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

Supplementary Information for:

The water – carbon monoxide dimer: new infrared spectra, *ab initio* rovibrational energy level calculations, and an interesting intermolecular mode

By:

A. Barclay,[†] A. van der Avoird,[‡] A.R.W. McKellar,[§] and N. Moazzen-Ahmadi

[†]*Department of Physics and Astronomy, University of Calgary, 2500 University Drive North West, Calgary, Alberta T2N 1N4, Canada,* [‡]*Theoretical Chemistry, Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135,6525 AJ Nijmegen, The Netherlands,* [§]*National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada.*

Table A-1. Calculated energy levels for the A state of CO-H_2O (*para* H_2O – CO), relative to dissociation (columns on left) and relative to the lowest level (columns on right) (in cm^{-1}).

K	*J* = 0	*J* = 1	*J* = 2	*J* = 0	*J* = 1	*J* = 2
Parity = *e*						
0	-315.9595	-315.7764	-315.4101	0.0000	0.1831	0.5494
1		-295.9991	-295.6306		19.9604	20.3289
1		-266.4385	-266.0694		49.5210	49.8901
0	-264.6893	-264.4997	-264.1205	51.2702	51.4598	51.8390
2			-258.4495			57.5100
0	-238.1530	-237.9762	-237.6227	77.8065	77.9833	78.3368
1		-235.3142	-234.9368		80.6453	81.0227
2			-229.1576			86.8019
0	-227.5408	-227.3511	-226.9716	88.4187	88.6084	88.9879
1		-219.3368	-218.9698		96.6227	96.9897
2			-212.7598			103.1997
1		-207.6071	-207.2321		108.3524	108.7274
0	-204.5711	-204.3823	-204.0045	111.3884	111.5772	111.9550
2			-198.8401			117.1194
Parity = *f*						
1		-295.9983	-295.6281		19.9612	20.3314
1		-266.4369	-266.0645		49.5226	49.8950
2			-258.4495			57.5100
0	-245.2553	-245.0701	-244.6999	70.7042	70.8894	71.2596
1		-235.3127	-234.9324		80.6468	81.0271
2			-229.1576			86.8019
1		-219.3355	-218.9660		96.6240	96.9935
2			-212.7598			103.1997
1		-207.6069	-207.2317		108.3526	108.7278
2			-198.8401			117.1194
1		-192.8147	-192.4286		123.1448	123.5309

Table A-2. Calculated energy levels for the B state of CO-H_2O (*ortho* H_2O – CO), relative to A state dissociation (columns on left) and relative to the lowest A state level (columns on right) (in cm^{-1}). (The B state dissociation threshold is +23.2994 cm^{-1}).

K	*J* = 0	*J* = 1	*J* = 2	*J* = 0	*J* = 1	*J* = 2
Parity = *e*						
0	-315.1644	-314.9812	-314.6148	0.7951	0.9783	1.3447
1		-296.2015	-295.8332		19.7580	20.1263
1		-267.3232	-266.9523		48.6363	49.0072
0	-263.4585	-263.2690	-262.8902	52.5010	52.6905	53.0693
2			-258.3207			57.6388
0	-236.8866	-236.7101	-236.3571	79.0729	79.2494	79.6024
1		-234.4441	-234.0663		81.5154	81.8932
2			-229.9466			86.0129
0	-226.2499	-226.0598	-225.6797	89.7096	89.8997	90.2798
1		-220.8027	-220.4364		95.1568	95.5231
2			-211.1363			104.8232
1		-208.7053	-208.3292		107.2542	107.6303
0	-203.0244	-202.8357	-202.4582	112.9351	113.1238	113.5013
2			-198.5718			117.3877
Parity = *f*						
1		-296.2009	-295.8314		19.7586	20.1281
1		-267.3224	-266.9502		48.6371	49.0093
2			-258.3207			57.6388
0	-246.9614	-246.7761	-246.4054	68.9981	69.1834	69.5541
1		-234.4430	-234.0628		81.5165	81.8967
2			-229.9466			86.0129
1		-220.8019	-220.4339		95.1576	95.5256
2			-211.1363			104.8232
1		-208.7061	-208.3315		107.2534	107.6280
2			-198.5718			117.3877
1		-192.5955	-192.2296		123.3640	123.7299
0	-191.0843	-190.8949	-190.5162	124.8752	125.0646	125.4433
1		-190.7663	-190.3866		125.1932	125.5729
2			-185.1680			130.7915
1		-176.2549	-175.8844		139.7046	140.0751

Table A-3. Calculated energy levels for the A state of CO-D_2O (*ortho* D_2O – CO), relative to dissociation (columns on left) and relative to the lowest level (columns on right) (in cm^{-1}).

K	*J* = 0	*J* = 1	*J* = 2	*J* = 0	*J* = 1	*J* = 2
Parity = *e*						
0	-368.4166	-368.2432	-367.8963	0.0000	0.1734	0.5203
1		-356.7124	-356.3660		11.7042	12.0506
2			-324.2084			44.2082
1		-322.8967	-322.5442		45.5199	45.8724
0	-320.0076	-319.8294	-319.4731	48.4090	48.5872	48.9435
2			-306.6043			61.8123
1		-292.5510	-292.1993		75.8656	76.2173
0	-291.3413	-291.1732	-290.8370	77.0753	77.2434	77.5796
0	-284.4091	-284.2302	-283.8723	84.0075	84.1864	84.5443
2			-279.0090			89.4076
1		-279.077	-278.7128		89.3396	89.7038
1		-273.1076	-272.7640		95.3090	95.6526
1		-264.0684	-263.7139		104.3482	104.7027
2			-259.5412			108.8754
Parity = *f*						
1		-356.7116	-356.3634		11.7050	12.0532
2			-324.2084			44.2082
1		-322.8957	-322.5410		45.5209	45.8756
0	-309.4110	-309.2353	-308.8841	59.0056	59.1813	59.5325
2			-306.6043			61.8123
1		-292.5501	-292.1966		75.8665	76.2200
2			-279.0089			89.4077
1		-279.0758	-278.7093		89.3408	89.7073
1		-273.1073	-272.7634		95.3093	95.6532
1		-264.0682	-263.7133		104.3484	104.7033
2			-259.5412			108.8754
0	-253.9484	-253.7691	-253.4105	114.4682	114.6475	115.0061
2			-247.3447			121.0719
1		-247.4532	-247.0963		120.9634	121.3203
1		-244.9276	-244.5752		123.4890	123.8414

Table A-4. Calculated energy levels for the B state of CO-D_2O (*para* D_2O – CO), relative to A state dissociation (columns on left) and relative to the lowest A state level (columns on right) (in cm^{-1}). (The B state dissociation threshold is +12.1183 cm^{-1}).

K	*J* = 0	*J* = 1	*J* = 2	*J* = 0	*J* = 1	*J* = 2
Parity = *e*						
0	-368.3866	-368.2132	-367.8663	0.03000	0.2034	0.5503
1		-356.7317	-356.3852		11.6849	12.0314
2			-324.2174			44.1992
1		-322.9799	-322.6270		45.4367	45.7896
0	-319.889	-319.7109	-319.3548	48.5276	48.7057	49.0618
2			-306.5157			61.9009
1		-292.515	-292.1633		75.9016	76.2533
0	-291.2868	-291.1188	-290.7828	77.1298	77.2978	77.6338
0	-284.0765	-283.8975	-283.5395	84.3401	84.5191	84.8771
2/1			-279.0124			89.4042
1/2		-279.3097	-278.9016		89.1069	89.5150
1		-273.1584	-272.8147		95.2582	95.6019
1		-263.9491	-263.5945		104.4675	104.8221
2			-259.5414			108.8752
Parity = *f*						
1		-356.7309	-356.3827		11.6857	12.0339
2			-324.2174			44.1992
1		-322.9799	-322.6243		45.4376	45.7923
0	-309.5019	-309.3262	-308.9748	58.9147	59.0904	59.4418
2			-306.5157			61.9009
1		-292.5142	-292.1608		75.9024	76.2558
2/1			-279.0110			89.4056
1/2		-279.3086	-278.9000		89.1080	89.5166
1		-273.1582	-272.8144		95.2584	95.6022
1		-263.9493	-263.5952		104.4673	104.8214
2			-259.5414			108.8752
0	-254.1514	-253.9719	-253.6130	114.2652	114.4447	114.8036
2			-247.5473			120.8693
1		-247.6461	-247.2889		120.7705	121.1277
1		-245.2796	-244.9290		123.1370	123.4876