Appendix to:

Infrared spectrum and intermolecular potential energy surface of the CO – O_2 dimer

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Table A-1. Observed transitions of CO-O_2 in group 1, correlating with ($n(O_2) = 1$, $j(O_2) = 0$) (units of cm^{-1}). Note: The "calculated" positions correspond to the "experimental" energy levels from Table 1 of the paper.

Upper *J*, *K e/f*	Lower *J*, *K e/f*	Observed	Calculated	Obs - Calc
1,1f	1,0	2145.411	2145.411	0.0000
2,1f	2,0	2145.427	2145.427	0.0000
3,1f	3,0	2145.451	2145.451	0.0000
4,1f	4,0	2145.480	2145.480	0.0000
5,1f	5,0	2145.516	2145.516	0.0000
6,1f	6,0	2145.555	2145.555	0.0000
7,1f	7,0	2145.593	2145.593	0.0000
8,1f	8,0	2145.628	2145.628	0.0000
1,1e	0,0	2145.557	2145.557	-0.0001
2,1e	1,0	2145.712	2145.712	0.0000
3,1e	2,0	2145.862	2145.862	0.0000
4,1e	3,0	2146.008	2146.008	-0.0001
5,1e	4,0	2146.147	2146.147	-0.0001
6,1e	5,0	2146.278	2146.278	0.0000
7,1e	6,0	2146.402	2146.402	0.0000
8,1e	7,0	2146.519	2146.519	0.0000
1,1e	2,0	2145.094	2145.094	0.0001
2,1e	3,0	2144.942	2144.942	0.0000
3,1e	4,0	2144.789	2144.789	0.0000
4,1e	5,0	2144.635	2144.635	0.0001
5,1e	6,0	2144.478	2144.478	0.0001
6,1e	7,0	2144.318	2144.318	-0.0001
7,1e	8,0	2144.157	2144.158	-0.0003
1,0	0,0	2142.849	2142.849	0.0001
2,0	1,0	2143.003	2143.003	0.0001
3,0	2,0	2143.156	2143.156	0.0000
4,0	3,0	2143.308	2143.307	0.0001
5,0	4,0	2143.457	2143.457	0.0000
6,0	5,0	2143.603	2143.603	0.0000
7,0	6,0	2143.748	2143.748	0.0000
8,0	8,1f	2139.758	2139.758	0.0000

0,0	1,0	2142.540	2142.540	-0.0001
1,0	2,0	2142.386	2142.386	-0.0002
2,0	3,0	2142.234	2142.234	0.0000
3,0	4,0	2142.083	2142.083	0.0002
4,0	5,0	2141.934	2141.934	-0.0001
5,0	6,0	2141.787	2141.787	-0.0001
6,0	7,0	2141.643	2141.643	0.0000
1,0	1,1f	2139.948	2139.948	0.0000
2,0	2,1f	2139.933	2139.933	0.0000
3,0	3,1f	2139.911	2139.911	0.0000
4,0	4,1f	2139.884	2139.884	0.0000
5,0	5,1f	2139.853	2139.853	0.0000
6,0	6,1f	2139.819	2139.819	0.0000
7,0	7,1f	2139.787	2139.787	0.0000
8,0	8,1f	2139.758	2139.758	0.0000
0,0	1,1e	2139.800	2139.800	0.0001
1,0	2,1e	2139.645	2139.645	0.0001
2,0	3,1e	2139.493	2139.493	0.0000
3,0	4,1e	2139.347	2139.347	-0.0001
4,0	5,1e	2139.207	2139.207	0.0000
5,0	6,1e	2139.075	2139.075	0.0000
6,0	7,1e	2138.951	2138.951	0.0000
2,0	1,1e	2140.263	2140.263	-0.0001
3,0	2,1e	2140.415	2140.415	-0.0001
4,0	3,1e	2140.567	2140.567	0.0000
5,0	4,1e	2140.721	2140.721	0.0001
6,0	5,1e	2140.876	2140.876	0.0000
7,0	6,1e	2141.036	2141.036	0.0000
1,0'	0,0	2151.963	2151.963	0.0000
2,0'	1,0	2152.087	2152.087	0.0000
3,0'	2,0	2152.193	2152.193	0.0000
4,0'	3,0	2152.281	2152.281	0.0000
5,0'	4,0	2152.349	2152.349	-0.0008
6,0'	5,0	2152.381	2152.381	0.0008
0,0'	1,0	2151.669	2151.669	0.0000
1,0'	2,0	2151.501	2151.501	0.0000
2,0'	3,0	2151.318	2151.318	0.0000
3,0'	4,0	2151.120	2151.120	0.0000
4,0'	5,0	2150.907	2150.907	0.0000

5,0'	6,0	2150.680	2150.680	0.0004
6,0'	7,0	2150.420	2150.420	-0.0006
2,2e	1,1e	2149.827	2149.827	-0.0005
3,2e	2,1e	2149.969	2149.969	-0.0001
4,2e	3,1e	2150.104	2150.104	-0.0002
5,2e	4,1e	2150.213	2150.213	-0.0001
6,2e	5,1e	2150.367	2150.371	-0.0035
2,2f	1,1f	2149.820	2149.820	0.0002
3,2f	2,1f	2149.948	2149.948	0.0002
4,2f	3,1f	2150.064	2150.064	0.0002
5,2f	4,1f	2150.169	2150.169	0.0002
6,2f	5,1f	2150.261	2150.262	-0.0001
2,2e	2,1f	2149.498	2149.497	0.0005
3,2e	3,1f	2149.466	2149.466	0.0001
4,2e	4,1f	2149.422	2149.422	0.0002
5,2e	5,1f	2149.345	2149.345	-0.0004
2,2f	2,1e	2149.517	2149.517	-0.0002
3,2f	3,1e	2149.508	2149.509	-0.0002
4,2f	4,1e	2149.499	2149.499	-0.0002
5,2f	5,1e	2149.491	2149.491	-0.0002
6,2f	6,1e	2149.484	2149.484	0.0001
5,2e	4,0	2152.949	2152.949	0.0002
6,2e	5,0	2153.094	2153.098	-0.0038
5,2e	6,0	2151.280	2151.279	0.0003
1,0"	0,0	2152.871	2152.870	0.0001
2,0"	1,0	2152.910	2152.910	0.0000
3,0"	2,0	2152.939	2152.939	0.0000
4,0"	3,0	2152.969	2152.969	-0.0001
5,0"	4,0	2153.031	2153.031	-0.0002
6,0"	5,0	2153.003	2153.003	0.0000
0,0"	1,0	2152.640	2152.640	0.0000
1,0"	2,0	2152.408	2152.408	-0.0001
2,0"	3,0	2152.141	2152.141	0.0000
3,0"	4,0	2151.865	2151.865	0.0000
4,0"	5,0	2151.595	2151.595	0.0001
5,0"	6,0	2151.362	2151.362	0.0005
6,0"	7,0	2151.043	2151.043	0.0000

4,0"	3,1e	2150.228	2150.229	-0.0005
5,0"	4,1e	2150.295	2940.295	-0.0003
6,0"	5,1e	2150.278	2150.276	0.0017
5,0"	5,1f	2149.427	2149.427	-0.0003
6,0"	6,1f	2149.219	2149.219	-0.0001

Table A-2. Observed transitions of CO-O_2 in group 2, correlating with ($n(O_2) = 1$, $j(O_2) = 2$) (units of cm^{-1}). Note: The "calculated" positions correspond to the "experimental" energy levels from Table 2 of the paper.

Upper *J, K e/f*	Lower *J, K e/f*	Observed	Calculated	Obs - Calc
3,3e	2,2e	2145.741	2145.741	-0.0002
4,3e	3,2e	2145.891	2145.892	-0.0011
5,3e	4,2e	2146.042	2146.043	-0.0007
6,3e	5,2e	2146.196	2146.193	0.0027
3,3f	2,2f	2145.741	2145.741	-0.0002
4,3f	3,2f	2145.894	2145.894	0.0007
5,3f	4,2f	2146.051	2146.050	0.0010
6,3f	5,2f	2146.212	2146.214	-0.0023
3,3e	3,2f	2145.303	2145.303	0.0003
4,3e	4,2f	2145.309	2145.309	-0.0002
5,3e	5,2f	2145.319	2145.319	-0.0002
3,3f	3,2e	2145.299	2145.298	0.0007
4,3f	4,2e	2145.296	2145.295	0.0002
5,3f	5,2e	2145.288	2145.288	-0.0005
3,2e	2,2e	2143.136	2143.137	-0.0004
4,2e	3,2e	2143.289	2143.289	0.0004
5,2e	4,2e	2143.447	2143.446	0.0012
6,2e	5,2e	2143.607	2143.608	-0.0007
3,2f	2,2f	2143.132	2143.134	-0.0014
4,2f	3,2f	2143.281	2143.281	0.0000
5,2f	4,2f	2143.431	2143.430	0.0011
6,2f	5,2f	2143.579	2143.580	-0.0005
2,2e	3,2e	2142.253	2142.252	0.0006
3,2e	4,2e	2142.100	2142.100	-0.0003
4,2e	5,2e	2141.943	2141.944	-0.0005
5,2e	6,2e	2141.782	2141.782	0.0003
2,2f	3,2f	2142.256	2142.255	0.0009

3,2f	4,2f	2142.108	2142.107	0.0001
4,2f	5,2f	2141.958	2141.959	-0.0012
5,2f	6,2f	2141.811	2141.810	0.0005
2,2e	3,3e	2139.629	2139.629	0.0003
3,2e	4,3e	2139.481	2139.480	0.0008
4,2e	5,3e	2139.333	2139.332	0.0003
5,2e	6,3e	2139.185	2139.186	-0.0018
2,2f	3,3f	2139.629	2139.628	0.0004
3,2f	4,3f	2139.478	2139.479	-0.0008
4,2f	5,3f	2139.324	2139.325	-0.0012
5,2f	6,3f	2139.168	2139.166	0.0025
3,2f	3,3e	2140.067	2140.067	-0.0004
4,2f	4,3e	2140.064	2140.064	0.0000
5,2f	5,3e	2140.057	2140.057	0.0003
3,2e	3,3f	2140.071	2140.072	-0.0004
4,2e	4,3f	2140.077	2140.077	0.0002
1,1e	2,2e	2145.512	2145.510	0.0014
2,1e	3,2e	2145.360	2145.360	-0.0002
3,1e	4,2e	2145.203	2145.203	-0.0001
4,1e	5,2e	2145.041	2145.035	0.0062
1,1f	2,2f	2145.516	2145.516	0.0000
2,1f	3,2f	2145.376	2145.379	-0.0022
3,1f	4,2f	2145.245	2145.244	0.0011
4,1f	5,2f	2145.115	2145.110	0.0051
3,1e	2,2e	2146.240	2146.240	0.0002
4,1e	3,2e	2146.387	2146.380	0.0069
3,1f	2,2f	2146.269	2146.270	-0.0008
4,1f	3,2f	2146.439	2146.432	0.0067
2,2e	1,1e	2139.859	2139.859	-0.0003
3,2e	2,1e	2140.011	2140.011	0.0006
4,2e	3,1e	2140.169	2140.169	-0.0002
2,2f	1,1f	2139.853	2139.854	-0.0007
3,2f	2,1f	2139.995	2139.993	0.0022
4,2f	3,1f	2140.128	2140.130	-0.0023
5,2f	4,1f	2140.268	2140.267	0.0008
2,2f	2,1e	2139.569	2139.567	0.0016
2,2e	3,1e	2139.132	2139.132	-0.0003
3,2e	4,1e	2138.985	2138.994	-0.0087

2,2f	3,1f	2139.103	2139.104	-0.0006
4,4e	3,3e	2149.849	2149.849	0.0004
5,4e	4,3e	2149.979	2149.978	0.0010
6,4e	5,3e	2150.104	2150.104	0.0007
7,4e	6,3e	2150.224	2150.224	0.0000
8,4e	7,3e	2150.341	2150.340	0.0014
4,4f	3,3f	2149.849	2149.850	-0.0005
5,4f	4,3f	2149.979	2149.981	-0.0012
6,4f	5,3f	2150.109	2150.108	0.0015
7,4f	6,3f	2150.228	2150.230	-0.0021
8,4f	7.3f	2150.345	2150.346	-0.0008
4,4e	4,3f	2149.261	2149.261	0.0002
5,4e	5,3f	2149.239	2149.240	-0.0011
6,4e	6,3f	2149.219	2149.213	0.0061
4,4f	4,3e	2149.261	2149.258	0.0024
5,4f	5,3e	2149.236	2149.236	0.0006
2,2'e	2,2f	2152.490	2152.491	-0.0006
3,2'e	3,2f	2152.503	2152.502	0.0012
4,2'e	4,2f	2152.530	2152.529	0.0007
2,2'f	2,2e	2152.483	2152.483	-0.0002
3,2'f	3,2e	2152.469	2152.470	-0.0012
4,2'f	4,2e	2152.442	2152.443	-0.0001
2,2'e	3,2e	2152.047	2152.048	-0.0007
3,2'e	4,2e	2151.904	2151.903	0.0006
4,2'e	5,2e	2151.766	2151.767	-0.0010
2,2'f	3,2f	2152.046	2152.045	0.0015
3,2'f	4,2f	2151.887	2151.888	-0.0006
4,2'f	5,2f	2151.719	2151.719	0.0001
4,2'e	3,2e	2153.112	2153.112	-0.0002
4,2'f	3,2f	2153.041	2153.041	0.0006

Table A-3. Calculated energy levels of CO-O_2 (in cm^{-1}) with $J = 0$ to 5, relative to the zero point energy (ZPE) of -81.9332 cm^{-1}. This ZPE corresponds to the forbidden level with $J = 0$, $K = 0$, $n(O_2) = 0$. Stack labels A, B, C, etc. correspond to those of Tables 5 and 6 in the paper. Permutation inversion group symmetry and spectroscopy parity *e*/*f* are also indicated. Only the allowed B+ and B− levels are given.

$J = 0$, $B^+(e)$			$J = 0$, $B^-(f)$		
calc	*K*	stack	calc	*K*	stack
4.6342	0	C	4.4928	0	B
8.3172	0	E	16.7199	0	
16.2495	0				

$J = 1$, $B^+(f)$			$J = 1$, $B^-(e)$		
calc	*K*	stack	calc	*K*	stack
1.8396	1	A	1.8322	1	A
4.6507	0	B	4.7915	0	C
9.6674	1	F	8.4632	0	E
11.6413	1	G	9.6652	1	F
11.8904	1	I	11.6342	1	G
16.3491	1		11.8904	1	I
16.9134	0		16.2400	1 + 0	
			16.5291	0 + 1	

$J = 2$, $B^+(e)$			$J = 2$, $B^-(f)$		
calc	*K*	stack	calc	*K*	stack
2.1410	1	A	2.1634	1	A
4.8824	2	D	4.8841	2	D
5.1076	0	C	4.9665	0	B
8.7552	0	E	9.9743	1	F
9.9676	1	F	11.9416	1	G
11.9207	1	G	12.1993	1	I
12.1989	1	I	15.4010	2	K
15.3988	2	K	16.5891	1	
16.4259	1 + 0		17.2837	0	
16.9096	0 + 1		17.6192	2	
17.6191	2		18.5848	2	
18.5843	2				

$J = 3$, $B^+(f)$			$J = 3$, $B^-(e)$		
calc	K	stack	calc	K	stack
2.6489	1	A	2.6040	1	A
5.3533	2	D	5.3455	2	D
5.4400	0	B	5.5853	0	C
10.4344	1	F	9.1930	0	E
12.0063	3	H	10.4206	1	F
12.3920	1	G	12.0062	3	H
12.6631	1	I	12.3514	1	G
14.8465	3	J	12.6617	1	I
15.8341	2	K	14.8465	3	J
16.9714	1		15.8232	2	K
17.8147	0		16.7708	1 + 0	
18.0735	2		17.4179	0 + 1	

$J = 4$, $B^+(e)$			$J = 4$, $B^-(f)$		
calc	K	stack	calc	K	stack
3.2210	1	A	3.2958	1	A
5.9565	2	D	5.9784	2	D
6.2278	0	C	6.0709	0	B
9.7765	0	E	11.0475	1	F
11.0238	1	F	12.6075	3	H
12.6066	3	H	12.9924	1	G
12.9277	1	G	13.2825	1	I
13.2787	1	I	15.4392	3	J
15.4386	3	J	16.4092	2	K
16.3772	2	K	17.5035	1	
17.2811	1 + 0		18.4947	0	
18.0481	0 + 1		18.0718	4	

$J = 5$, $B^{+}(f)$			$J = 5$, $B^{-}(e)$		
calc	K	stack	calc	K	stack
4.1037	1	A	3.9914	1	A
6.7588	2	D	6.7128	2	D
6.8588	0	B	7.0367	0	C
11.8129	1	F	10.5055	0	E
13.3553	3	H	11.7761	1	F
13.7425	1	G	13.3518	3	H
14.0577	1	I	13.6515	1	G
16.1796	3	J	14.0498	1	I
17.1249	2	K	16.1770	3	J
18.1882	1		17.0549	2	K
18.8435	4		17.9622	1 + 0	
19.3113	0		18.7969	0 + 1	
19.4490	2		18.8535	4	