

Table S1. Rovibrational energy levels with $J \leq 4$ of *para*H₂-CO₂ for CO₂ in its vibrational ground state. Energies are given in cm⁻¹.

J	Even +1	Even -1	Odd +1	Odd -1
0	-50.383 (000)		-28.316	
	-23.544		-20.235	
	-15.116		-7.107	
	-3.335			
1	-26.838	-49.385(111)	-49.230(110)	-49.727(101)
	-14.373	-27.545	-20.313	-27.241
		-21.927	-8.371	-22.354
		-17.805	-0.594	-17.186
		-10.884		-11.607
		-4.297		-3.863
		-0.647		-0.291
2	-48.456(202)	-47.768(211)	-48.232(212)	-46.747(221)
	-46.706(220)	-24.380	-26.100	-25.192
	-26.257	-18.114	-24.507	-17.335
	-20.131	-10.474	-21.069	-11.298
	-18.961	-4.230	-14.659	-3.602
	-14.967		-13.081	
	-7.891		-6.898	
	-5.935		-1.950	
3	-44.804(322)	-46.523(313)	-45.604(312)	-46.638(303)
	-22.747	-42.702(331)	-42.695(330)	-44.616(321)
	-20.607	-24.355	-22.637	-24.615
	-15.180	-22.675	-14.995	-20.934
	-7.513	-19.001	-13.155	-18.157
	-5.441	-14.900	-7.661	-16.974
		-10.979	-0.597	-11.856
		-10.462		-8.302
		-3.182		-3.252
		-1.531		-2.146

Table S1. continued.

J	Even +1	Even -1	Odd +1	Odd -1
4	-44.324(404)	-42.782(413)	-44.278(414)	-42.238(423)
	-41.745(422)	-40.047(431)	-40.093(432)	-37.245(441)
	-37.244(440)	-20.143	-22.434	-19.651
	-22.331	-15.762	-19.614	-18.682
	-19.768	-11.049	-16.386	-12.065
	-16.018	-10.862	-15.863	-7.957
	-13.006	-3.851	-13.804	-3.207
	-9.870	-0.144	-7.574	-2.222
	-7.869		-5.955	
	-5.644		-2.721	

Table S2. Rovibrational energy levels with $J \leq 4$ of *ortho*H₂-CO₂ for CO₂ in its vibrational ground state. Energies are given in cm⁻¹. Note that *ortho*H₂-CO₂ dissociates into the $j_{\text{H}_2} = 1$ channel, so that states with energies lower than $2B(\text{H}_2) = 118.644 \text{ cm}^{-1}$ are bound.

J	Even +1	Even -1	Odd +1	Odd -1
0	72.172	93.651	46.939	67.576
	82.951	109.418	80.807	102.472
	93.097		86.855	113.653
	100.276		99.545	
	108.919		105.813	
	112.902		111.507	
	116.858		117.429	
1	48.098	47.562	68.338	47.981
	68.264	68.506	73.553	72.827
	83.022	73.376	87.446	81.858
	92.803	81.739	94.343	84.977
	94.841	85.147	100.545	90.184
	102.899	89.939	101.256	94.974
	105.121	96.781	103.778	96.542
	107.465	101.060	107.814	100.973
	111.427	103.522	111.950	103.769
	112.129	103.642	115.889	106.127
	116.217	107.186	117.724	108.545
	117.461	109.216		112.019
		111.810		114.697
		115.223		115.757
	116.652		117.206	
	117.993		118.450	
	118.396		118.585	
2	49.108	50.712	48.784	49.456
	70.366	69.539	50.732	69.530
	74.107	75.005	70.041	70.474
	76.557	85.178	74.486	76.540
	82.621	90.170	83.549	84.834
	87.686	95.643	83.990	90.536
	88.374	96.956	87.058	95.824
	93.454	98.046	93.499	96.700
	96.577	102.882	94.224	103.311
	100.524	104.162	97.807	104.220
	101.524	105.281	100.279	104.550

Table S2. continued.

J	Even +1	Even -1	Odd +1	Odd -1
2	102.255	107.333	102.299	107.446
	103.617	109.089	104.821	108.247
	106.709	112.585	106.386	110.054
	107.286	114.885	107.959	111.683
	109.016	115.878	109.484	114.887
	110.386	116.634	110.169	115.508
	113.137		112.311	117.409
	114.224		113.567	
	116.733		114.148	
	118.194		117.035	
		118.010		
		118.567		
3	51.481	50.572	52.566	50.784
	54.955	52.668	71.287	54.953
	71.294	72.245	73.602	72.382
	72.795	73.641	77.168	75.945
	78.385	76.163	81.157	78.488
	87.516	81.125	86.935	84.338
	88.414	84.589	93.639	87.073
	93.148	86.327	94.708	90.259
	97.497	89.754	97.523	91.423
	100.887	92.317	99.858	96.964
	101.758	97.533	101.110	98.905
	102.560	97.854	105.255	98.967
	105.101	99.664	106.090	102.217
	106.469	103.995	107.172	103.930
	107.805	104.607	108.246	105.044
	109.382	105.939	109.643	105.600
	109.954	107.043	110.307	106.055
	111.554	107.488	112.163	107.926
	112.917	109.629	113.016	109.668
	114.429	110.496	115.173	110.749
116.181	110.938	115.982	112.430	
118.475	113.140		113.816	
	114.193		114.055	
	115.888		116.391	
	116.560		117.585	

Table S2. continued.

J	Even +1	Even -1	Odd +1	Odd -1
4	53.004	55.028	52.880	54.153
	57.444	60.718	55.310	57.459
	74.987	73.554	60.717	73.555
	78.092	76.365	74.968	75.891
	78.303	80.018	76.592	78.113
	81.207	83.458	78.398	80.874
	86.499	89.610	83.300	86.969
	87.115	92.706	86.286	90.295
	88.088	97.263	89.883	91.042
	93.065	98.114	91.166	96.631
	95.764	99.783	93.305	99.472
	97.234	102.666	94.627	99.929
	101.163	105.432	100.956	104.116
	101.925	107.132	101.919	105.855
	102.698	107.653	103.000	106.189
	104.232	108.116	104.502	107.688
	106.191	108.753	106.224	109.346
	108.861	109.838	107.750	110.246
	109.228	112.261	109.060	111.318
	110.018	113.038	109.185	112.150
	110.570	113.591	110.264	112.886
	111.688	114.095	111.002	114.741
	112.430	115.452	111.780	116.182
	113.452	117.326	112.616	116.695
	114.262	117.570	114.203	117.699