329	2377.0321	
CO2-86Kr	6	0	6	7	0	7	2377.0329	2377.0326	
							Blend	2377.0322	0.0006
CO2-84Kr	6	2	4	7	2	5	2377.0770	2377.0766	0.0004
CO2-84Kr	6	2	5	7	2	6	2377.0792	2377.0792	0.0000
CO2-86Kr	5	0	5	6	0	6	2377.1356	2377.1343	
CO2-84Kr	5	0	5	6	0	6	2377.1356	2377.1345	
							Blend	2377.1345	0.0011
CO2-84Kr	5	2	4	6	2	5	2377.1835	2377.1844	
CO2-84Kr	5	2	3	6	2	4	2377.1835	2377.1827	
CO2-86Kr	5	2	4	6	2	5	2377.1835	2377.1841	
CO2-86Kr	5	2	3	6	2	4	2377.1835	2377.1826	
							Blend	2377.1835	0.0000
CO2-84Kr	4	0	4	5	0	5	2377.2342	2377.2341	0.0001
CO2-84Kr	4	2	2	5	2	3	2377.2855	2377.2852	
CO2-86Kr	4	2	2	5	2	3	2377.2855	2377.2842	
CO2-86Kr	4	2	3	5	2	4	2377.2855	2377.2851	
CO2-84Kr	4	2	3	5	2	4	2377.2855	2377.2861	
							Blend	2377.2854	0.0000
CO2-84Kr	3	0	3	4	0	4	2377.3306	2377.3308	-0.0002
CO2-84Kr	3	2	1	4	2	2	2377.3839	2377.3840	
CO2-86Kr	3	2	2	4	2	3	2377.3839	2377.3827	
CO2-84Kr	3	2	2	4	2	3	2377.3839	2377.3845	
							Blend	2377.3840	-0.0001
CO2-84Kr	2	0	2	3	0	3	2377.4241	2377.4245	-0.0004
CO2-84Kr	2	2	1	3	2	2	2377.4789	2377.4794	

CO2-84Kr	2	2	0	3	2	1	2377.4789	2377.4792	
							Blend	2377.4793	-0.0004
CO2-84Kr	1	0	1	2	0	2	2377.5147	2377.5152	-0.0006
CO2-86Kr	0	0	0	1	0	1	2377.5986	2377.5992	-0.0006
CO2-84Kr	0	0	0	1	0	1	2377.6021	2377.6029	-0.0008
CO2-84Kr	7	2	6	7	2	5	2377.6388	2377.6401	-0.0014
CO2-84Kr	7	2	5	7	2	6	2377.6512	2377.6521	-0.0010
CO2-84Kr	6	2	5	6	2	4	2377.6672	2377.6671	0.0001
CO2-84Kr	6	2	4	6	2	5	2377.6737	2377.6738	-0.0001
CO2-86Kr	5	2	3	5	2	4	2377.6895	2377.6889	
CO2-84Kr	5	2	4	5	2	3	2377.6895	2377.6897	
							Blend	2377.6895	0.0000
CO2-84Kr	5	2	3	5	2	4	2377.6929	2377.6930	-0.0001
CO2-86Kr	4	2	3	4	2	2	2377.7047	2377.7039	
CO2-86Kr	4	2	2	4	2	3	2377.7047	2377.7052	
							Blend	2377.7046	0.0002
CO2-84Kr	4	2	2	4	2	3	2377.7091	2377.7094	
CO2-84Kr	4	2	3	4	2	2	2377.7091	2377.7080	
							Blend	2377.7087	0.0004
CO2-86Kr	3	2	1	3	2	2	2377.7187	2377.7186	
CO2-86Kr	3	2	2	3	2	1	2377.7187	2377.7181	
							Blend	2377.7183	0.0003
CO2-84Kr	3	2	1	3	2	2	2377.7230	2377.7229	
CO2-84Kr	3	2	2	3	2	1	2377.7230	2377.7224	
							Blend	2377.7226	0.0004
CO2-86Kr	2	2	0	2	2	1	2377.7289	2377.7287	
CO2-86Kr	2	2	1	2	2	0	2377.7289	2377.7286	
							Blend	2377.7287	0.0002
CO2-84Kr	2	2	1	2	2	0	2377.7335	2377.7330	
CO2-84Kr	2	2	0	2	2	1	2377.7335	2377.7331	
							Blend	2377.7330	0.0004
CO2-80Kr	2	2	0	2	2	1	2377.7421	2377.7418	
CO2-80Kr	2	2	1	2	2	0	2377.7421	2377.7417	
							Blend	2377.7417	0.0004
CO2-86Kr	1	0	1	0	0	0	2377.7646	2377.7640	0.0007
CO2-84Kr	1	0	1	0	0	0	2377.7693	2377.7690	0.0003
CO2-86Kr	3	0	3	2	0	2	2377.9164	2377.9161	0.0003
CO2-84Kr	3	0	3	2	0	2	2377.9222	2377.9222	0.0000
CO2-82Kr	3	0	3	2	0	2	2377.9282	2377.9285	-0.0003
CO2-80Kr	3	0	3	2	0	2	2377.9348	2377.9348	0.0000
CO2-86Kr	3	2	1	2	2	0	2377.9703	2377.9703	
CO2-86Kr	3	2	2	2	2	1	2377.9703	2377.9701	
							Blend	2377.9702	0.0001
CO2-84Kr	3	2	2	2	2	1	2377.9763	2377.9763	
CO2-84Kr	3	2	1	2	2	0	2377.9763	2377.9765	
							Blend	2377.9764	-0.0001
CO2-82Kr	3	2	1	2	2	0	2377.9825	2377.9827	
CO2-82Kr	3	2	2	2	2	1	2377.9825	2377.9825	

							Blend	2377.9826	-0.0001
CO2-86Kr	4	0	4	3	0	3	2377.9877	2377.9873	0.0004
CO2-84Kr	4	0	4	3	0	3	2377.9940	2377.9939	0.0001
CO2-82Kr	4	0	4	3	0	3	2378.0006	2378.0007	-0.0002
CO2-80Kr	4	0	4	3	0	3	2378.0076	2378.0077	-0.0001
CO2-86Kr	4	2	3	3	2	2	2378.0403	2378.0402	
CO2-86Kr	4	2	2	3	2	1	2378.0403	2378.0406	
							Blend	2378.0404	-0.0001
CO2-84Kr	4	2	3	3	2	2	2378.0470	2378.0469	
CO2-84Kr	4	2	2	3	2	1	2378.0470	2378.0473	
							Blend	2378.0471	-0.0001
CO2-83Kr	4	2	3	3	2	2	2378.0505	2378.0503	
CO2-83Kr	4	2	2	3	2	1	2378.0505	2378.0507	
							Blend	2378.0505	0.0000
CO2-86Kr	5	0	5	4	0	4	2378.0552	2378.0551	0.0001
CO2-84Kr	5	0	5	4	0	4	2378.0623	2378.0623	0.0001
CO2-83Kr	5	0	5	4	0	4	2378.0657	2378.0659	-0.0002
CO2-82Kr	5	0	5	4	0	4	2378.0696	2378.0696	0.0000
CO2-80Kr	5	0	5	4	0	4	2378.0771	2378.0771	0.0000
CO2-86Kr	5	2	4	4	2	3	2378.1070	2378.1067	
CO2-86Kr	5	2	3	4	2	2	2378.1070	2378.1076	
							Blend	2378.1072	-0.0002
CO2-84Kr	5	2	3	4	2	2	2378.1143	2378.1149	
CO2-84Kr	5	2	4	4	2	3	2378.1143	2378.1139	
							Blend	2378.1144	-0.0001
CO2-86Kr	6	0	6	5	0	5	2378.1198	2378.1195	0.0003
CO2-84Kr	6	0	6	5	0	5	2378.1273	2378.1272	0.0001
CO2-83Kr	6	0	6	5	0	5	2378.1309	2378.1310	-0.0001
CO2-82Kr	6	0	6	5	0	5	2378.1348	2378.1350	-0.0002
CO2-80Kr	6	0	6	5	0	5	2378.1430	2378.1431	-0.0001
CO2-84Kr	7	0	7	6	0	6	2378.1885	2378.1886	0.0000
CO2-83Kr	7	0	7	6	0	6	2378.1926	2378.1927	-0.0001
CO2-82Kr	7	0	7	6	0	6	2378.1968	2378.1968	0.0000
CO2-80Kr	7	0	7	6	0	6	2378.2058	2378.2055	0.0003
CO2-86Kr	7	2	6	6	2	5	2378.2288	2378.2292	-0.0004
CO2-86Kr	7	2	5	6	2	4	2378.2309	2378.2319	-0.0010
CO2-84Kr	8	0	8	7	0	7	2378.2463	2378.2464	-0.0001
CO2-83Kr	8	0	8	7	0	7	2378.2504	2378.2507	-0.0004
CO2-82Kr	8	0	8	7	0	7	2378.2551	2378.2551	0.0000
CO2-86Kr	8	2	7	7	2	6	2378.2853	2378.2851	0.0002
CO2-86Kr	8	2	6	7	2	5	2378.2891	2378.2892	-0.0001
CO2-84Kr	8	2	7	7	2	6	2378.2939	2378.2937	0.0002
CO2-84Kr	8	2	6	7	2	5	2378.2983	2378.2978	0.0005
CO2-84Kr	9	0	9	8	0	8	2378.3010	2378.3006	0.0004
CO2-82Kr	9	0	9	8	0	8	2378.3098	2378.3097	0.0000
CO2-86Kr	9	2	8	8	2	7	2378.3379	2378.3375	0.0004
CO2-86Kr	10	0	10	9	0	9	2378.3426	2378.3420	
CO2-86Kr	9	2	7	8	2	6	2378.3426	2378.3432	

							Blend	2378.3424	0.0002
CO2-84Kr	9	2	8	8	2	7	2378.3472	2378.3464	0.0008
CO2-84Kr	10	0	10	9	0	9	2378.3519	2378.3512	
CO2-84Kr	9	2	7	8	2	6	2378.3519	2378.3524	
							Blend	2378.3516	0.0003
CO2-83Kr	9	2	7	8	2	6	2378.3568	2378.3570	
CO2-83Kr	10	0	10	9	0	9	2378.3568	2378.3559	
CO2-82Kr	9	2	8	8	2	7	2378.3568	2378.3556	
							Blend	2378.3561	0.0007
CO2-82Kr	9	2	7	8	2	6	2378.3613	2378.3617	
CO2-82Kr	10	0	10	9	0	9	2378.3613	2378.3606	
							Blend	2378.3610	0.0003

Table A-5. Observed and fitted (01¹1) ← (01¹0) hot band transitions of CO₂-Kr (cm⁻¹).Transitions with $K_a'' = 0$ and 2 belong to the in-plane band.Transitions with $K_a'' = 1$ and 3 belong to the out-of-plane band.

J'	K_a'	K_c'	J''	K_a''	K_c''	Observed	Calculated	Obs - Calc
3	1	2	4	2	3	2334.3979	2334.3975	0.0004
3	1	3	4	2	2	2334.4012	2334.4011	0.0001
2	1	1	3	2	2	2334.4625	2334.4621	0.0003
2	1	2	3	2	1	2334.4651	2334.4652	-0.0001
1	1	0	2	2	1	2334.5278	2334.5270	
1	1	1	2	2	0	2334.5278	2334.5286	
						Blend	2334.5278	0.0000
2	1	1	2	2	0	2334.6813	2334.6815	-0.0002
2	1	2	2	2	1	2334.6912	2334.6911	
3	1	2	3	2	1	2334.6912	2334.6916	
						Blend	2334.6914	-0.0002
4	1	3	4	2	2	2334.7000	2334.7001	-0.0001
4	1	4	4	2	3	2334.7351	2334.7353	-0.0002
5	1	5	5	2	4	2334.7586	2334.7588	-0.0002
6	1	6	6	2	5	2334.7818	2334.7819	-0.0001
8	1	8	8	2	7	2334.8243	2334.8241	0.0002
4	0	4	5	1	5	2334.9609	2334.9612	-0.0003
3	0	3	4	1	4	2335.0452	2335.0453	-0.0001
2	0	2	3	1	3	2335.1336	2335.1336	0.0000
10	1	10	11	0	11	2335.2033	2335.2027	
6	1	5	5	2	4	2335.2033	2335.2036	
						Blend	2335.2033	0.0000
6	0	6	6	1	5	2335.2610	2335.2610	0.0000
9	1	9	10	0	10	2335.2897	2335.2897	0.0001
5	0	5	5	1	4	2335.2966	2335.2966	-0.0001
0	0	0	1	1	1	2335.3203	2335.3203	-0.0001
4	0	4	4	1	3	2335.3287	2335.3287	0.0000
3	0	3	3	1	2	2335.3576	2335.3576	0.0000
8	1	8	9	0	9	2335.3749	2335.3749	0.0001
2	0	2	2	1	1	2335.3830	2335.3830	-0.0001
1	0	1	1	1	0	2335.4032	2335.4032	0.0000
5	1	5	6	0	6	2335.6216	2335.6218	-0.0002
3	0	3	2	1	2	2335.6846	2335.6845	0.0001
4	1	4	5	0	5	2335.7021	2335.7020	0.0001
4	0	4	3	1	3	2335.7728	2335.7724	0.0005
3	1	3	4	0	4	2335.7821	2335.7816	0.0005
2	1	2	3	0	3	2335.8613	2335.8610	0.0003
1	1	1	2	0	2	2335.9394	2335.9403	-0.0009
5	1	4	5	0	5	2336.0734	2336.0735	-0.0001
4	1	3	4	0	4	2336.0806	2336.0806	0.0000
3	1	2	3	0	3	2336.0873	2336.0874	0.0000

2	1	1	2	0	2	2336.0933	2336.0933	0.0000
1	1	0	1	0	1	2336.0976	2336.0976	0.0000
1	1	1	0	0	0	2336.1806	2336.1805	0.0000
2	1	2	1	0	1	2336.2617	2336.2616	0.0001
3	1	3	2	0	2	2336.3433	2336.3433	0.0001
4	1	4	3	0	3	2336.4252	2336.4252	0.0001
5	1	5	4	0	4	2336.5073	2336.5071	0.0001
6	1	6	5	0	5	2336.5890	2336.5889	0.0001
2	2	0	2	1	1	2336.7678	2336.7679	-0.0001
2	2	1	2	1	2	2336.7945	2336.7945	0.0000
9	1	9	8	0	8	2336.8298	2336.8300	-0.0001
10	1	10	9	0	9	2336.9078	2336.9080	-0.0001
2	2	1	1	1	0	2336.9718	2336.9719	-0.0002
2	2	0	1	1	1	2336.9813	2336.9815	-0.0002
5	3	2	5	1	4	2337.0424	2337.0427	-0.0002
4	2	2	3	1	3	2337.0499	2337.0501	-0.0002
12	1	12	11	0	11	2337.0593	2337.0592	0.0000
4	3	1	4	1	3	2337.0651	2337.0649	0.0002
4	3	2	4	1	4	2337.1453	2337.1452	0.0000
5	3	3	5	1	5	2337.1579	2337.1579	-0.0001
6	3	4	6	1	6	2337.1733	2337.1730	0.0003
6	2	5	6	2	5	2337.2120	2337.2122	-0.0002
7	2	6	7	2	6	2337.2229	2337.2229	-0.0001
8	2	7	8	2	7	2337.2349	2337.2348	0.0000
3	3	1	2	1	1	2337.3841	2337.3841	0.0000
3	3	0	2	1	2	2337.4104	2337.4109	
3	2	1	2	2	1	2337.4104	2337.4107	
3	2	2	2	2	0	2337.4104	2337.4086	
						Blend	2337.4100	0.0004
4	3	2	3	1	2	2337.4577	2337.4576	0.0002
4	2	3	3	2	1	2337.4895	2337.4892	0.0002
4	2	2	3	2	2	2337.4969	2337.4965	0.0004
4	3	1	3	1	3	2337.5088	2337.5086	0.0002
5	3	3	4	1	3	2337.5257	2337.5254	0.0002
5	2	4	4	2	2	2337.5704	2337.5706	-0.0001
3	3	0	3	2	1	2337.5759	2337.5760	-0.0001
3	3	1	3	2	2	2337.5812	2337.5811	0.0001
6	3	4	5	1	4	2337.5876	2337.5887	
5	2	3	4	2	3	2337.5876	2337.5870	
						Blend	2337.5876	0.0000
5	3	2	4	1	4	2337.6068	2337.6071	-0.0003
3	3	0	2	2	1	2337.8007	2337.8019	
3	3	1	2	2	0	2337.8007	2337.8005	
						Blend	2337.8012	-0.0005
4	3	2	3	2	1	2337.9496	2337.9495	0.0001
4	3	1	3	2	2	2337.9548	2337.9550	-0.0002
5	3	3	4	2	2	2338.1046	2338.1045	0.0001
5	3	2	4	2	3	2338.1172	2338.1173	0.0000

6	3	4	5	2	3	2338.2629	2338.2628	0.0001
6	3	3	5	2	4	2338.2863	2338.2864	-0.0001
7	3	5	6	2	4	2338.4231	2338.4232	-0.0001
4	4	0	3	3	1	2338.5236	2338.5236	
4	4	1	3	3	0	2338.5236	2338.5236	
						Blend	2338.5236	0.0000
5	4	1	4	3	2	2338.6113	2338.6112	
5	4	2	4	3	1	2338.6113	2338.6112	
						Blend	2338.6112	0.0001
6	4	2	5	3	3	2338.6996	2338.6997	
6	4	3	5	3	2	2338.6996	2338.6996	
						Blend	2338.6997	0.0000
